Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 10:08 PM EDT

PDB ID	:	3EVJ
Title	:	Intermediate structure of antithrombin bound to the natural pentasaccharide
Authors	:	Huntington, J.A.; Belzar, K.J.
Deposited on	:	2008-10-13
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

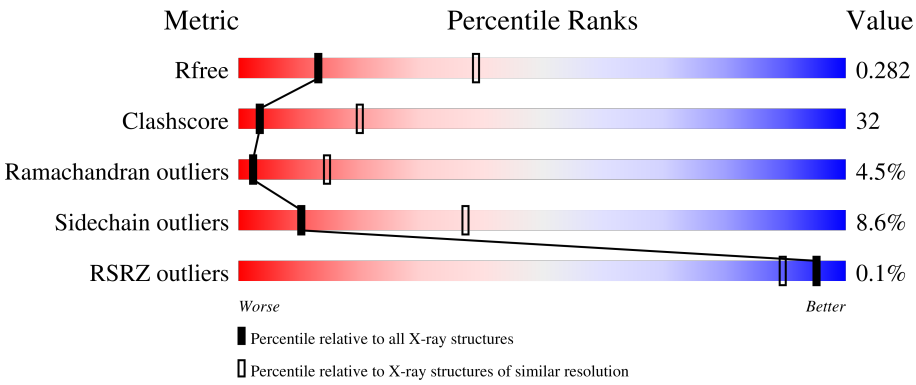
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	I	432	44% 43% 7% 6%
1	L	432	48% 43% 5% •
2	A	3	33% 33% 33%
3	B	2	50% 50%
3	C	2	100%

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Mol	Chain	Length	Quality of chain
4	D	5	20% 60% 20%
5	E	5	20% 40% 40%
5	F	5	60% 40%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	A	3	X	-	-	-
3	NAG	B	2	-	-	-	X
4	MAN	D	3	X	-	-	-

2 Entry composition (i)

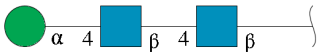
There are 7 unique types of molecules in this entry. The entry contains 6574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	404	3016	1922	498	579	17	0	0	0
1	L	417	3148	2009	517	605	17	0	0	0

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

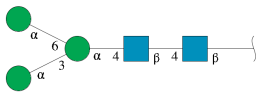


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	3	38	21	2	15	0	0	0

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

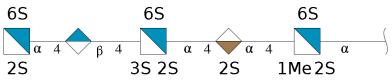
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	2	28	16	2	10	0	0	0
3	C	2	28	16	2	10	0	0	0

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



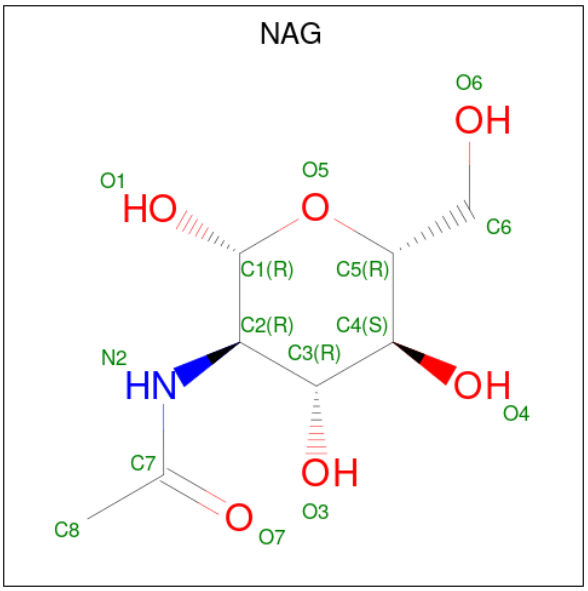
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	5	61	34	2	25	0	0	0

- Molecule 5 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	5	91	31	3	49	8	0	0	0
5	F	5	91	31	3	49	8	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	I	1	14	8	1	5	6	0
			Total	C	N	O		
6	L	1	14	8	1	5	0	0

- Molecule 7 is water.

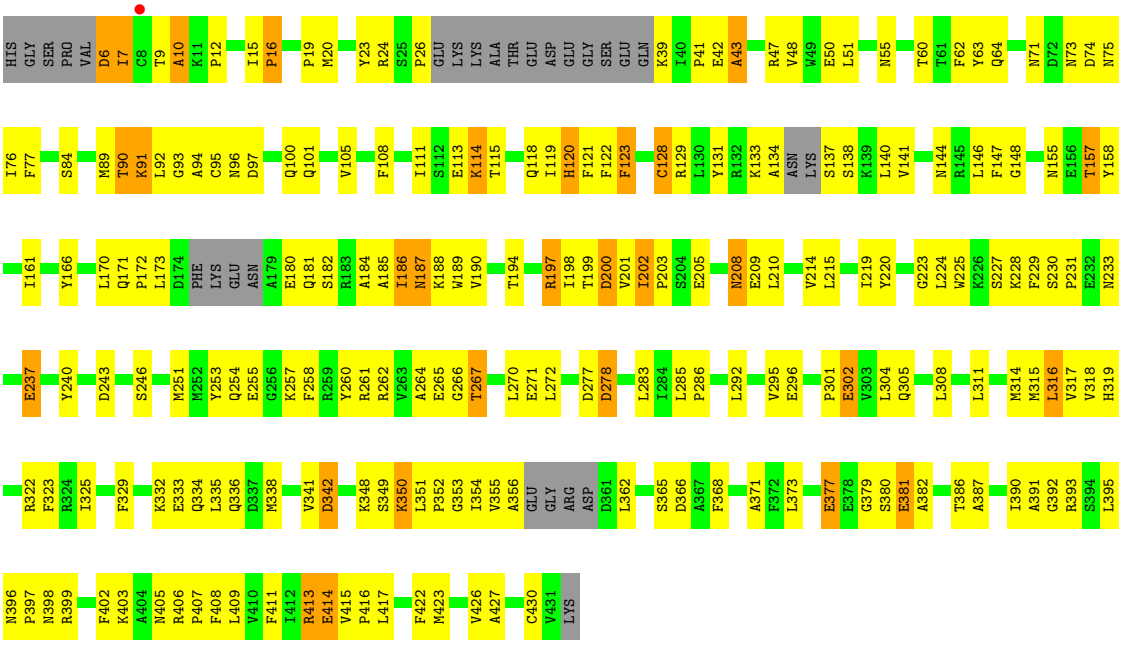
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	I	24	24	24	0	0
			Total	O		
7	L	21	21	21	0	0

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.

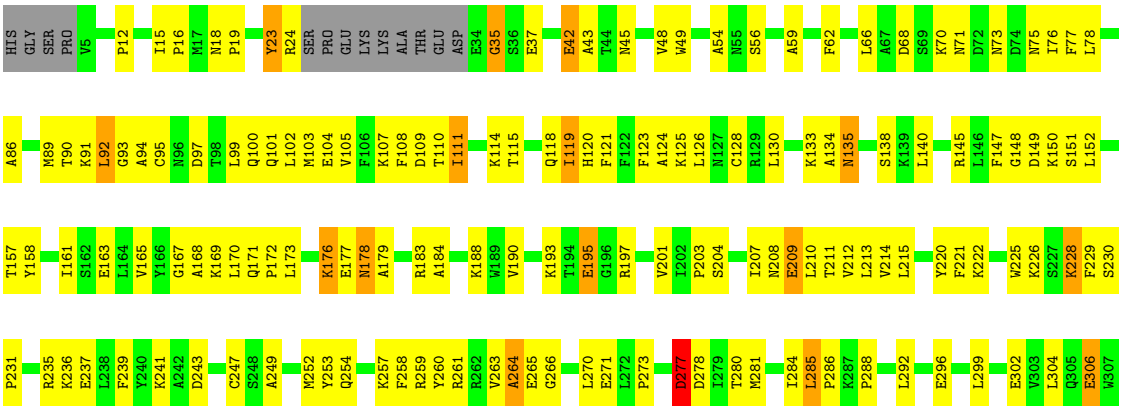
- Molecule 1: Antithrombin-III

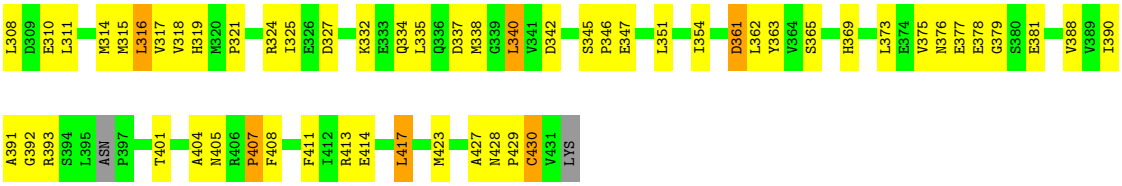
Chain I:



- Molecule 1: Antithrombin-III

Chain L:





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

Chain A: 33% 33% 33%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside

Chain E: 20% 40% 40%

• Molecule 5: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alph

a-L-idopyranuronic acid-(1-4)-methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranosid
e

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.85Å 87.06Å 92.38Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	63.24 – 3.00 63.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (63.24-3.00) 99.1 (63.24-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.289 0.221 , 0.282	Depositor DCC
R_{free} test set	1016 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6574	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SGN, ZDO, BDP, MAN, SUS, IDS

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	I	0.43	0/3076	0.67	0/4187
1	L	0.46	0/3211	0.74	2/4365 (0.0%)
All	All	0.44	0/6287	0.70	2/8552 (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	I	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	35	GLY	N-CA-C	6.30	128.86	113.10
1	L	95	CYS	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	63	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3016	0	2762	223	0
1	L	3148	0	2933	169	0
2	A	38	0	30	8	0
3	B	28	0	25	2	0
3	C	28	0	25	2	0
4	D	61	0	52	4	0
5	E	91	0	27	3	0
5	F	91	0	27	3	0
6	I	14	0	13	0	0
6	L	14	0	13	0	0
7	I	24	0	0	2	0
7	L	21	0	0	0	0
All	All	6574	0	5907	399	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 32.

