Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 12:14 PM BST

PDB ID	:	3I6S
Title	:	Crystal Structure of the plant subtilisin-like protease SBT3
Authors	:	Rose, R.; Ottmann, C.
Deposited on	:	2009-07-07
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

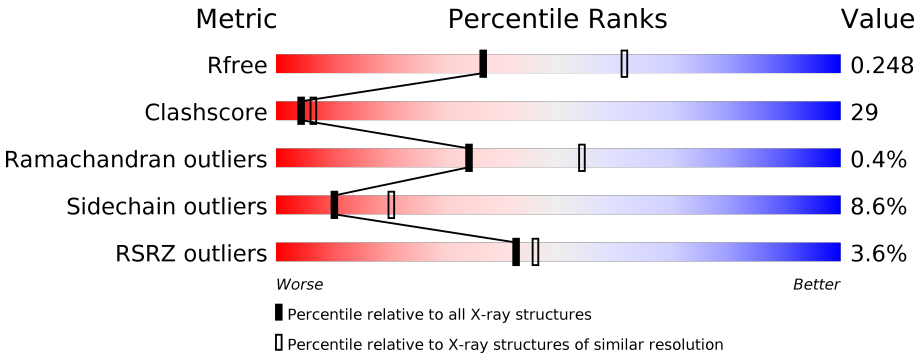
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	A	649	4% 59% 34% 5%
1	B	649	3% 61% 32% 5%
2	C	2	100%
3	D	3	33% 67%
3	E	3	67% 33%
3	G	3	100%

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Mol	Chain	Length	Quality of chain
3	H	3	33% 33% 33%
4	F	2	100%

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	NAG	C	2	-	-	-	X
3	NAG	G	1	-	-	X	-
3	NAG	G	3	-	-	X	-
4	NAG	F	1	X	-	-	-
4	FUC	F	2	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10372 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.

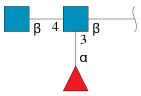
- Molecule 1 is a protein called Subtilisin-like protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			4844	3057	833	933	21			
1	B	639	Total	C	N	O	S	0	0	0
			4822	3047	830	924	21			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is water.

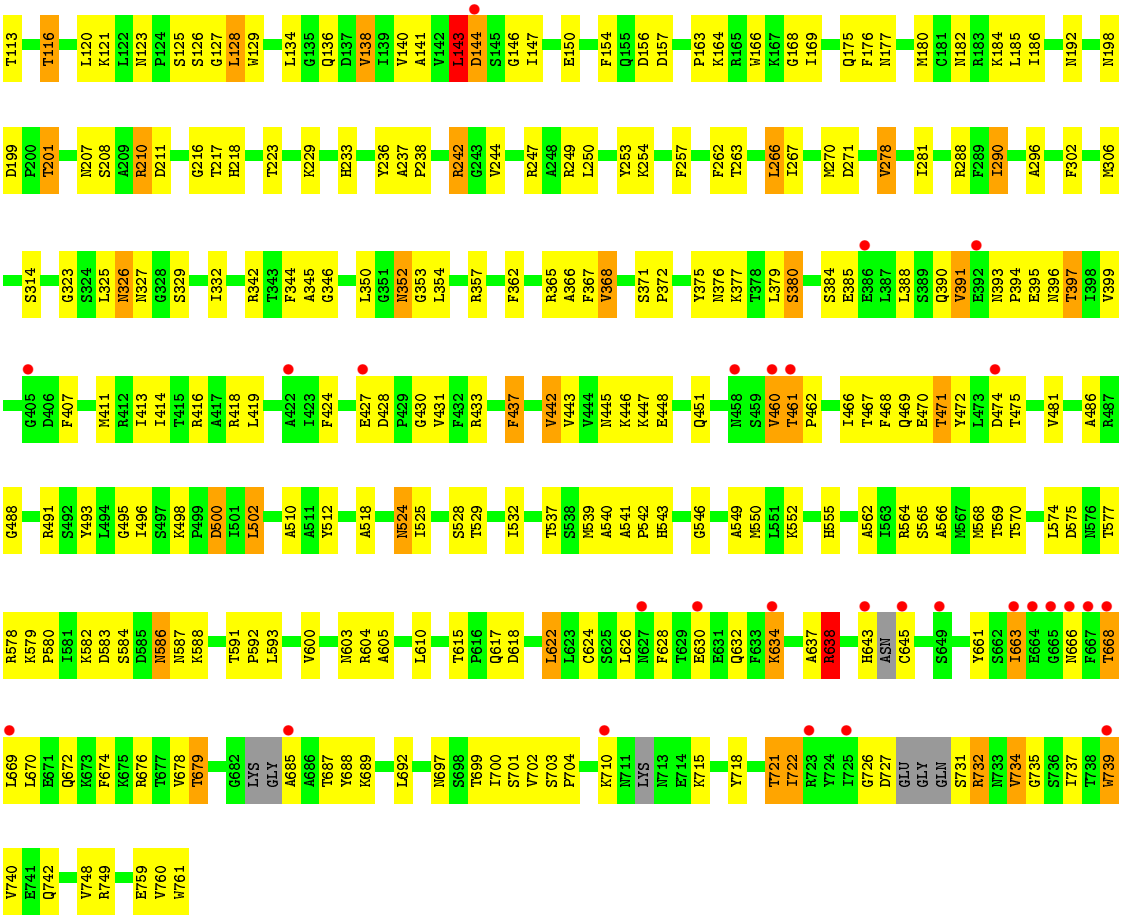
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	212	Total	O	0	0
			212	212		
5	B	290	Total	O	0	0
			290	290		

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.