All (399) 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:I:332:LYS:O	1:I:336:GLN:HG3	1.71	0.89
1:L:258:PHE:HB2	1:L:316:LEU:HD21	1.55	0.88
1:L:178:ASN:N	1:L:178:ASN:HD22	1.68	0.88
4:D:1:NAG:H62	4:D:2:NAG:HN2	1.39	0.88
1:L:102:LEU:HD23	1:L:340:LEU:HD21	1.56	0.87
1:L:171:GLN:HE21	1:L:173:LEU:HD21	1.39	0.85
1:L:365:SER:HB3	1:L:392:GLY:H	1.41	0.85
1:I:316:LEU:HD23	1:I:316:LEU:H	1.45	0.80
1:I:390:ILE:HG12	1:L:319:HIS:HB2	1.61	0.80
1:I:93:GLY:HA2	1:I:353:GLY:HA3	1.64	0.80
1:I:186:ILE:O	1:I:189:TRP:N	2.14	0.79
1:L:292:LEU:HD23	1:L:407:PRO:HG2	1.65	0.79
1:I:258:PHE:HB2	1:I:316:LEU:HD21	1.63	0.79
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.65	0.78
1:L:292:LEU:CD2	1:L:407:PRO:HG2	2.14	0.78
1:L:286:PRO:HG3	1:L:292:LEU:HD13	1.67	0.77
4:D:1:NAG:C6	4:D:2:NAG:HN2	1.99	0.75
1:I:90:THR:C	1:I:92:LEU:H	1.90	0.74
1:I:395:LEU:HB2	1:I:399:ARG:HH12	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:GLY:HA3	1:I:170:LEU:HD21	1.70	0.74
1:L:172:PRO:O	1:L:173:LEU:HD23	1.88	0.74
1:I:47:ARG:HH21	1:I:114:LYS:HZ3	1.37	0.73
1:I:302:GLU:CD	1:I:302:GLU:H	1.90	0.73
1:L:428:ASN:OD1	1:L:430:CYS:HB2	1.88	0.73
3:C:1:NAG:H62	3:C:2:NAG:O5	1.89	0.72
1:I:93:GLY:CA	1:I:353:GLY:HA3	2.19	0.72
2:A:2:NAG:C3	2:A:2:NAG:N2	2.53	0.72
1:I:354:ILE:N	1:I:354:ILE:HD12	2.04	0.72
1:I:286:PRO:HB3	1:I:295:VAL:HG21	1.72	0.72
1:L:158:TYR:CE2	1:L:354:ILE:HG23	2.26	0.71
1:L:190:VAL:HG11	1:L:201:VAL:HG21	1.70	0.71
1:I:386:THR:HG22	1:I:387:ALA:N	2.05	0.71
1:L:114:LYS:NZ	5:F:3:SUS:O9S	2.24	0.71
1:I:187:ASN:ND2	1:I:200:ASP:HA	2.05	0.70
1:I:147:PHE:CE1	1:I:186:ILE:HG12	2.27	0.69
1:L:111:ILE:HD12	1:L:115:THR:HG22	1.73	0.69
1:L:91:LYS:HE2	1:L:103:MET:HE3	1.72	0.69
1:I:380:SER:C	1:I:382:ALA:H	1.95	0.69
1:I:415:VAL:HG13	1:I:416:PRO:HA	1.74	0.69
1:L:119:ILE:HD12	1:L:120:HIS:H	1.58	0.69
1:L:299:LEU:HD11	1:L:304:LEU:HD21	1.75	0.69
1:L:177:GLU:C	1:L:178:ASN:HD22	1.94	0.69
1:L:92:LEU:HD11	1:L:161:ILE:HG21	1.75	0.69
1:I:47:ARG:NH2	1:I:114:LYS:HZ3	1.90	0.68
1:I:202:ILE:HG22	1:I:203:PRO:HD2	1.74	0.68
1:I:229:PHE:HB2	1:I:377:GLU:HA	1.76	0.68
1:I:134:ALA:HB1	1:I:137:SER:N	2.08	0.68
1:L:15:ILE:N	1:L:16:PRO:HD3	2.08	0.68
1:L:178:ASN:N	1:L:178:ASN:ND2	2.40	0.68
1:I:148:GLY:CA	1:I:170:LEU:HD21	2.24	0.68
1:I:386:THR:HG22	1:I:387:ALA:H	1.59	0.68
1:I:148:GLY:N	1:I:170:LEU:HD21	2.09	0.67
1:L:93:GLY:O	1:L:351:LEU:HA	1.94	0.67
1:L:270:LEU:HD12	1:L:271:GLU:N	2.10	0.67
1:I:51:LEU:HD21	1:I:123:PHE:CD2	2.29	0.67
1:I:187:ASN:HD22	1:I:200:ASP:HA	1.59	0.67
1:L:119:ILE:HD12	1:L:120:HIS:N	2.09	0.67
1:I:395:LEU:HB2	1:I:399:ARG:NH1	2.10	0.66
1:I:194:THR:HG21	1:I:198:ILE:HB	1.78	0.66
1:I:332:LYS:HG2	1:I:336:GLN:NE2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:GLN:O	1:L:104:GLU:HG3	1.96	0.65
2:A:2:NAG:N2	2:A:2:NAG:C1	2.60	0.65
1:I:94:ALA:HA	1:I:351:LEU:HD23	1.79	0.65
1:I:60:THR:O	1:I:64:GLN:HG3	1.97	0.65
4:D:5:MAN:O2	4:D:5:MAN:H62	1.95	0.64
1:L:70:LYS:HE2	1:L:75:ASN:O	1.98	0.64
1:I:181:GLN:O	1:I:184:ALA:HB3	1.97	0.64
1:I:352:PRO:HA	1:I:355:VAL:HG22	1.80	0.64
1:L:119:ILE:O	1:L:123:PHE:HB2	1.98	0.64
1:L:229:PHE:HB2	1:L:377:GLU:HA	1.80	0.64
1:I:47:ARG:HH21	1:I:114:LYS:NZ	1.95	0.64
1:L:195:GLU:HG3	1:L:220:TYR:CZ	2.32	0.64
1:L:209:GLU:OE1	1:L:210:LEU:HG	1.98	0.64
1:L:270:LEU:HD12	1:L:271:GLU:H	1.60	0.64
1:L:179:ALA:HB1	1:L:207:ILE:O	1.97	0.63
1:I:186:ILE:CG2	1:I:202:ILE:HD11	2.29	0.63
1:I:285:LEU:HD12	1:I:286:PRO:HD2	1.81	0.63
1:I:214:VAL:HG13	1:I:366:ASP:O	2.00	0.62
1:I:71:ASN:HD21	1:I:73:ASN:HB2	1.64	0.62
1:L:171:GLN:NE2	1:L:173:LEU:HD21	2.13	0.62
1:I:23:TYR:O	1:I:24:ARG:NH1	2.31	0.62
1:I:12:PRO:HG3	1:I:121:PHE:CE2	2.35	0.62
1:I:302:GLU:CD	1:I:302:GLU:N	2.54	0.61
1:I:180:GLU:C	1:I:182:SER:N	2.52	0.61
1:L:111:ILE:HD12	1:L:115:THR:CG2	2.30	0.61
1:L:124:ALA:HB2	1:L:165:VAL:HG13	1.82	0.61
1:L:91:LYS:CD	1:L:103:MET:HE3	2.31	0.61
1:I:7:ILE:HD12	1:I:7:ILE:H	1.66	0.61
1:I:96:ASN:OD1	1:I:97:ASP:N	2.28	0.61
1:I:120:HIS:HD2	1:I:121:PHE:H	1.49	0.60
1:I:377:GLU:H	1:I:377:GLU:CD	2.05	0.60
1:I:224:LEU:HD23	1:I:382:ALA:CB	2.32	0.60
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.84	0.60
1:I:396:ASN:HD21	1:I:398:ASN:HB3	1.65	0.60
1:I:101:GLN:O	1:I:105:VAL:HG23	2.02	0.60
1:I:101:GLN:OE1	1:I:342:ASP:HB2	2.01	0.59
1:I:47:ARG:NH2	1:I:114:LYS:NZ	2.48	0.59
1:L:226:LYS:HD2	1:L:277:ASP:OD1	2.02	0.59
1:L:110:THR:O	1:L:111:ILE:HG23	2.01	0.59
1:I:47:ARG:HD2	1:I:115:THR:OG1	2.03	0.59
1:I:225:TRP:NE1	1:I:379:GLY:HA2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:ILE:HG23	1:I:120:HIS:N	2.18	0.59
1:I:77:PHE:CE2	1:I:373:LEU:HB2	2.38	0.58
1:L:335:LEU:HD23	1:L:338:MET:HE3	1.84	0.58
1:I:120:HIS:CD2	1:I:121:PHE:H	2.22	0.58
1:L:104:GLU:HG2	1:L:109:ASP:OD2	2.03	0.58
1:L:375:VAL:HG12	1:L:376:ASN:N	2.19	0.58
1:I:180:GLU:C	1:I:182:SER:H	2.04	0.58
1:L:92:LEU:HD11	1:L:161:ILE:CG2	2.34	0.58
4:D:1:NAG:H62	4:D:2:NAG:N2	2.13	0.57
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.04	0.57
1:L:184:ALA:O	1:L:188:LYS:HB2	2.04	0.57
1:L:273:PRO:HA	1:L:280:THR:HG22	1.85	0.57
1:I:146:LEU:HG	1:I:215:LEU:HD13	1.86	0.57
1:I:147:PHE:CD1	1:I:186:ILE:HG12	2.39	0.57
1:I:380:SER:O	1:I:382:ALA:N	2.36	0.57
1:L:365:SER:CB	1:L:392:GLY:H	2.16	0.57
1:I:386:THR:HG23	1:L:315:MET:O	2.05	0.57
1:L:263:VAL:CG1	1:L:264:ALA:N	2.68	0.56
1:I:140:LEU:HD11	1:I:219:ILE:HD11	1.86	0.56
1:L:285:LEU:HD12	1:L:408:PHE:HB2	1.87	0.56
1:L:77:PHE:CE2	1:L:373:LEU:HB2	2.40	0.56
1:L:91:LYS:CE	1:L:103:MET:HE3	2.34	0.56
2:A:2:NAG:C3	2:A:2:NAG:C1	2.83	0.56
1:I:90:THR:O	1:I:92:LEU:N	2.38	0.56
1:I:71:ASN:HB3	1:I:74:ASP:OD2	2.06	0.56
1:I:391:ALA:O	1:L:321:PRO:HD3	2.04	0.56
1:I:90:THR:C	1:I:92:LEU:N	2.59	0.56
1:I:197:ARG:HG3	1:I:220:TYR:CZ	2.41	0.56
1:I:390:ILE:HG12	1:L:319:HIS:CB	2.33	0.55
1:I:186:ILE:HD12	1:I:202:ILE:CD1	2.36	0.55
1:L:188:LYS:O	1:L:188:LYS:HD3	2.06	0.55
1:L:121:PHE:O	1:L:124:ALA:HB3	2.07	0.55
1:I:266:GLY:O	1:I:267:THR:C	2.45	0.55
1:L:286:PRO:CG	1:L:292:LEU:HD13	2.36	0.55
1:L:130:LEU:HD23	1:L:414:GLU:OE1	2.07	0.55
3:B:1:NAG:O7	3:B:1:NAG:H3	2.06	0.55
1:L:123:PHE:O	1:L:126:LEU:HB3	2.06	0.54
1:L:140:LEU:HD12	1:L:220:TYR:O	2.08	0.54
1:L:284:ILE:HD12	1:L:411:PHE:HE1	1.72	0.54
1:L:236:LYS:HA	1:L:249:ALA:O	2.08	0.54
1:I:20:MET:HE3	2:A:1:NAG:H2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:GLY:O	1:I:172:PRO:HA	2.07	0.54
1:I:225:TRP:CD1	1:I:379:GLY:HA2	2.42	0.54
1:I:301:PRO:HB2	1:I:302:GLU:OE2	2.07	0.54
1:I:415:VAL:CG1	1:I:416:PRO:HA	2.38	0.54
1:I:270:LEU:HD12	1:I:271:GLU:N	2.22	0.54
1:I:366:ASP:HB3	1:I:368:PHE:CZ	2.43	0.54
1:L:208:ASN:HD22	1:L:393:ARG:HD3	1.73	0.54
1:L:404:ALA:HB3	1:L:427:ALA:HB1	1.90	0.54
1:I:146:LEU:HG	1:I:215:LEU:CD1	2.38	0.54
1:I:237:GLU:OE1	1:I:403:LYS:HE3	2.08	0.54
1:L:103:MET:HE1	1:L:108:PHE:CD2	2.43	0.53
1:I:240:TYR:CD1	1:I:246:SER:HB3	2.43	0.53
1:L:15:ILE:N	1:L:16:PRO:CD	2.71	0.53
1:I:48:VAL:HG21	5:E:5:SGN:O5S	2.08	0.53
1:I:278:ASP:O	1:I:414:GLU:HG2	2.08	0.53
1:I:197:ARG:HE	1:I:197:ARG:HA	1.72	0.53
1:L:91:LYS:HD3	1:L:103:MET:CE	2.38	0.53
1:I:197:ARG:HG3	1:I:220:TYR:OH	2.09	0.53
1:I:19:PRO:HB3	1:I:92:LEU:HD12	1.91	0.52
1:I:285:LEU:HD11	1:I:406:ARG:HG3	1.91	0.52
1:I:292:LEU:O	1:I:296:GLU:HG3	2.09	0.52
1:L:56:SER:O	1:L:59:ALA:HB3	2.09	0.52
1:I:396:ASN:ND2	1:I:398:ASN:HB3	2.24	0.52
1:L:404:ALA:O	1:L:405:ASN:HB2	2.10	0.52
1:I:335:LEU:O	1:I:338:MET:HB2	2.09	0.52
1:L:176:LYS:O	1:L:209:GLU:HB3	2.10	0.52
1:L:261:ARG:CB	1:L:311:LEU:HD23	2.40	0.52
1:L:259:ARG:NH2	1:L:311:LEU:O	2.41	0.52
1:L:149:ASP:HB3	1:L:152:LEU:HD12	1.92	0.52
1:I:23:TYR:C	1:I:24:ARG:HH11	2.12	0.52
1:I:62:PHE:CD2	1:I:338:MET:HE2	2.45	0.52
1:I:131:TYR:C	1:I:133:LYS:H	2.13	0.52
1:I:184:ALA:O	1:I:188:LYS:CB	2.58	0.51
1:I:224:LEU:HD23	1:I:382:ALA:HB1	1.93	0.51
1:L:77:PHE:CZ	1:L:373:LEU:HB2	2.45	0.51
1:L:125:LYS:O	1:L:128:CYS:HB2	2.10	0.51
1:I:119:ILE:HG23	1:I:120:HIS:H	1.74	0.51
1:L:302:GLU:CD	1:L:302:GLU:H	2.14	0.51
1:L:148:GLY:O	1:L:172:PRO:HA	2.10	0.51
1:I:386:THR:CG2	1:I:387:ALA:H	2.23	0.51
1:L:62:PHE:HD1	1:L:338:MET:CE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:THR:O	1:I:200:ASP:C	2.49	0.51
1:I:272:LEU:HD12	1:I:283:LEU:HD11	1.92	0.50
1:I:71:ASN:ND2	1:I:73:ASN:HB2	2.26	0.50
1:L:211:THR:HA	1:L:391:ALA:O	2.11	0.50
1:L:91:LYS:HE2	1:L:119:ILE:HD11	1.93	0.50
1:L:24:ARG:HH12	1:L:109:ASP:HB2	1.77	0.50
1:I:386:THR:CG2	1:I:387:ALA:N	2.72	0.50
1:L:213:LEU:HD22	1:L:354:ILE:HG21	1.93	0.50
1:I:144:ASN:HB3	1:I:166:TYR:OH	2.12	0.50
1:I:243:ASP:OD1	1:I:243:ASP:N	2.43	0.50
1:L:225:TRP:NE1	1:L:376:ASN:O	2.41	0.50
1:I:335:LEU:HD23	1:I:338:MET:CE	2.42	0.50
1:I:325:ILE:HD11	1:I:426:VAL:HG22	1.94	0.50
1:I:186:ILE:HD12	1:I:202:ILE:HD11	1.94	0.49
1:I:187:ASN:OD1	1:I:202:ILE:HG13	2.12	0.49
1:I:270:LEU:HD23	1:I:402:PHE:CD1	2.47	0.49
1:I:219:ILE:HG12	1:I:220:TYR:N	2.27	0.49
1:L:48:VAL:HG21	5:F:5:SGN:O5S	2.12	0.49
1:I:155:ASN:OD1	1:I:356:ALA:HA	2.13	0.49
1:L:90:THR:OG1	1:L:215:LEU:HD22	2.11	0.49
1:L:401:THR:HG22	1:L:401:THR:O	2.12	0.49
1:L:145:ARG:HG2	1:L:147:PHE:CZ	2.48	0.49
1:I:138:SER:CB	1:I:223:GLY:HA2	2.42	0.49
1:I:197:ARG:HA	1:I:197:ARG:NE	2.28	0.49
1:L:78:LEU:HB2	1:L:369:HIS:NE2	2.27	0.49
1:L:125:LYS:HA	1:L:125:LYS:HE2	1.93	0.49
1:L:261:ARG:HB3	1:L:311:LEU:HD23	1.94	0.49
1:I:51:LEU:HD12	1:I:51:LEU:O	2.13	0.49
1:L:257:LYS:HA	1:L:314:MET:O	2.13	0.49
1:L:316:LEU:HD23	1:L:316:LEU:H	1.78	0.49
1:L:228:LYS:O	1:L:254:GLN:NE2	2.45	0.49
1:I:161:ILE:HD11	2:A:2:NAG:H82	1.95	0.48
1:L:62:PHE:HD1	1:L:338:MET:HE2	1.78	0.48
1:L:163:GLU:OE2	1:L:169:LYS:HG2	2.13	0.48
1:L:345:SER:O	1:L:347:GLU:N	2.46	0.48
1:I:403:LYS:HD3	1:I:405:ASN:ND2	2.28	0.48
1:L:263:VAL:HG12	1:L:264:ALA:N	2.27	0.48
1:L:163:GLU:HA	1:L:168:ALA:H	1.78	0.48
1:I:23:TYR:CE2	1:I:100:GLN:HG3	2.48	0.48
1:I:39:LYS:O	1:I:41:PRO:HD3	2.13	0.48
1:I:219:ILE:O	1:I:371:ALA:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:350:LYS:C	1:I:352:PRO:HD3	2.34	0.48
3:B:1:NAG:O7	3:B:1:NAG:C3	2.62	0.48
1:I:20:MET:CE	2:A:1:NAG:H2	2.43	0.48
1:I:120:HIS:CD2	1:I:121:PHE:N	2.81	0.48
1:I:329:PHE:HB2	7:I:876:HOH:O	2.12	0.48
1:L:92:LEU:CD2	1:L:120:HIS:CE1	2.96	0.48
1:I:62:PHE:HD2	1:I:338:MET:CE	2.27	0.48
1:L:18:ASN:O	1:L:161:ILE:HD11	2.14	0.48
1:I:89:MET:SD	1:I:166:TYR:HB2	2.53	0.48
1:L:149:ASP:OD2	1:L:151:SER:N	2.43	0.48
1:L:281:MET:HA	1:L:411:PHE:O	2.14	0.48
1:L:91:LYS:CE	1:L:119:ILE:HD11	2.43	0.48
1:I:51:LEU:HD11	1:I:123:PHE:CE2	2.49	0.48
1:I:208:ASN:C	1:I:210:LEU:H	2.15	0.48
1:I:161:ILE:HD11	2:A:2:NAG:C8	2.44	0.47
1:I:411:PHE:CE2	1:I:423:MET:HE3	2.49	0.47
1:I:186:ILE:CB	1:I:202:ILE:HD11	2.45	0.47
1:I:316:LEU:H	1:I:316:LEU:CD2	2.20	0.47
1:L:324:ARG:O	1:L:325:ILE:HG22	2.14	0.47
1:I:283:LEU:HD23	1:I:408:PHE:CE2	2.49	0.47
1:I:316:LEU:HD23	1:I:316:LEU:N	2.20	0.47
1:L:208:ASN:HB3	1:L:393:ARG:CZ	2.43	0.47
1:L:221:PHE:CG	1:L:222:LYS:N	2.82	0.47
1:I:180:GLU:CG	1:I:180:GLU:O	2.63	0.47
1:I:190:VAL:HG21	1:I:201:VAL:HG21	1.97	0.47
1:I:351:LEU:N	1:I:352:PRO:HD3	2.29	0.47
1:L:23:TYR:CG	1:L:24:ARG:N	2.80	0.47
1:L:214:VAL:HA	1:L:388:VAL:O	2.14	0.47
1:L:253:TYR:CE1	1:L:317:VAL:HG13	2.49	0.47
1:I:23:TYR:HE2	1:I:100:GLN:HG3	1.80	0.47
1:I:155:ASN:N	1:I:354:ILE:O	2.37	0.47
1:L:304:LEU:O	1:L:308:LEU:HG	2.15	0.47
1:I:93:GLY:O	1:I:351:LEU:HA	2.15	0.47
1:I:352:PRO:HA	1:I:355:VAL:CG2	2.44	0.47
1:I:319:HIS:CE1	1:I:403:LYS:HZ2	2.32	0.47
1:L:225:TRP:CD1	1:L:379:GLY:HA2	2.50	0.47
1:I:260:TYR:CG	1:I:261:ARG:N	2.82	0.46
1:L:120:HIS:HB3	1:L:165:VAL:HG11	1.97	0.46
1:L:230:SER:O	1:L:231:PRO:C	2.53	0.46
2:A:1:NAG:H5	2:A:2:NAG:O7	2.14	0.46
1:I:305:GLN:O	1:I:308:LEU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:97:ASP:O	1:L:101:GLN:HG3	2.15	0.46
1:I:214:VAL:HG22	1:I:365:SER:OG	2.16	0.46
1:L:91:LYS:HD3	1:L:103:MET:HE2	1.97	0.46
1:I:7:ILE:HD13	1:I:128:CYS:SG	2.56	0.46
1:I:120:HIS:N	1:I:120:HIS:CD2	2.83	0.46
1:I:148:GLY:O	1:I:173:LEU:N	2.49	0.46
1:I:224:LEU:CD2	1:I:382:ALA:HB1	2.46	0.46
1:L:91:LYS:CD	1:L:103:MET:CE	2.93	0.46
1:L:110:THR:O	1:L:111:ILE:CG2	2.63	0.46
1:I:75:ASN:OD1	1:I:427:ALA:N	2.48	0.45
1:I:237:GLU:CD	1:I:251:MET:HG2	2.37	0.45
1:L:259:ARG:CZ	1:L:311:LEU:HB2	2.45	0.45
1:I:319:HIS:HB2	1:I:403:LYS:HA	1.97	0.45
1:I:380:SER:C	1:I:382:ALA:N	2.64	0.45
1:I:158:TYR:CD2	1:I:354:ILE:HG23	2.51	0.45
1:I:228:LYS:O	1:I:254:GLN:NE2	2.50	0.45
1:I:257:LYS:HA	1:I:314:MET:O	2.17	0.45
1:L:91:LYS:HG3	1:L:99:LEU:CD1	2.47	0.45
1:L:259:ARG:NH1	1:L:311:LEU:HB2	2.31	0.45
1:I:157:THR:O	1:I:161:ILE:HG13	2.16	0.45
1:I:170:LEU:C	1:I:170:LEU:HD23	2.36	0.45
1:I:406:ARG:HB2	1:I:407:PRO:HD2	1.98	0.45
1:L:12:PRO:HB3	1:L:118:GLN:OE1	2.17	0.45
1:I:264:ALA:O	1:I:265:GLU:HB2	2.17	0.45
1:I:271:GLU:OE2	1:I:413:ARG:NH1	2.50	0.45
1:I:9:THR:O	1:I:10:ALA:O	2.35	0.44
1:I:185:ALA:O	1:I:189:TRP:HB2	2.16	0.44
1:L:71:ASN:HD21	1:L:73:ASN:HB2	1.81	0.44
1:L:302:GLU:CD	1:L:302:GLU:N	2.71	0.44
1:L:321:PRO:HG3	1:L:429:PRO:HB3	1.99	0.44
1:L:417:LEU:N	1:L:417:LEU:CD2	2.80	0.44
1:I:77:PHE:CE1	1:I:422:PHE:HB3	2.52	0.44
1:I:209:GLU:O	1:I:209:GLU:HG2	2.17	0.44
1:I:286:PRO:HB3	1:I:295:VAL:CG2	2.45	0.44
1:L:345:SER:C	1:L:347:GLU:H	2.19	0.44
5:E:3:SUS:N2	5:E:3:SUS:O9S	2.51	0.44
1:I:261:ARG:HB3	1:I:311:LEU:HD23	2.00	0.44
1:L:292:LEU:HD22	1:L:407:PRO:O	2.17	0.44
1:L:375:VAL:CG1	1:L:376:ASN:N	2.80	0.44
1:I:322:ARG:O	1:I:323:PHE:HB3	2.18	0.44
1:I:108:PHE:O	1:I:111:ILE:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ASP:HA	7:I:886:HOH:O	2.17	0.44
1:I:197:ARG:NH2	1:I:381:GLU:OE1	2.50	0.44
1:L:23:TYR:O	1:L:24:ARG:CB	2.65	0.44
1:I:89:MET:O	1:I:92:LEU:N	2.51	0.44
1:I:129:ARG:NH1	5:E:5:SGN:O6S	2.51	0.44
1:I:202:ILE:HG23	1:I:368:PHE:CD2	2.53	0.44
1:L:94:ALA:HA	1:L:351:LEU:HD23	2.00	0.44
1:L:163:GLU:OE2	1:L:169:LYS:CG	2.66	0.44
1:L:170:LEU:C	1:L:170:LEU:HD23	2.37	0.43
1:I:411:PHE:HE2	1:I:423:MET:HE3	1.82	0.43
1:L:91:LYS:HD3	1:L:103:MET:HE3	2.00	0.43
1:L:241:LYS:CE	1:L:247:CYS:SG	3.06	0.43
5:F:4:BDP:O3	5:F:5:SGN:C1	2.66	0.43
1:L:66:LEU:HD12	1:L:66:LEU:HA	1.90	0.43
1:L:101:GLN:O	1:L:105:VAL:HG23	2.18	0.43
1:L:197:ARG:NH2	1:L:381:GLU:OE1	2.51	0.43
1:L:310:GLU:O	1:L:311:LEU:C	2.57	0.43
1:I:329:PHE:N	1:I:329:PHE:CD2	2.86	0.43
1:L:212:VAL:HG12	1:L:213:LEU:N	2.32	0.43
1:I:42:GLU:O	1:I:43:ALA:C	2.56	0.43
1:I:231:PRO:HG3	1:I:377:GLU:HG2	2.00	0.43
1:L:134:ALA:O	1:L:135:ASN:C	2.57	0.43
1:I:89:MET:O	1:I:90:THR:C	2.58	0.43
1:I:390:ILE:HG12	1:L:319:HIS:ND1	2.34	0.43
1:I:50:GLU:OE1	1:I:111:ILE:HB	2.19	0.42
1:I:186:ILE:O	1:I:188:LYS:N	2.52	0.42
1:I:197:ARG:HD3	1:I:381:GLU:OE1	2.18	0.42
1:L:345:SER:C	1:L:347:GLU:N	2.72	0.42
1:I:76:ILE:HG22	1:I:77:PHE:N	2.34	0.42
1:I:315:MET:CE	1:I:395:LEU:HD21	2.49	0.42
1:L:42:GLU:HB3	1:L:43:ALA:H	1.51	0.42
1:I:55:ASN:O	1:I:55:ASN:ND2	2.53	0.42
1:I:253:TYR:CE1	1:I:317:VAL:HG13	2.53	0.42
1:I:351:LEU:HB3	1:I:354:ILE:HD13	2.01	0.42
1:I:171:GLN:NE2	1:I:172:PRO:HD2	2.34	0.42
1:I:262:ARG:HD3	1:I:266:GLY:O	2.19	0.42
1:I:354:ILE:N	1:I:354:ILE:CD1	2.76	0.42
1:L:260:TYR:CG	1:L:261:ARG:N	2.87	0.42
1:I:47:ARG:HG3	1:I:122:PHE:CE1	2.54	0.42
1:I:316:LEU:CD2	1:I:316:LEU:N	2.80	0.42
1:I:332:LYS:HE2	1:I:336:GLN:HE22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:TRP:CD1	1:L:417:LEU:HB2	2.54	0.42
1:L:221:PHE:CD1	1:L:222:LYS:N	2.88	0.42
1:I:317:VAL:HG12	1:I:318:VAL:N	2.34	0.42
1:L:193:LYS:HA	1:L:193:LYS:HD3	1.85	0.42
1:L:308:LEU:HA	1:L:311:LEU:HG	2.01	0.42
1:I:24:ARG:O	1:I:26:PRO:HD3	2.19	0.42
1:I:353:GLY:C	1:I:354:ILE:HD12	2.38	0.42
1:I:395:LEU:CB	1:I:399:ARG:NH1	2.81	0.42
1:I:231:PRO:C	1:I:233:ASN:H	2.23	0.42
1:I:323:PHE:HE2	1:I:373:LEU:HD23	1.85	0.42
1:I:335:LEU:HD23	1:I:338:MET:HE1	2.00	0.42
1:L:163:GLU:O	1:L:167:GLY:HA2	2.20	0.42
1:I:92:LEU:HD23	1:I:158:TYR:CE1	2.55	0.41
1:I:341:VAL:HG13	1:I:342:ASP:N	2.34	0.41
1:I:230:SER:HA	1:I:231:PRO:HD3	1.95	0.41
1:L:273:PRO:CA	1:L:280:THR:HG22	2.49	0.41
1:L:423:MET:HE2	1:L:423:MET:HB2	1.91	0.41
1:L:252:MET:O	1:L:319:HIS:HA	2.21	0.41
1:L:346:PRO:HG3	1:L:363:TYR:CE2	2.55	0.41
1:I:332:LYS:CE	1:I:336:GLN:HE22	2.33	0.41
1:L:125:LYS:O	1:L:128:CYS:N	2.53	0.41
1:L:302:GLU:O	1:L:306:GLU:HB2	2.20	0.41
1:I:15:ILE:O	1:I:16:PRO:C	2.59	0.41
1:L:45:ASN:HB3	1:L:48:VAL:HG23	2.02	0.41
1:L:264:ALA:C	1:L:266:GLY:H	2.24	0.41
1:I:186:ILE:CD1	1:I:202:ILE:HD11	2.51	0.41
1:I:255:GLU:HG2	1:I:395:LEU:HD12	2.03	0.41
3:C:2:NAG:O7	3:C:2:NAG:H3	2.19	0.41
1:I:62:PHE:CD2	1:I:338:MET:CE	3.02	0.41
1:I:89:MET:O	1:I:91:LYS:N	2.54	0.41
1:L:12:PRO:HD3	1:L:121:PHE:CZ	2.56	0.41
1:L:278:ASP:OD1	1:L:278:ASP:N	2.47	0.41
1:L:292:LEU:O	1:L:296:GLU:HG3	2.21	0.41
1:L:76:ILE:HA	1:L:327:ASP:OD2	2.21	0.41
1:L:253:TYR:HA	1:L:318:VAL:O	2.21	0.41
1:L:378:GLU:N	1:L:378:GLU:OE1	2.54	0.41
1:I:148:GLY:H	1:I:170:LEU:HD21	1.82	0.40
1:I:332:LYS:HG2	1:I:336:GLN:HE21	1.86	0.40
1:L:86:ALA:O	1:L:89:MET:HB2	2.21	0.40
1:I:92:LEU:HD13	1:I:120:HIS:CE1	2.56	0.40
1:L:286:PRO:HD3	1:L:292:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ASN:OD1	1:I:426:VAL:HA	2.21	0.40
1:I:332:LYS:CG	1:I:336:GLN:NE2	2.83	0.40
1:I:335:LEU:O	1:I:338:MET:N	2.50	0.40
1:I:336:GLN:C	1:I:338:MET:N	2.73	0.40
1:I:392:GLY:O	1:L:239:PHE:CE2	2.74	0.40
1:I:393:ARG:NH2	1:L:237:GLU:OE1	2.54	0.40
1:L:54:ALA:HB1	1:L:107:LYS:O	2.21	0.40
1:L:363:TYR:O	1:L:390:ILE:HG23	2.21	0.40
1:I:93:GLY:HA3	1:I:353:GLY:HA3	2.02	0.40
1:I:96:ASN:CG	1:I:97:ASP:H	2.10	0.40
1:L:91:LYS:HD2	1:L:99:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	394/432 (91%)	315 (80%)	63 (16%)	16 (4%)	3 16
1	L	411/432 (95%)	336 (82%)	55 (13%)	20 (5%)	2 13
All	All	805/864 (93%)	651 (81%)	118 (15%)	36 (4%)	2 14