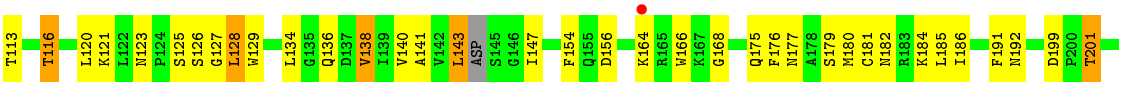
- Molecule 1: Subtilisin-like protease

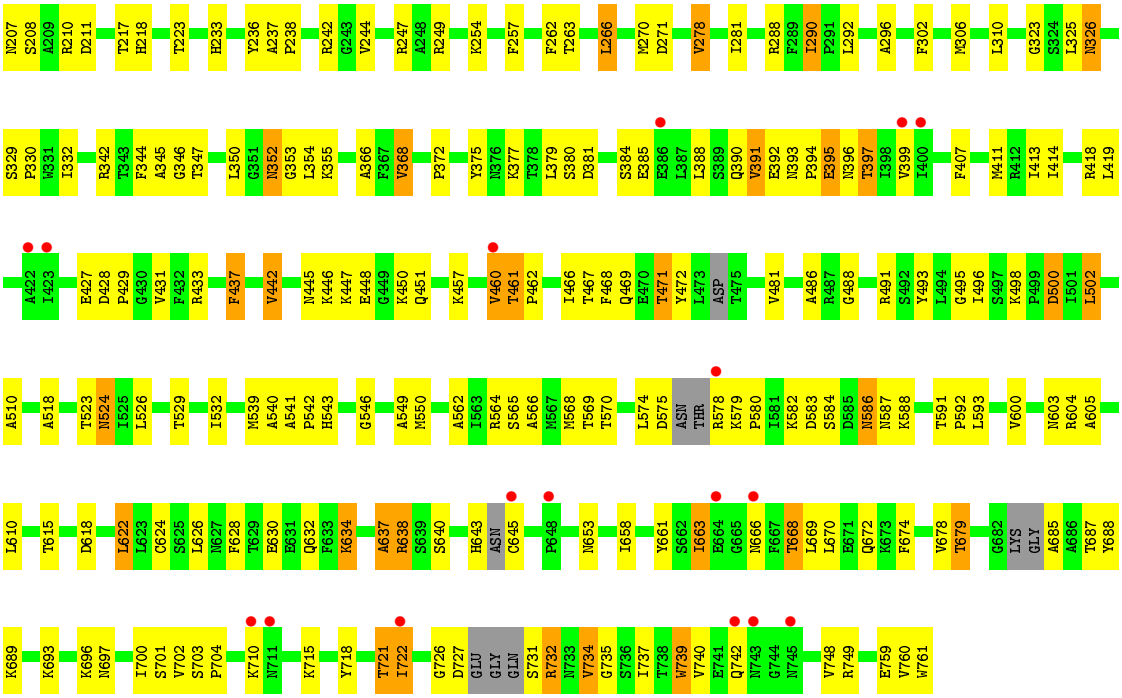
Chain A:



- Molecule 1: Subtilisin-like protease

Chain B:





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

Chain C:

• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

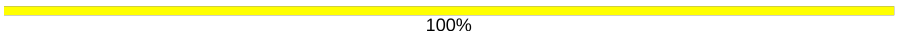
Chain D:

• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

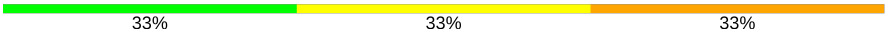
• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.89Å 143.89Å 195.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.50) 99.8 (19.99-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.249 , 0.283 0.247 , 0.248	Depositor DCC
R_{free} test set	4014 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10372	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC

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	0.31	0/4951	0.47	0/6737
1	B	0.29	0/4927	0.46	0/6699
All	All	0.30	0/9878	0.46	0/13436

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	LEU	Peptide
1	A	210	ARG	Sidechain
1	A	637	ALA	Peptide
1	B	637	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4783	284	0
1	B	4822	0	4773	261	0
2	C	28	0	25	2	0
3	D	38	0	34	1	0
3	E	38	0	33	8	0
3	G	38	0	35	13	1
3	H	38	0	34	1	0
4	F	24	0	22	3	0
5	A	212	0	0	47	1
5	B	290	0	0	44	0
All	All	10372	0	9739	563	1

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 29.

All (563) 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:699:THR:HA	5:A:781:HOH:O	1.35	1.25
1:A:475:THR:HA	5:A:908:HOH:O	1.35	1.22
1:B:395:GLU:HG3	5:B:9:HOH:O	1.40	1.18
1:A:591:THR:HG22	1:A:593:LEU:H	1.05	1.17
1:A:674:PHE:HE2	1:A:722:ILE:CD1	1.57	1.17
1:B:674:PHE:HE2	1:B:722:ILE:CD1	1.57	1.16
1:B:591:THR:HG22	1:B:593:LEU:H	1.05	1.15
1:B:674:PHE:CE2	1:B:722:ILE:HD11	1.82	1.14
1:B:591:THR:HG23	1:B:592:PRO:HD2	1.28	1.13
1:A:591:THR:HG23	1:A:592:PRO:HD2	1.22	1.13
1:A:674:PHE:CE2	1:A:722:ILE:HD11	1.84	1.12
1:B:143:LEU:HD21	1:B:270:MET:HG2	1.32	1.11
1:A:144:ASP:HB3	1:A:146:GLY:H	1.12	1.10
1:A:674:PHE:HE2	1:A:722:ILE:HD11	1.13	1.09
1:A:143:LEU:HD21	1:A:270:MET:HG2	1.31	1.09
1:A:433:ARG:HD2	5:A:854:HOH:O	1.53	1.08
1:B:674:PHE:HE2	1:B:722:ILE:HD11	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HG22	5:A:76:HOH:O	1.56	1.05
1:A:679:THR:HG22	5:A:52:HOH:O	1.55	1.04
1:A:674:PHE:CE2	1:A:722:ILE:CD1	2.39	1.03
1:B:375:TYR:HD2	5:B:821:HOH:O	1.38	1.03
1:B:393:ASN:O	1:B:397:THR:HG22	1.58	1.03
1:B:674:PHE:CE2	1:B:722:ILE:CD1	2.38	1.03
1:A:393:ASN:O	1:A:397:THR:HG22	1.59	1.02
1:B:693:LYS:HD2	5:B:977:HOH:O	1.58	1.01
1:A:689:LYS:HD2	1:A:742:GLN:CD	1.86	0.96
1:B:721:THR:HG22	5:B:784:HOH:O	1.64	0.95
1:B:689:LYS:HD2	1:B:742:GLN:CD	1.85	0.95
1:A:638:ARG:HD3	5:A:812:HOH:O	1.69	0.92
1:A:591:THR:CG2	1:A:592:PRO:HD2	2.00	0.92
1:A:591:THR:HG23	1:A:592:PRO:CD	2.00	0.92
1:A:672:GLN:HG2	1:A:674:PHE:CZ	2.05	0.92
1:A:555:HIS:CD2	5:A:878:HOH:O	2.23	0.91
1:B:461:THR:O	1:B:461:THR:HG22	1.70	0.91
3:G:1:NAG:H62	3:G:3:NAG:C1	2.00	0.91
1:A:175:GLN:O	1:A:210:ARG:NH1	2.04	0.90
3:G:1:NAG:H62	3:G:3:NAG:O7	1.69	0.90
1:B:591:THR:CG2	1:B:592:PRO:HD2	2.01	0.90
1:B:591:THR:HG22	1:B:593:LEU:N	1.88	0.89
1:B:262:PHE:HE1	5:B:835:HOH:O	1.55	0.89
1:A:591:THR:HG22	1:A:593:LEU:N	1.88	0.89
1:A:555:HIS:HD2	5:A:878:HOH:O	1.56	0.88
1:B:591:THR:HG23	1:B:592:PRO:CD	2.05	0.87
1:A:141:ALA:HB2	1:A:278:VAL:HG21	1.56	0.87
1:A:323:GLY:O	1:A:491:ARG:HD2	1.75	0.87
1:A:461:THR:HG22	1:A:461:THR:O	1.72	0.86
1:B:574:LEU:HD12	5:B:875:HOH:O	1.75	0.86
1:A:143:LEU:CD2	1:A:270:MET:HG2	2.06	0.85
1:B:181:CYS:HB3	5:B:98:HOH:O	1.76	0.85
1:B:175:GLN:O	1:B:210:ARG:NH1	2.11	0.84
1:A:471:THR:CG2	5:A:851:HOH:O	2.24	0.84
1:B:381:ASP:HB3	5:B:841:HOH:O	1.77	0.84
1:B:141:ALA:HB2	1:B:278:VAL:HG21	1.57	0.84
1:B:672:GLN:HG2	1:B:674:PHE:CZ	2.12	0.83
1:B:143:LEU:CD2	1:B:270:MET:HG2	2.07	0.83
1:A:674:PHE:HE2	1:A:722:ILE:HD13	1.44	0.83
1:B:447:LYS:CE	5:B:829:HOH:O	2.27	0.82