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	10	ALA
1	I	186	ILE
1	I	348	LYS
1	I	430	CYS
1	L	42	GLU
1	L	264	ALA
1	I	43	ALA

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Mol	Chain	Res	Type
1	I	237	GLU
1	I	349	SER
1	I	350	LYS
1	L	19	PRO
1	L	133	LYS
1	L	203	PRO
1	L	277	ASP
1	L	361	ASP
1	L	430	CYS
1	I	91	LYS
1	I	187	ASN
1	I	377	GLU
1	L	135	ASN
1	L	138	SER
1	L	150	LYS
1	L	332	LYS
1	I	90	THR
1	I	381	GLU
1	L	37	GLU
1	L	119	ILE
1	L	228	LYS
1	I	16	PRO
1	I	267	THR
1	L	195	GLU
1	I	208	ASN
1	L	35	GLY
1	L	68	ASP
1	L	111	ILE
1	L	288	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	299/383 (78%)	270 (90%)	29 (10%)	8 31
1	L	318/383 (83%)	294 (92%)	24 (8%)	13 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	617/766 (80%)	564 (91%)	53 (9%)	10 37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	6	ASP
1	I	7	ILE
1	I	84	SER
1	I	95	CYS
1	I	113	GLU
1	I	114	LYS
1	I	118	GLN
1	I	120	HIS
1	I	123	PHE
1	I	128	CYS
1	I	141	VAL
1	I	157	THR
1	I	197	ARG
1	I	200	ASP
1	I	202	ILE
1	I	205	GLU
1	I	227	SER
1	I	277	ASP
1	I	278	ASP
1	I	302	GLU
1	I	304	LEU
1	I	316	LEU
1	I	333	GLU
1	I	334	GLN
1	I	342	ASP
1	I	362	LEU
1	I	413	ARG
1	I	414	GLU
1	I	417	LEU
1	L	23	TYR
1	L	92	LEU
1	L	157	THR
1	L	176	LYS
1	L	178	ASN
1	L	183	ARG
1	L	204	SER
1	L	209	GLU

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Mol	Chain	Res	Type
1	L	235	ARG
1	L	243	ASP
1	L	265	GLU
1	L	277	ASP
1	L	285	LEU
1	L	306	GLU
1	L	316	LEU
1	L	334	GLN
1	L	337	ASP
1	L	340	LEU
1	L	342	ASP
1	L	361	ASP
1	L	362	LEU
1	L	407	PRO
1	L	413	ARG
1	L	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	71	ASN
1	I	118	GLN
1	I	120	HIS
1	I	171	GLN
1	I	181	GLN
1	I	254	GLN
1	I	336	GLN
1	I	405	ASN
1	L	71	ASN
1	L	171	GLN
1	L	178	ASN
1	L	334	GLN
1	L	405	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

22 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	A	1	1,2	14,14,15	0.64	0	17,19,21	1.02	2 (11%)
2	NAG	A	2	2	11,11,15	0.49	0	11,12,21	0.86	0
2	MAN	A	3	2	11,11,12	0.62	0	15,15,17	0.46	0
3	NAG	B	1	1,3	14,14,15	0.77	0	17,19,21	0.82	0
3	NAG	B	2	3	14,14,15	0.57	0	17,19,21	0.61	0
3	NAG	C	1	1,3	14,14,15	0.78	0	17,19,21	1.17	2 (11%)
3	NAG	C	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.59	0
4	NAG	D	1	1,4	14,14,15	0.65	0	17,19,21	0.61	0
4	NAG	D	2	4	14,14,15	0.58	0	17,19,21	0.65	0
4	MAN	D	3	4	11,11,12	0.71	0	15,15,17	0.93	1 (6%)
4	MAN	D	4	4	11,11,12	0.65	0	15,15,17	0.59	0
4	MAN	D	5	4	11,11,12	0.74	0	15,15,17	1.22	1 (6%)
5	ZDO	E	1	5	20,21,21	2.74	5 (25%)	25,32,32	1.32	3 (12%)
5	IDS	E	2	5	16,16,17	1.52	2 (12%)	17,24,26	1.42	2 (11%)
5	SUS	E	3	5	22,23,24	2.77	5 (22%)	24,36,38	1.42	3 (12%)
5	BDP	E	4	5	12,12,13	0.66	0	14,17,19	0.67	0
5	SGN	E	5	5	18,19,20	2.83	4 (22%)	22,29,31	1.32	3 (13%)
5	ZDO	F	1	5	20,21,21	2.72	5 (25%)	25,32,32	1.35	3 (12%)
5	IDS	F	2	5	16,16,17	1.51	2 (12%)	17,24,26	1.62	2 (11%)
5	SUS	F	3	5	22,23,24	2.79	5 (22%)	24,36,38	1.55	3 (12%)
5	BDP	F	4	5	12,12,13	0.66	0	14,17,19	0.81	0
5	SGN	F	5	5	18,19,20	2.83	4 (22%)	22,29,31	1.24	1 (4%)