1:A:352:ASN:ND2	1:A:354:LEU:H	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:HB3	1:A:580:PRO:HD2	1.60	0.81
1:A:727:ASP:OD1	1:A:731:SER:HB3	1.81	0.81
1:A:144:ASP:HB3	1:A:146:GLY:N	1.94	0.80
1:B:323:GLY:O	1:B:491:ARG:HD2	1.81	0.80
1:B:523:THR:HG23	5:B:945:HOH:O	1.81	0.79
1:B:674:PHE:HE2	1:B:722:ILE:HD13	1.46	0.79
2:C:1:NAG:O6	2:C:2:NAG:C1	2.30	0.79
1:A:731:SER:HA	5:A:785:HOH:O	1.83	0.79
1:B:579:LYS:HB3	1:B:580:PRO:HD2	1.63	0.79
1:B:238:PRO:HD2	5:B:106:HOH:O	1.81	0.79
1:B:352:ASN:ND2	1:B:354:LEU:H	1.79	0.78
1:B:450:LYS:HG2	5:B:912:HOH:O	1.83	0.78
1:B:446:LYS:HD3	5:B:901:HOH:O	1.83	0.78
1:A:352:ASN:HD22	1:A:352:ASN:C	1.86	0.78
1:B:447:LYS:HE3	5:B:829:HOH:O	1.84	0.78
1:A:669:LEU:HD13	1:A:669:LEU:C	2.04	0.78
1:A:471:THR:HG22	5:A:851:HOH:O	1.83	0.77
1:B:388:LEU:O	1:B:391:VAL:HG12	1.85	0.77
1:A:591:THR:CG2	1:A:592:PRO:CD	2.61	0.76
1:A:388:LEU:O	1:A:391:VAL:HG12	1.84	0.76
1:A:346:GLY:HA2	1:A:467:THR:O	1.85	0.76
1:B:591:THR:CG2	1:B:592:PRO:CD	2.63	0.76
1:B:346:GLY:HA2	1:B:467:THR:O	1.86	0.76
1:B:727:ASP:OD1	1:B:731:SER:HB3	1.85	0.76
1:B:116:THR:HG21	1:B:543:HIS:NE2	2.01	0.76
1:B:663:ILE:H	1:B:663:ILE:HD13	1.49	0.76
1:B:352:ASN:C	1:B:352:ASN:HD22	1.90	0.75
1:A:663:ILE:HD13	1:A:663:ILE:H	1.50	0.75
1:B:493:TYR:CE1	5:B:845:HOH:O	2.39	0.75
1:A:552:LYS:CD	5:A:837:HOH:O	2.34	0.75
1:B:634:LYS:O	1:B:638:ARG:HA	1.85	0.74
3:G:1:NAG:C4	3:G:3:NAG:C1	2.66	0.74
1:A:116:THR:HG21	1:A:543:HIS:NE2	2.03	0.74
1:B:669:LEU:HD13	1:B:669:LEU:C	2.09	0.73
1:A:365:ARG:NE	5:A:913:HOH:O	2.20	0.73
3:G:1:NAG:O4	3:G:3:NAG:O5	2.07	0.73
1:B:381:ASP:CB	5:B:841:HOH:O	2.35	0.72
1:A:460:VAL:O	1:A:461:THR:HB	1.89	0.72
1:A:552:LYS:HD2	5:A:837:HOH:O	1.90	0.72
1:A:123:ASN:HD22	1:A:125:SER:H	1.38	0.72
1:A:393:ASN:O	1:A:397:THR:CG2	2.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASN:HD22	1:B:587:ASN:N	1.88	0.71
1:B:393:ASN:O	1:B:397:THR:CG2	2.37	0.71
1:B:460:VAL:O	1:B:461:THR:HB	1.90	0.71
1:A:472:TYR:HB3	5:A:782:HOH:O	1.91	0.71
1:A:577:THR:O	1:A:578:ARG:HB2	1.91	0.71
1:A:302:PHE:O	1:A:306:MET:HG2	1.92	0.70
1:A:586:ASN:HD22	1:A:587:ASN:N	1.91	0.69
1:B:450:LYS:CG	5:B:912:HOH:O	2.41	0.69
1:B:375:TYR:CD2	5:B:821:HOH:O	2.24	0.69
1:B:177:ASN:H	1:B:180:MET:CE	2.06	0.69
1:B:384:SER:O	1:B:388:LEU:HD23	1.93	0.69
1:A:384:SER:O	1:A:388:LEU:HD23	1.93	0.68
5:A:829:HOH:O	3:E:1:NAG:H83	1.93	0.68
1:A:578:ARG:HA	1:A:578:ARG:HE	1.59	0.68
1:A:470:GLU:HA	5:A:10:HOH:O	1.93	0.68
1:B:218:HIS:CE1	1:B:510:ALA:HB3	2.29	0.68
3:G:1:NAG:C6	3:G:3:NAG:C1	2.72	0.68
1:A:570:THR:HG21	1:A:605:ALA:HB2	1.75	0.68
1:B:674:PHE:CE2	1:B:722:ILE:HD13	2.24	0.68
1:A:591:THR:HG22	1:A:592:PRO:N	2.09	0.67
1:A:578:ARG:NE	1:A:578:ARG:HA	2.09	0.67
1:A:129:TRP:CG	1:A:134:LEU:HD22	2.30	0.67
1:A:702:VAL:HG22	1:A:703:SER:N	2.10	0.67
1:B:123:ASN:HD21	1:B:126:SER:H	1.42	0.67
1:B:591:THR:HG22	1:B:592:PRO:N	2.09	0.67
1:B:570:THR:HG21	1:B:605:ALA:HB2	1.75	0.67
1:B:721:THR:CG2	5:B:784:HOH:O	2.29	0.67
1:B:129:TRP:CG	1:B:134:LEU:HD22	2.30	0.67
1:B:302:PHE:O	1:B:306:MET:HG2	1.94	0.67
1:A:199:ASP:OD1	1:A:201:THR:HB	1.94	0.66
1:B:199:ASP:OD1	1:B:201:THR:HB	1.95	0.66
1:A:634:LYS:O	1:A:638:ARG:HA	1.95	0.66
1:B:123:ASN:HD22	1:B:125:SER:H	1.41	0.66
1:B:433:ARG:NH2	5:B:101:HOH:O	2.28	0.66
3:G:2:FUC:C6	3:G:3:NAG:H2	2.26	0.66
1:A:460:VAL:HG22	5:A:863:HOH:O	1.96	0.66
1:B:702:VAL:HG22	1:B:703:SER:N	2.11	0.66
1:A:575:ASP:C	1:A:575:ASP:OD1	2.34	0.65
1:B:491:ARG:HG3	5:B:976:HOH:O	1.96	0.65
1:A:502:LEU:O	1:A:600:VAL:HG23	1.96	0.65
1:A:218:HIS:CE1	1:A:510:ALA:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:H	1:B:471:THR:HG21	1.60	0.65
1:B:128:LEU:HD22	1:B:550:MET:HB3	1.78	0.65
1:A:591:THR:CG2	1:A:592:PRO:N	2.60	0.65
1:B:177:ASN:H	1:B:180:MET:HE2	1.61	0.65
1:A:237:ALA:H	1:A:471:THR:HG21	1.60	0.65
1:A:177:ASN:HD22	2:C:1:NAG:C1	2.01	0.64
1:B:502:LEU:O	1:B:600:VAL:HG23	1.98	0.64
1:A:674:PHE:CD2	1:A:722:ILE:HD11	2.31	0.64
1:B:461:THR:CG2	1:B:461:THR:O	2.44	0.64
1:A:123:ASN:HD21	1:A:126:SER:H	1.45	0.63
1:A:136:GLN:HA	1:A:247:ARG:O	1.98	0.63
1:B:674:PHE:CD2	1:B:722:ILE:HD11	2.31	0.63
1:A:177:ASN:H	1:A:180:MET:CE	2.11	0.62
1:A:352:ASN:ND2	1:A:352:ASN:C	2.52	0.62
3:G:3:NAG:O7	3:G:3:NAG:C1	2.47	0.62
1:B:136:GLN:HA	1:B:247:ARG:O	1.99	0.62
1:B:591:THR:CG2	1:B:592:PRO:N	2.63	0.62
1:B:583:ASP:HB3	1:B:586:ASN:HD21	1.64	0.62
1:A:583:ASP:HB3	1:A:586:ASN:HD21	1.65	0.62
1:B:375:TYR:OH	1:B:377:LYS:HE3	2.00	0.61
1:B:700:ILE:HG22	1:B:722:ILE:HG23	1.82	0.61
1:A:177:ASN:H	1:A:180:MET:HE2	1.65	0.61
1:A:524:ASN:H	1:A:524:ASN:HD22	1.48	0.61
1:A:129:TRP:HB3	1:A:134:LEU:CD2	2.30	0.61
1:A:375:TYR:OH	1:A:377:LYS:HE3	2.01	0.61
1:A:591:THR:CG2	1:A:593:LEU:H	1.97	0.60
1:B:121:LYS:HD3	5:B:780:HOH:O	2.01	0.60
1:B:181:CYS:CB	5:B:98:HOH:O	2.39	0.60
1:B:689:LYS:HD2	1:B:742:GLN:OE1	2.00	0.60
1:A:701:SER:OG	1:A:721:THR:HG23	2.00	0.60
1:B:129:TRP:HB3	1:B:134:LEU:CD2	2.31	0.60
1:A:700:ILE:HG22	1:A:722:ILE:HG23	1.82	0.60
1:A:674:PHE:CE2	1:A:722:ILE:HD13	2.23	0.60
1:B:175:GLN:NE2	5:B:897:HOH:O	2.35	0.60
1:A:428:ASP:OD1	1:A:428:ASP:C	2.39	0.60
1:A:345:ALA:HB3	1:A:472:TYR:HE1	1.66	0.60
1:A:689:LYS:HD2	1:A:742:GLN:OE1	2.02	0.60