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	A	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/10/10/26	-
2	MAN	A	3	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	MAN	D	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	MAN	D	5	4	-	2/2/19/22	1/1/1/1
5	ZDO	E	1	5	-	8/13/33/33	0/1/1/1
5	IDS	E	2	5	-	0/9/26/29	0/1/1/1
5	SUS	E	3	5	-	7/16/33/36	0/1/1/1
5	BDP	E	4	5	-	0/4/21/24	0/1/1/1
5	SGN	E	5	5	-	0/11/28/31	0/1/1/1
5	ZDO	F	1	5	-	4/13/33/33	0/1/1/1
5	IDS	F	2	5	-	0/9/26/29	0/1/1/1
5	SUS	F	3	5	-	8/16/33/36	0/1/1/1
5	BDP	F	4	5	-	1/4/21/24	0/1/1/1
5	SGN	F	5	5	-	2/11/28/31	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	5	SGN	O2S-S1	7.37	1.50	1.42
5	F	3	SUS	O1S-S1	7.32	1.50	1.42
5	E	1	ZDO	OSB-S2	7.31	1.50	1.42
5	E	5	SGN	O2S-S1	7.30	1.50	1.42
5	E	3	SUS	O1S-S1	7.29	1.50	1.42
5	E	5	SGN	O1S-S1	7.29	1.50	1.42
5	E	1	ZDO	OSA-S2	7.28	1.50	1.42
5	F	3	SUS	O3S-S1	7.27	1.50	1.42
5	F	5	SGN	O1S-S1	7.26	1.50	1.42
5	F	1	ZDO	OSB-S2	7.26	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	ZDO	OSA-S2	7.24	1.50	1.42
5	E	3	SUS	O3S-S1	7.24	1.50	1.42
5	E	1	ZDO	O6-S6	-4.95	1.43	1.56
5	F	5	SGN	O6-S2	-4.88	1.43	1.56
5	F	1	ZDO	O6-S6	-4.88	1.43	1.56
5	E	5	SGN	O6-S2	-4.87	1.43	1.56
5	E	3	SUS	O6-S2	-4.86	1.43	1.56
5	F	3	SUS	O6-S2	-4.83	1.43	1.56
5	F	2	IDS	O2-S	-4.66	1.43	1.57
5	E	2	IDS	O2-S	-4.63	1.43	1.57
5	E	3	SUS	O3-S3	-4.62	1.43	1.57
5	F	3	SUS	O3-S3	-4.62	1.43	1.57
5	F	3	SUS	S1-N2	3.17	1.63	1.59
5	E	1	ZDO	S2-N2	3.04	1.63	1.59
5	F	1	ZDO	S2-N2	2.99	1.63	1.59
5	E	5	SGN	S1-N2	2.95	1.63	1.59
5	F	5	SGN	S1-N2	2.84	1.63	1.59
5	E	3	SUS	S1-N2	2.79	1.63	1.59
5	F	2	IDS	O2-C2	-2.55	1.43	1.47
5	E	2	IDS	O2-C2	-2.46	1.43	1.47
5	E	1	ZDO	O1-C1	2.19	1.43	1.40
5	F	1	ZDO	O1-C1	2.11	1.43	1.40
3	C	2	NAG	C1-C2	2.02	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	2	IDS	C2-O2-S	-5.67	110.52	117.91
5	E	2	IDS	C2-O2-S	-4.95	111.45	117.91
5	F	3	SUS	O1S-S1-O3S	-4.88	108.63	120.16
5	E	1	ZDO	OSA-S2-OSB	-4.62	109.24	120.16
5	F	1	ZDO	OSA-S2-OSB	-4.51	109.50	120.16
5	E	3	SUS	O1S-S1-O3S	-4.46	109.62	120.16
5	E	5	SGN	O1S-S1-O2S	-4.45	109.64	120.16
5	F	5	SGN	O1S-S1-O2S	-4.42	109.71	120.16
5	F	3	SUS	C3-O3-S3	-4.12	110.92	118.88
4	D	5	MAN	C1-O5-C5	4.10	117.75	112.19
5	E	3	SUS	C3-O3-S3	-3.58	111.96	118.88
5	F	1	ZDO	C1M-O1-C1	-2.83	108.91	113.27
5	E	1	ZDO	C1M-O1-C1	-2.77	109.00	113.27
5	E	5	SGN	O6-C6-C5	2.76	112.77	107.62
3	C	1	NAG	C3-C4-C5	2.52	114.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3	MAN	C1-C2-C3	2.47	112.70	109.67
5	F	2	IDS	O2-C2-C3	2.30	110.16	106.95
2	A	1	NAG	C2-N2-C7	-2.28	119.65	122.90
5	E	2	IDS	O2-C2-C3	2.25	110.10	106.95
5	E	3	SUS	O6-C6-C5	2.19	111.71	107.62
2	A	1	NAG	O5-C5-C6	-2.18	103.79	107.20
5	E	1	ZDO	C3-C4-C5	-2.10	106.49	110.24
5	F	3	SUS	O6-C6-C5	2.10	111.53	107.62
5	F	1	ZDO	O1-C1-C2	2.09	111.34	108.14
3	C	1	NAG	C4-C3-C2	2.08	114.07	111.02
5	E	5	SGN	C6-C5-C4	-2.08	107.75	112.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	3	MAN	C1
4	D	3	MAN	C1

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
3	B	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	1	ZDO	C2-C1-O1-C1M
5	E	1	ZDO	O5-C1-O1-C1M
5	E	1	ZDO	C2-N2-S2-OSA
5	E	3	SUS	C2-N2-S1-O2S
5	F	1	ZDO	C2-N2-S2-OSA
5	F	1	ZDO	C6-O6-S6-OS3
5	F	3	SUS	C2-N2-S1-O1S
5	F	3	SUS	C2-N2-S1-O2S
3	B	1	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	3	MAN	C4-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
5	F	1	ZDO	C6-O6-S6-OS1
5	F	3	SUS	C6-O6-S2-O4S
2	A	3	MAN	O5-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	E	1	ZDO	O5-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
5	E	1	ZDO	C6-O6-S6-OS3
5	E	3	SUS	C6-O6-S2-O6S
5	F	3	SUS	C6-O6-S2-O6S
5	F	3	SUS	C3-C2-N2-S1
5	E	1	ZDO	C6-O6-S6-OS2
5	F	1	ZDO	C6-O6-S6-OS2
3	B	1	NAG	O7-C7-N2-C2
5	E	1	ZDO	C6-O6-S6-OS1
5	F	3	SUS	C6-O6-S2-O5S
5	F	3	SUS	C1-C2-N2-S1
5	E	3	SUS	C6-O6-S2-O4S
4	D	3	MAN	C4-C5-C6-O6
5	E	3	SUS	C3-C2-N2-S1
4	D	5	MAN	C4-C5-C6-O6
5	F	5	SGN	C6-O6-S2-O5S
5	E	3	SUS	C1-C2-N2-S1
5	E	3	SUS	C6-O6-S2-O5S
3	C	2	NAG	C3-C2-N2-C7
5	E	3	SUS	C2-N2-S1-O1S
5	F	3	SUS	C2-N2-S1-O3S
5	E	1	ZDO	C4-C5-C6-O6
5	F	5	SGN	C6-O6-S2-O4S
4	D	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C1-C2-N2-C7
3	B	2	NAG	C3-C2-N2-C7
5	F	4	BDP	O5-C5-C6-O6B

All (2) ring outliers are listed below:

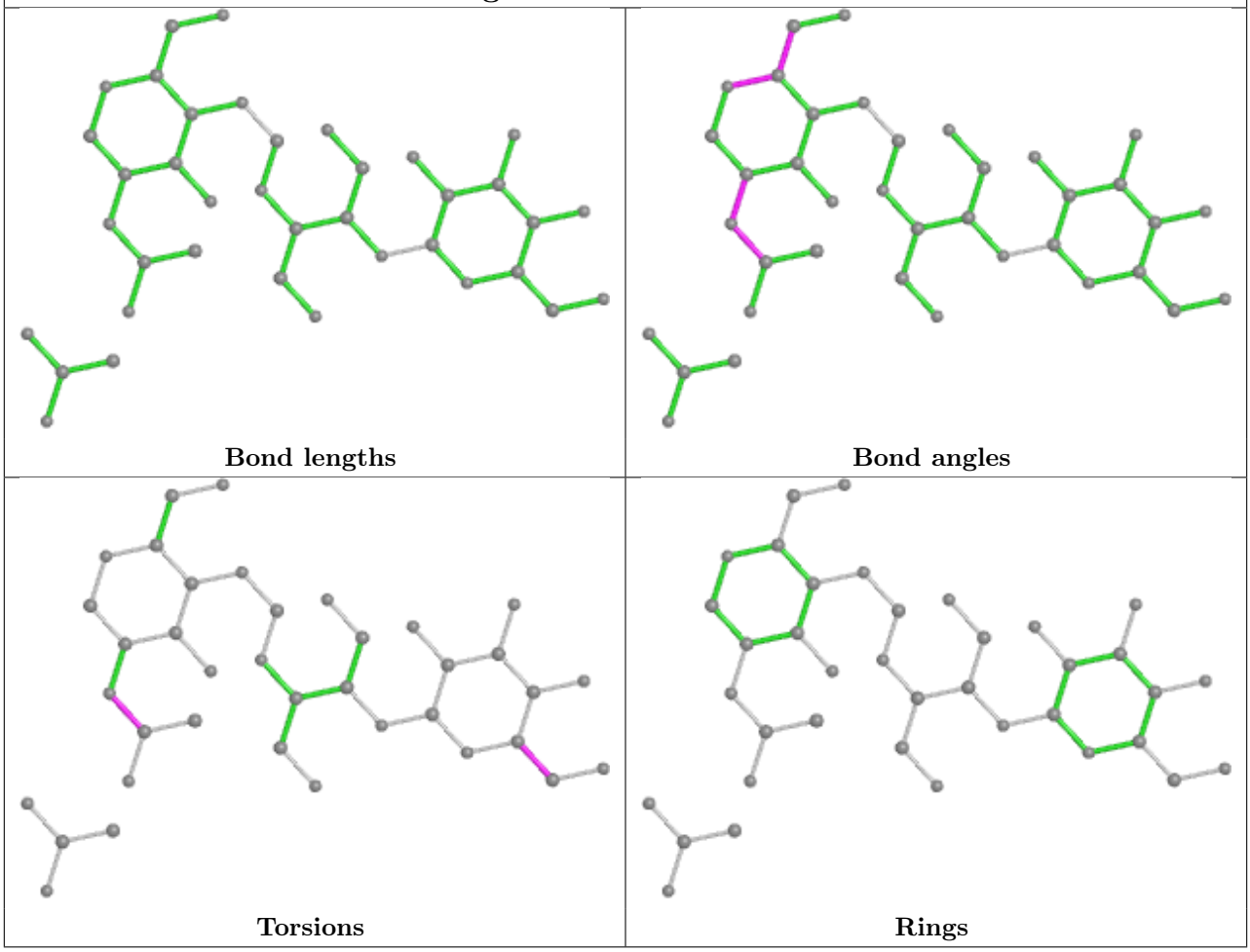
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	D	5	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 22 short contacts:

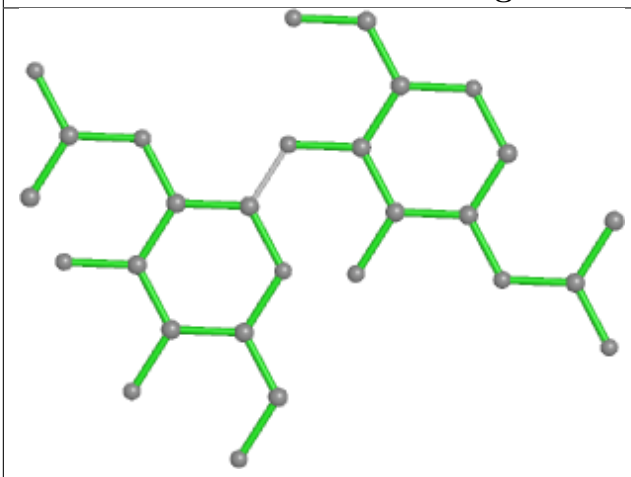
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	3	0
3	C	2	NAG	2	0
5	F	4	BDP	1	0
3	B	1	NAG	2	0
5	F	3	SUS	1	0
5	E	5	SGN	2	0
4	D	2	NAG	3	0
2	A	2	NAG	6	0
3	C	1	NAG	1	0
5	F	5	SGN	2	0
4	D	5	MAN	1	0
2	A	1	NAG	3	0
5	E	3	SUS	1	0