1:B:457:LYS:HE3	5:B:821:HOH:O	2.01	0.60
1:B:610:LEU:HB3	1:B:678:VAL:HG22	1.83	0.59
1:B:266:LEU:O	1:B:266:LEU:HD12	2.02	0.59
1:B:352:ASN:C	1:B:352:ASN:ND2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:NH2	5:A:95:HOH:O	2.33	0.59
1:A:569:THR:HA	1:A:749:ARG:O	2.01	0.59
1:A:610:LEU:HB3	1:A:678:VAL:HG22	1.84	0.59
1:B:461:THR:N	1:B:462:PRO:CD	2.65	0.59
1:A:622:LEU:O	1:A:626:LEU:HD13	2.03	0.59
1:B:138:VAL:HG11	1:B:549:ALA:HB1	1.84	0.59
1:B:679:THR:HB	1:B:715:LYS:HG2	1.85	0.59
1:B:737:ILE:HD11	1:B:739:TRP:CZ3	2.37	0.59
4:F:1:NAG:H3	4:F:2:FUC:H5	1.85	0.59
1:B:524:ASN:H	1:B:524:ASN:HD22	1.49	0.58
1:B:566:ALA:O	1:B:570:THR:HG22	2.03	0.58
1:A:138:VAL:HG11	1:A:549:ALA:HB1	1.85	0.58
3:G:1:NAG:C4	3:G:3:NAG:O5	2.50	0.58
1:B:722:ILE:HD12	1:B:722:ILE:H	1.69	0.58
1:B:737:ILE:CD1	1:B:739:TRP:CZ3	2.86	0.58
1:B:388:LEU:O	1:B:391:VAL:CG1	2.52	0.58
1:A:679:THR:HB	1:A:715:LYS:HG2	1.83	0.58
1:A:737:ILE:HD11	1:A:739:TRP:CZ3	2.39	0.58
1:B:345:ALA:HB3	1:B:472:TYR:HE1	1.68	0.58
1:B:701:SER:OG	1:B:721:THR:HG23	2.04	0.58
1:A:461:THR:N	1:A:462:PRO:CD	2.67	0.58
1:A:630:GLU:HB3	1:A:643:HIS:CD2	2.38	0.58
1:A:737:ILE:CD1	1:A:739:TRP:CZ3	2.87	0.58
1:B:518:ALA:CB	1:B:529:THR:HG22	2.34	0.58
1:A:352:ASN:HD22	1:A:354:LEU:H	1.49	0.57
1:A:388:LEU:O	1:A:391:VAL:CG1	2.52	0.57
1:A:385:GLU:HG2	1:A:413:ILE:HD12	1.85	0.57
5:A:829:HOH:O	3:E:1:NAG:C8	2.51	0.57
1:A:564:ARG:O	1:A:568:MET:HG3	2.04	0.57
1:A:672:GLN:CG	1:A:674:PHE:CZ	2.86	0.57
1:B:570:THR:HG21	1:B:605:ALA:CB	2.35	0.57
1:A:722:ILE:HD12	1:A:722:ILE:H	1.69	0.57
1:A:428:ASP:OD1	1:A:430:GLY:N	2.33	0.57
1:A:570:THR:HG21	1:A:605:ALA:CB	2.35	0.57
1:B:591:THR:CG2	1:B:593:LEU:H	1.97	0.57
1:B:290:ILE:H	1:B:290:ILE:HD13	1.69	0.56
1:B:123:ASN:ND2	1:B:126:SER:H	2.02	0.56
1:A:666:ASN:ND2	5:A:884:HOH:O	2.37	0.56
1:A:128:LEU:HD22	1:A:550:MET:HB3	1.85	0.56
1:A:229:LYS:CG	5:A:94:HOH:O	2.53	0.56
1:B:325:LEU:HA	1:B:486:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CE2	1:A:180:MET:HB3	2.41	0.56
1:A:702:VAL:HG22	1:A:703:SER:H	1.70	0.56
1:B:622:LEU:CD2	1:B:622:LEU:C	2.74	0.56
1:B:732:ARG:N	1:B:732:ARG:HD3	2.20	0.56
1:A:150:GLU:OE2	1:A:210:ARG:NH2	2.39	0.56
1:A:586:ASN:ND2	1:A:588:LYS:H	2.04	0.56
1:A:669:LEU:CD1	1:A:669:LEU:C	2.74	0.56
1:B:352:ASN:HD22	1:B:354:LEU:H	1.51	0.56
1:B:574:LEU:CD1	5:B:875:HOH:O	2.42	0.56
1:A:722:ILE:HD12	1:A:722:ILE:N	2.21	0.56
1:B:630:GLU:HB3	1:B:643:HIS:CD2	2.41	0.56
3:G:2:FUC:H62	3:G:3:NAG:H2	1.88	0.56
1:A:566:ALA:O	1:A:570:THR:HG22	2.06	0.56
1:B:569:THR:HA	1:B:749:ARG:O	2.06	0.56
1:B:486:ALA:HB2	5:B:796:HOH:O	2.05	0.56
1:A:176:PHE:HA	1:A:180:MET:HE2	1.87	0.55
1:A:493:TYR:CE2	1:A:495:GLY:HA3	2.40	0.55
1:A:737:ILE:HD11	1:A:739:TRP:CH2	2.41	0.55
1:B:201:THR:O	1:B:201:THR:CG2	2.55	0.55
1:A:266:LEU:HD12	1:A:266:LEU:O	2.06	0.55
1:A:123:ASN:HD22	1:A:125:SER:N	2.04	0.55
1:A:461:THR:CG2	1:A:461:THR:O	2.46	0.55
3:E:2:FUC:H5	3:E:3:NAG:O5	2.06	0.55
1:B:428:ASP:OD1	1:B:428:ASP:C	2.45	0.55
1:A:352:ASN:HD22	1:A:353:GLY:N	2.04	0.55
1:A:622:LEU:C	1:A:622:LEU:CD2	2.75	0.55
1:B:722:ILE:N	1:B:722:ILE:HD12	2.22	0.55
1:B:570:THR:HG21	1:B:605:ALA:CA	2.37	0.55
1:B:622:LEU:O	1:B:626:LEU:HD13	2.06	0.55
1:A:201:THR:O	1:A:201:THR:CG2	2.54	0.55
1:B:325:LEU:HD12	1:B:325:LEU:C	2.27	0.55
1:A:570:THR:HG21	1:A:605:ALA:CA	2.36	0.55
1:B:385:GLU:HG2	1:B:413:ILE:HD12	1.88	0.55
1:B:570:THR:OG1	1:B:604:ARG:HB3	2.07	0.55
1:A:518:ALA:CB	1:A:529:THR:HG22	2.36	0.55
1:B:737:ILE:HD11	1:B:739:TRP:CH2	2.41	0.55
1:A:144:ASP:OD1	1:A:216:GLY:HA2	2.07	0.55
1:A:290:ILE:H	1:A:290:ILE:HD13	1.72	0.55
1:A:199:ASP:CG	5:A:872:HOH:O	2.45	0.54
1:A:325:LEU:HD12	1:A:325:LEU:C	2.28	0.54
1:B:123:ASN:HD22	1:B:125:SER:N	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:VAL:CG1	1:A:761:TRP:N	2.70	0.54
1:A:390:GLN:HE22	3:E:3:NAG:HN2	1.54	0.54
1:A:325:LEU:HA	1:A:486:ALA:HB1	1.89	0.54
1:A:579:LYS:HB2	5:A:950:HOH:O	2.07	0.54
1:A:460:VAL:CG2	5:A:863:HOH:O	2.54	0.54
1:B:760:VAL:CG1	1:B:761:TRP:N	2.70	0.54
1:B:179:SER:HB3	4:F:1:NAG:H82	1.89	0.54
1:A:570:THR:OG1	1:A:604:ARG:HB3	2.06	0.53
1:A:669:LEU:HD13	1:A:670:LEU:N	2.23	0.53
1:B:697:ASN:ND2	5:B:970:HOH:O	2.41	0.53
1:B:586:ASN:ND2	1:B:588:LYS:H	2.07	0.53
1:B:679:THR:HG22	5:B:790:HOH:O	2.09	0.53
1:B:760:VAL:HG12	1:B:761:TRP:N	2.23	0.53
1:A:233:HIS:O	1:A:233:HIS:CD2	2.62	0.53
1:B:541:ALA:N	1:B:542:PRO:HD2	2.24	0.53
1:A:357:ARG:HH12	1:A:474:ASP:CG	2.11	0.53
1:B:120:LEU:O	1:B:121:LYS:HB2	2.09	0.53
1:A:390:GLN:NE2	3:E:1:NAG:O6	2.42	0.53
1:A:661:TYR:CD2	1:A:726:GLY:HA3	2.44	0.53
1:A:688:TYR:CB	1:A:739:TRP:HD1	2.22	0.53
1:A:760:VAL:HG12	1:A:761:TRP:N	2.24	0.53
1:B:564:ARG:O	1:B:568:MET:HG3	2.09	0.53
1:B:658:ILE:HG22	5:B:782:HOH:O	2.08	0.53
1:A:288:ARG:HG3	1:A:326:ASN:HB3	1.91	0.53
1:A:610:LEU:HB2	1:A:748:VAL:HG21	1.90	0.53
1:A:123:ASN:ND2	1:A:126:SER:H	2.05	0.53
1:A:749:ARG:HB3	5:A:844:HOH:O	2.08	0.53
1:B:352:ASN:HD22	1:B:353:GLY:N	2.07	0.53
1:A:732:ARG:N	1:A:732:ARG:HD3	2.23	0.52
1:B:218:HIS:ND1	1:B:510:ALA:HB3	2.24	0.52
1:B:392:GLU:N	5:B:921:HOH:O	2.42	0.52
1:A:120:LEU:O	1:A:121:LYS:HB2	2.09	0.52