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

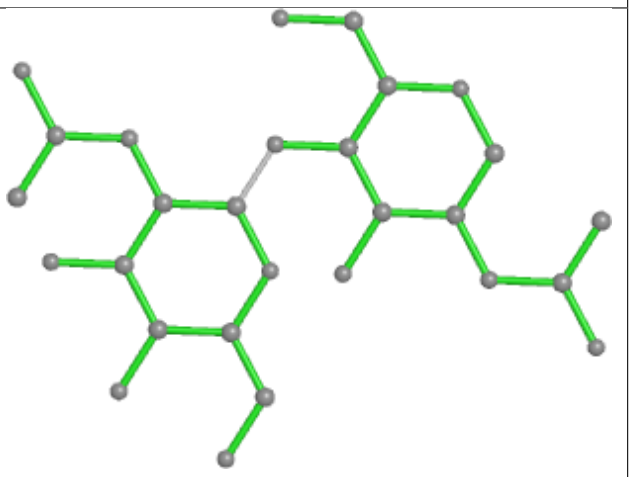
Oligosaccharide Chain A



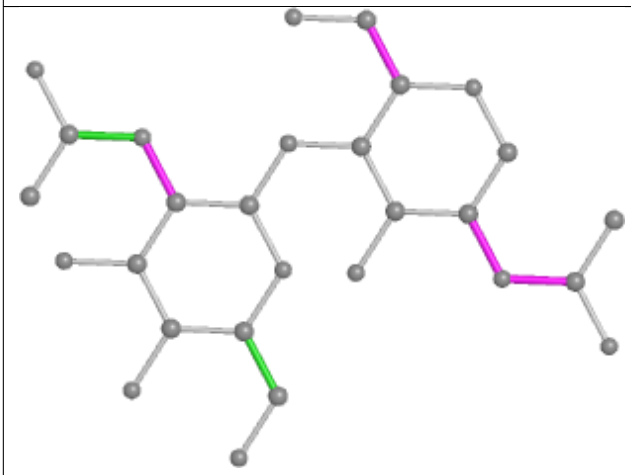
Oligosaccharide Chain B



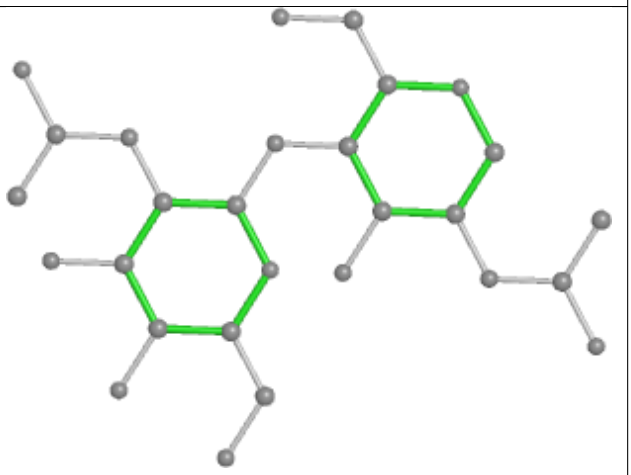
Bond lengths



Bond angles

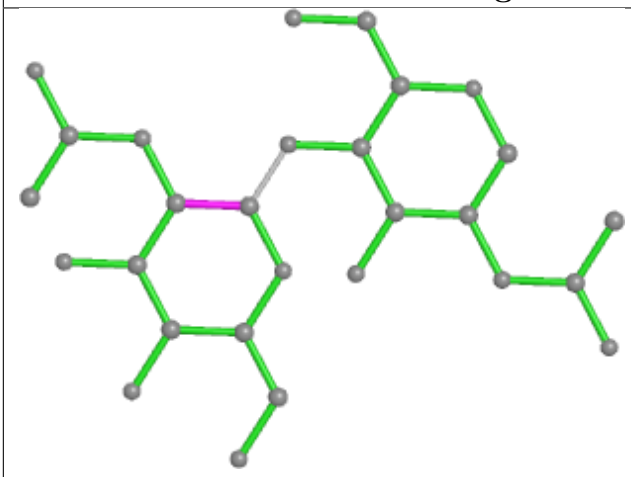


Torsions

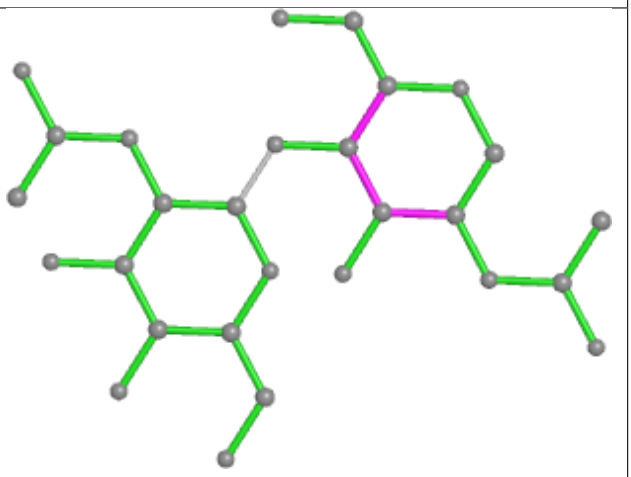


Rings

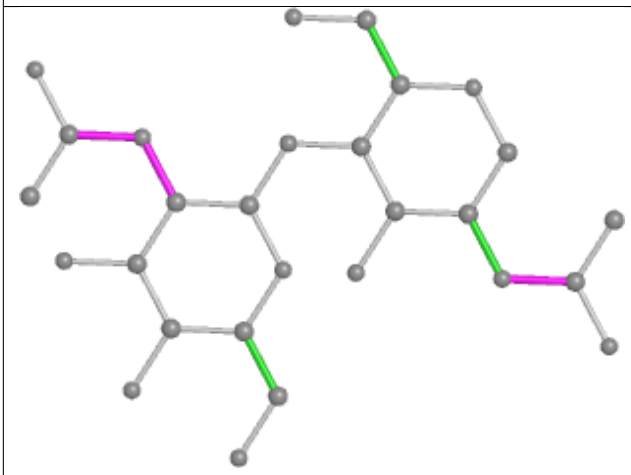
Oligosaccharide Chain C



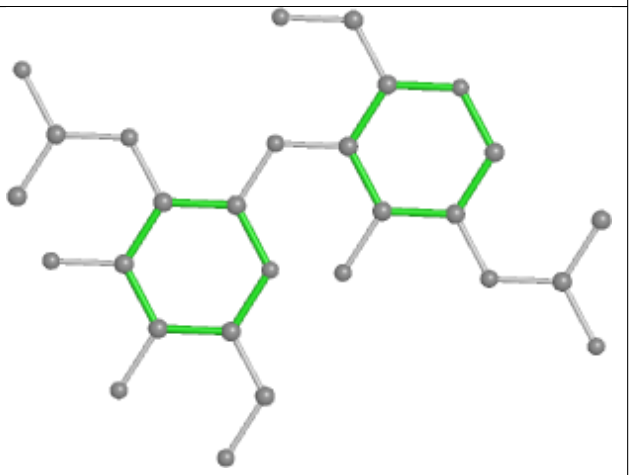
Bond lengths



Bond angles

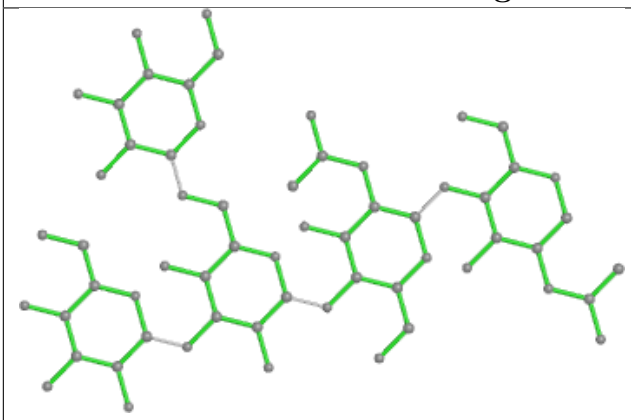


Torsions

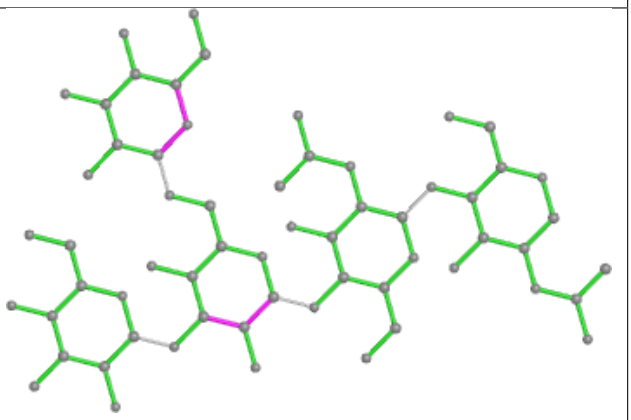


Rings

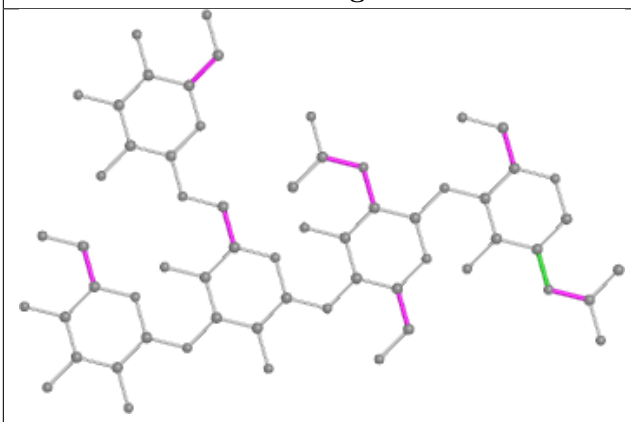
Oligosaccharide Chain D



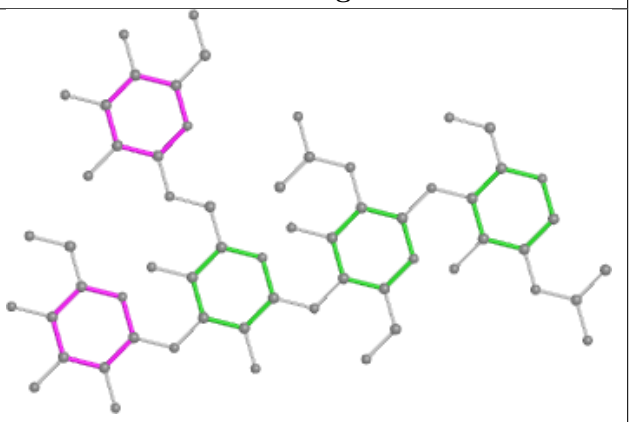
Bond lengths



Bond angles

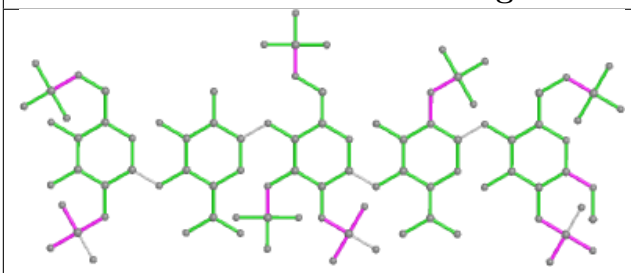


Torsions

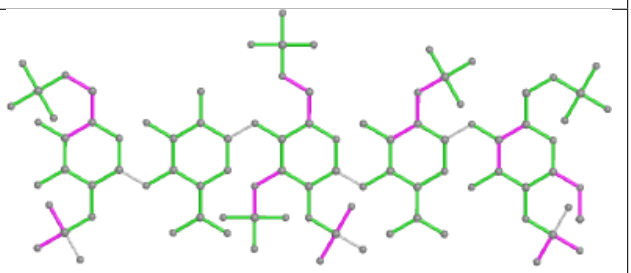


Rings

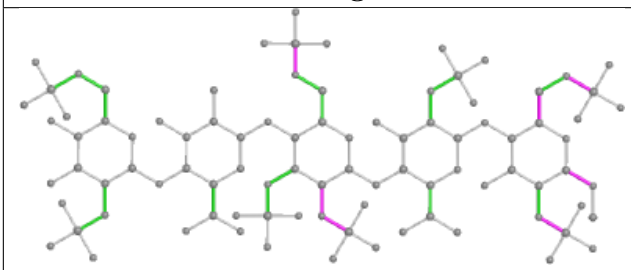
Oligosaccharide Chain E



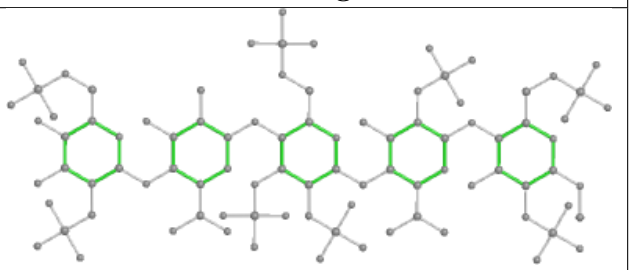
Bond lengths



Bond angles

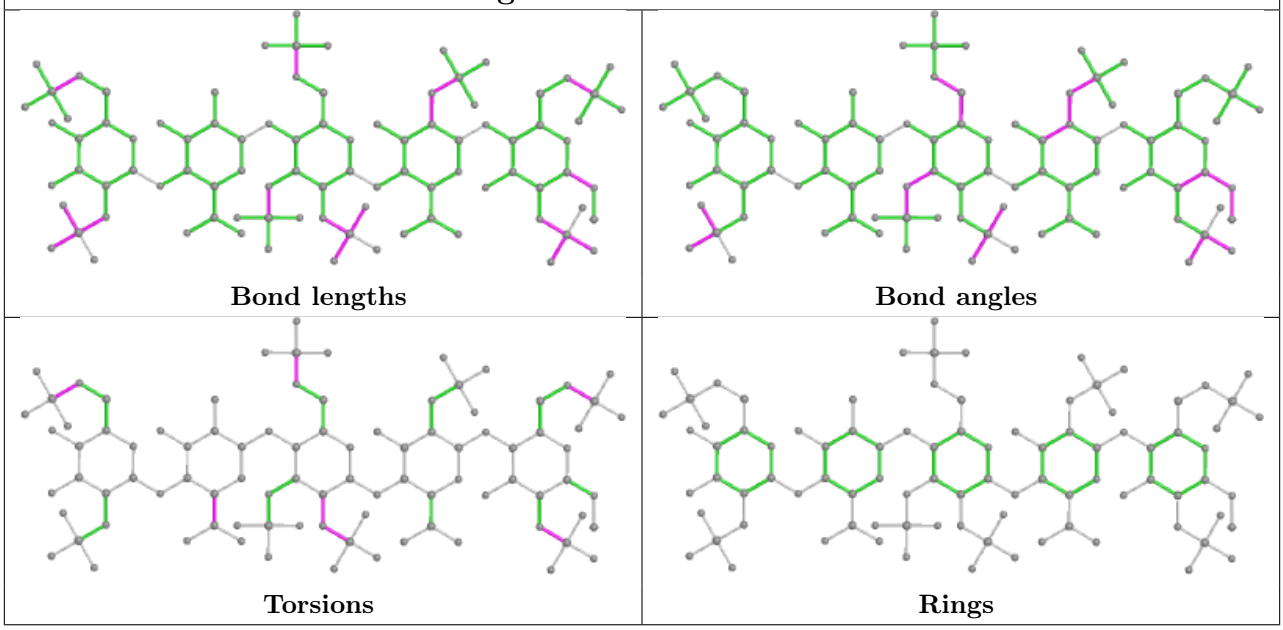


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
6	NAG	I	801	1	14,14,15	0.58	0	17,19,21	0.76	0
6	NAG	L	801	1	14,14,15	0.55	0	17,19,21	0.86	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
6	NAG	I	801	1	-	4/6/23/26	0/1/1/1
6	NAG	L	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	801	NAG	C8-C7-N2-C2
6	L	801	NAG	O7-C7-N2-C2
6	I	801	NAG	C3-C2-N2-C7
6	I	801	NAG	C8-C7-N2-C2
6	I	801	NAG	C4-C5-C6-O6
6	I	801	NAG	O7-C7-N2-C2

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 (i)

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	I	404/432 (93%)	-0.39	1 (0%) 95 87	37, 65, 90, 100	0
1	L	417/432 (96%)	-0.40	0 100 100	33, 59, 90, 106	0
All	All	821/864 (95%)	-0.40	1 (0%) 95 89	33, 62, 90, 106	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	8	CYS	2.4

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
3	NAG	B	2	14/15	0.39	0.40	128,132,134,134	0
3	NAG	C	2	14/15	0.67	0.38	87,90,92,92	0
5	IDS	E	2	16/17	0.74	0.29	101,108,116,116	0
4	MAN	D	4	11/12	0.82	0.19	76,81,83,84	0
3	NAG	B	1	14/15	0.82	0.20	110,114,118,123	0
5	SUS	F	3	23/24	0.82	0.25	97,104,112,113	0
2	MAN	A	3	11/12	0.83	0.20	82,85,87,87	0
4	MAN	D	5	11/12	0.84	0.17	90,91,92,92	0

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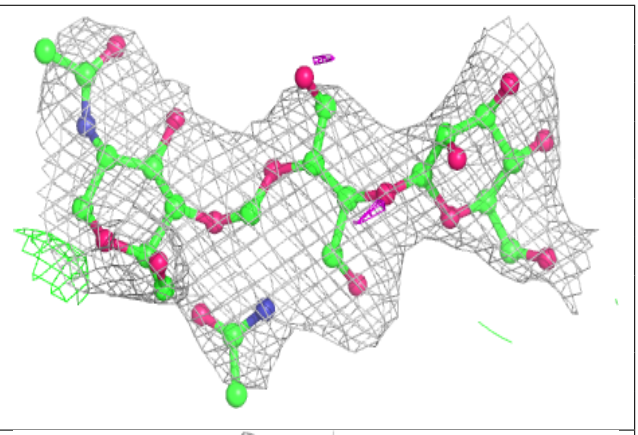
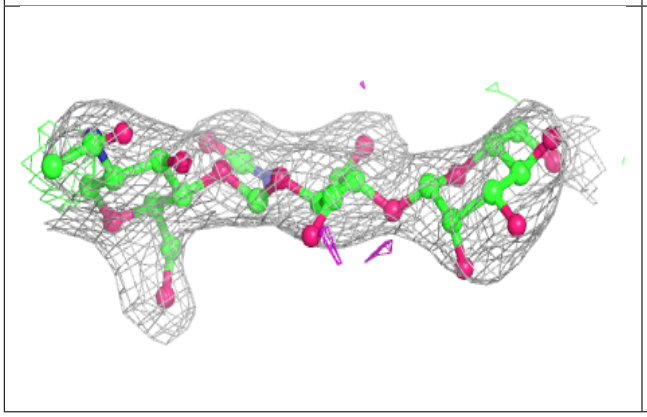
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BDP	F	4	12/13	0.84	0.24	92,94,96,98	0
5	IDS	F	2	16/17	0.85	0.23	97,101,103,104	0
4	MAN	D	3	11/12	0.87	0.18	79,81,85,89	0
5	ZDO	E	1	21/21	0.88	0.19	103,104,110,110	0
3	NAG	C	1	14/15	0.88	0.21	63,71,75,82	0
5	ZDO	F	1	21/21	0.88	0.20	86,90,99,101	0
5	SGN	F	5	19/20	0.88	0.17	96,100,110,110	0
5	BDP	E	4	12/13	0.89	0.24	88,91,94,96	0
2	NAG	A	2	13/15	0.89	0.30	63,71,74,79	0
5	SGN	E	5	19/20	0.90	0.21	76,90,98,99	0
4	NAG	D	1	14/15	0.90	0.18	64,67,68,71	0
2	NAG	A	1	14/15	0.91	0.19	69,72,75,76	0
4	NAG	D	2	14/15	0.91	0.17	68,74,77,79	0
5	SUS	E	3	23/24	0.94	0.19	87,92,101,102	0

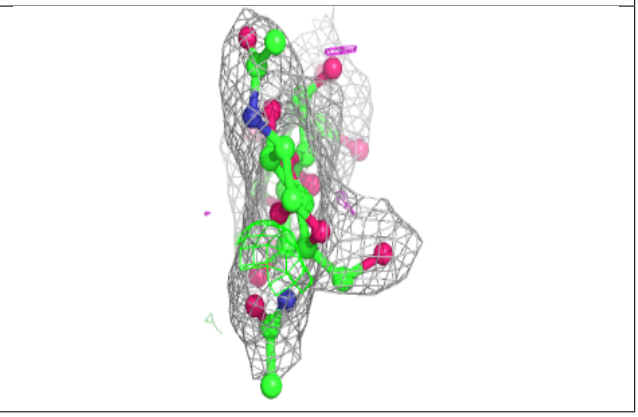
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

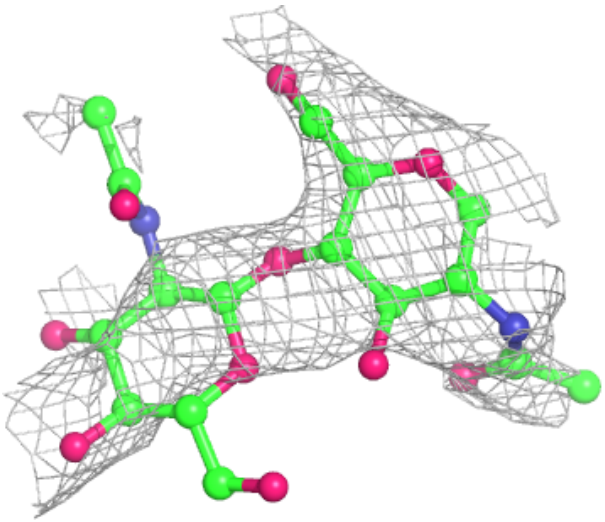


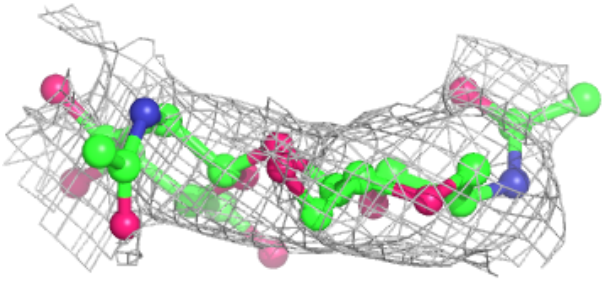


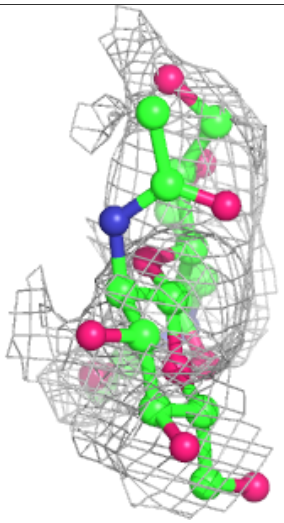


Electron density around Chain B:

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

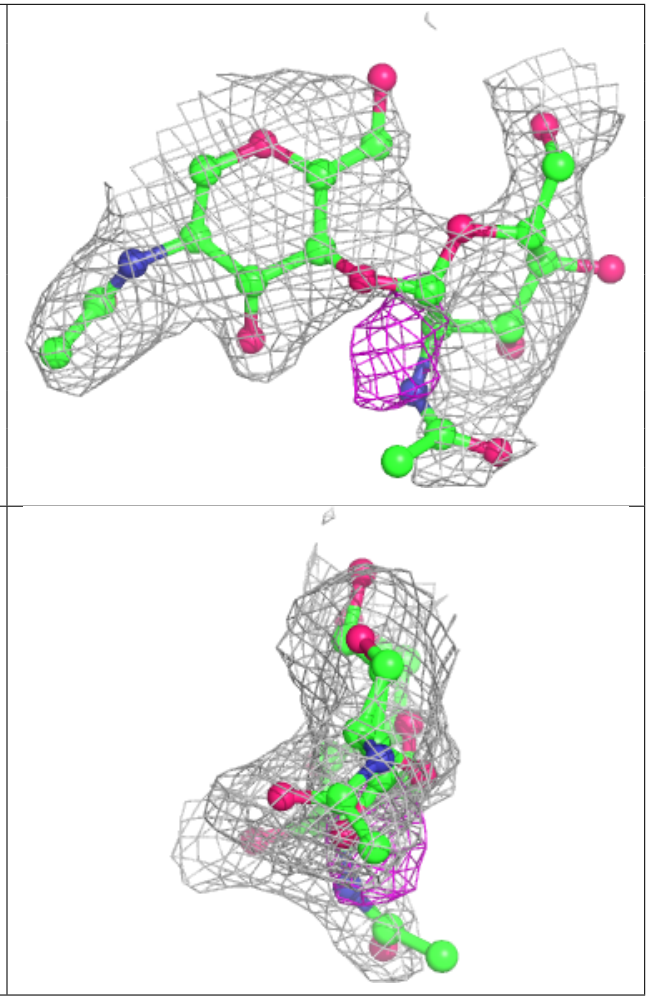






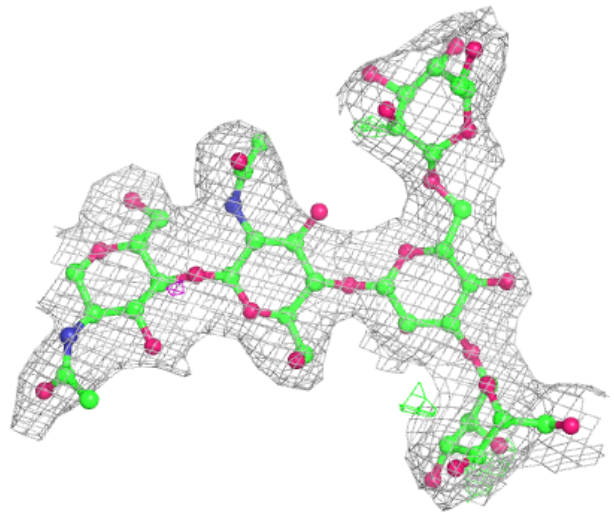
Electron density around Chain C:

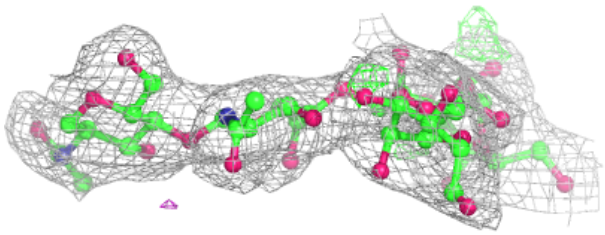
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

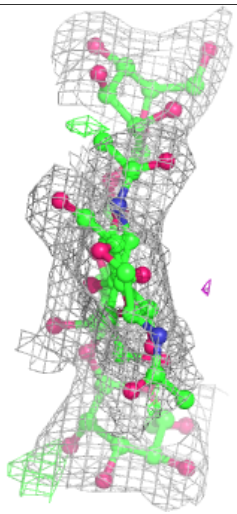


Electron density around Chain D:

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

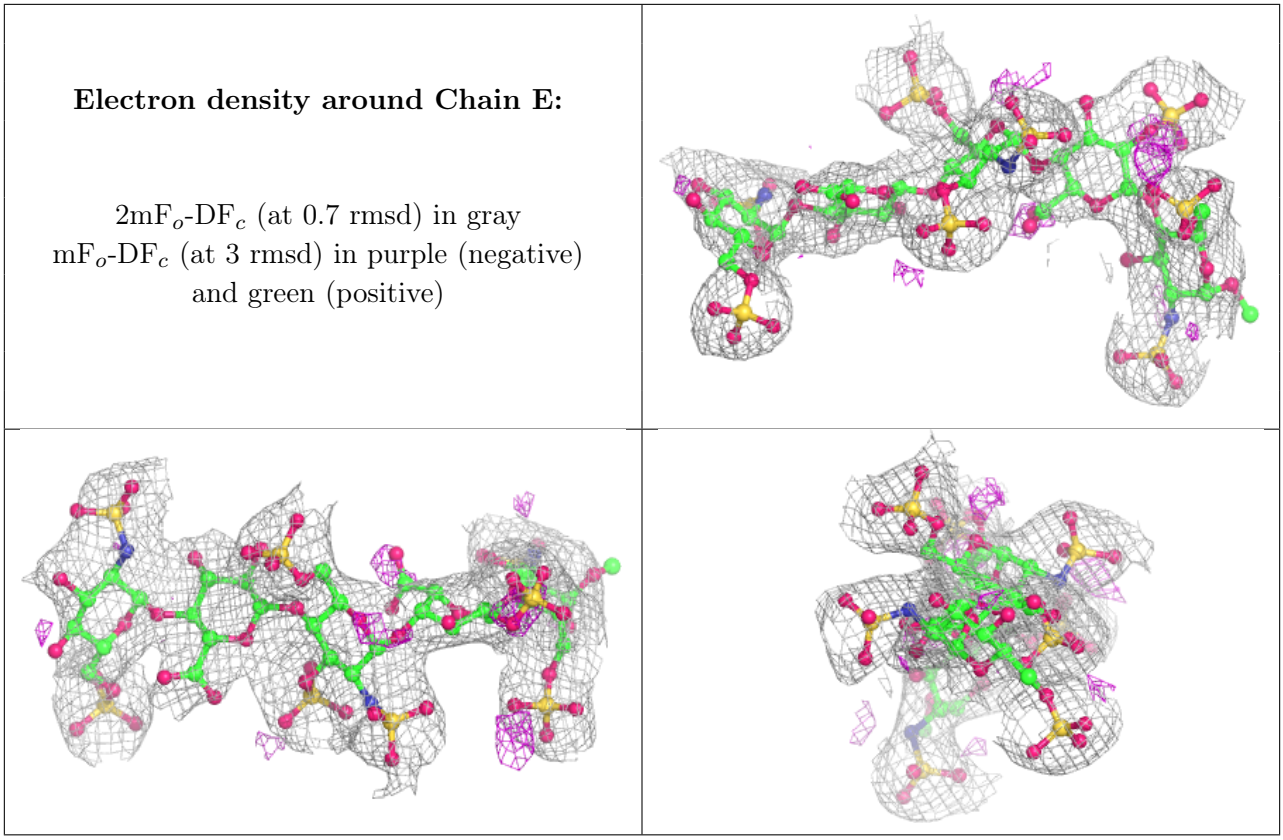






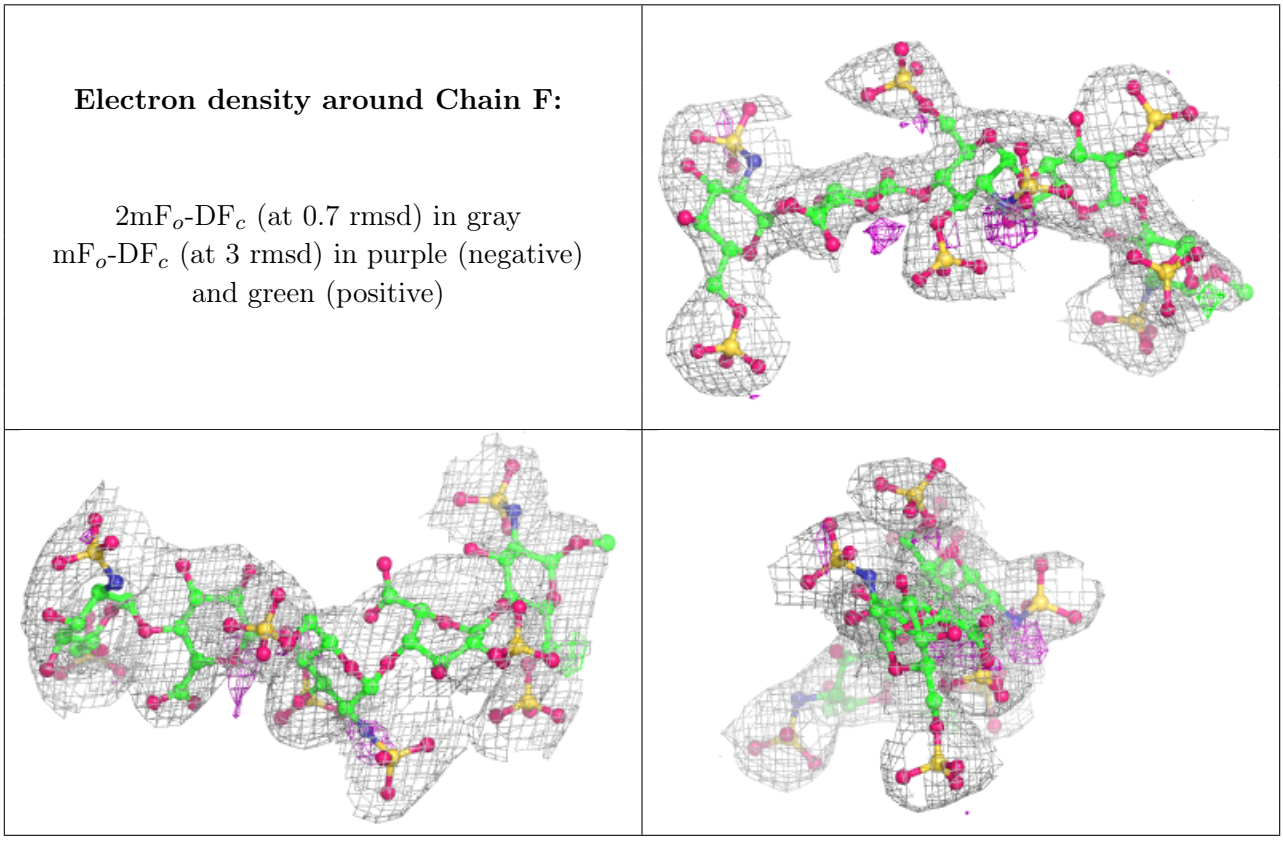
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands (i)

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
6	NAG	I	801	14/15	0.71	0.21	105,107,108,109	6
6	NAG	L	801	14/15	0.88	0.22	80,81,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.