1:A:427:GLU:OE2	1:A:445:ASN:HB2	2.09	0.52
3:G:1:NAG:H4	3:G:3:NAG:O5	2.09	0.52
1:B:666:ASN:HB2	5:B:899:HOH:O	2.07	0.52
1:B:610:LEU:HB2	1:B:748:VAL:HG21	1.92	0.52
1:A:541:ALA:N	1:A:542:PRO:HD2	2.25	0.52
1:A:169:ILE:HG12	5:A:952:HOH:O	2.08	0.52
1:A:418:ARG:HG3	1:B:418:ARG:NH2	2.25	0.52
1:A:566:ALA:O	1:A:570:THR:CG2	2.58	0.52
1:B:702:VAL:HG22	1:B:703:SER:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:TYR:CZ	1:B:739:TRP:CZ3	2.98	0.52
1:B:266:LEU:HD12	1:B:266:LEU:C	2.30	0.51
1:B:688:TYR:CB	1:B:739:TRP:HD1	2.23	0.51
1:A:263:THR:HG23	1:A:296:ALA:HB2	1.92	0.51
1:B:669:LEU:CD1	1:B:669:LEU:C	2.78	0.51
1:A:345:ALA:CB	1:A:472:TYR:HE1	2.22	0.51
1:A:342:ARG:HD3	1:A:344:PHE:CE2	2.46	0.51
1:B:491:ARG:HH21	1:B:759:GLU:HB2	1.75	0.51
1:A:266:LEU:HD12	1:A:266:LEU:C	2.31	0.51
1:A:718:TYR:CZ	1:A:739:TRP:CZ3	2.98	0.51
1:B:566:ALA:O	1:B:570:THR:CG2	2.58	0.51
1:B:610:LEU:HB3	1:B:678:VAL:CG2	2.40	0.51
1:B:688:TYR:HB3	1:B:739:TRP:HD1	1.76	0.51
1:B:669:LEU:HD13	1:B:670:LEU:N	2.26	0.51
1:A:634:LYS:HB3	1:A:634:LYS:HZ3	1.76	0.50
1:B:288:ARG:HG3	1:B:326:ASN:HB3	1.92	0.50
1:A:540:ALA:O	1:A:543:HIS:HB2	2.11	0.50
1:A:610:LEU:HB3	1:A:678:VAL:CG2	2.40	0.50
1:A:689:LYS:NZ	5:A:862:HOH:O	2.39	0.50
1:A:352:ASN:HD21	1:A:354:LEU:CB	2.24	0.50
1:B:342:ARG:HD3	1:B:344:PHE:CE2	2.46	0.50
1:B:176:PHE:CE2	1:B:180:MET:HB3	2.47	0.50
1:B:368:VAL:O	1:B:368:VAL:HG22	2.12	0.50
1:B:366:ALA:HB3	1:B:468:PHE:CE1	2.46	0.50
1:B:637:ALA:O	1:B:640:SER:OG	2.26	0.50
1:B:427:GLU:OE2	1:B:445:ASN:HB2	2.11	0.50
1:B:661:TYR:CD2	1:B:726:GLY:HA3	2.47	0.50
1:A:562:ALA:O	1:A:565:SER:HB3	2.12	0.50
1:A:577:THR:O	1:A:578:ARG:CB	2.58	0.49
1:B:622:LEU:HD23	1:B:622:LEU:O	2.11	0.49
1:A:368:VAL:O	1:A:368:VAL:HG22	2.12	0.49
1:A:622:LEU:O	1:A:622:LEU:HD23	2.10	0.49
1:B:586:ASN:O	1:B:587:ASN:HB2	2.12	0.49
1:B:663:ILE:HD13	1:B:663:ILE:N	2.23	0.49
1:A:143:LEU:CD2	1:A:270:MET:CG	2.86	0.49
1:B:176:PHE:HA	1:B:180:MET:HE2	1.93	0.49
1:B:731:SER:N	5:B:960:HOH:O	2.44	0.49
3:D:1:NAG:H61	3:D:3:NAG:O7	2.13	0.49
3:G:2:FUC:H61	3:G:3:NAG:H2	1.95	0.49
1:A:346:GLY:O	1:A:442:VAL:HG11	2.13	0.49
1:A:512:TYR:HE1	5:A:773:HOH:O	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ILE:N	1:B:211:ASP:HB2	2.28	0.49
1:A:418:ARG:NH2	1:B:418:ARG:HG3	2.28	0.49
1:B:433:ARG:HD2	5:B:51:HOH:O	2.11	0.49
1:B:448:GLU:HA	1:B:451:GLN:HE21	1.78	0.49
1:B:128:LEU:CD2	1:B:550:MET:HB3	2.42	0.49
1:A:357:ARG:NH1	1:A:474:ASP:OD2	2.40	0.49
1:B:562:ALA:O	1:B:565:SER:HB3	2.12	0.49
1:A:166:TRP:CZ2	1:A:168:GLY:HA3	2.48	0.49
1:B:129:TRP:CB	1:B:134:LEU:CD2	2.90	0.48
1:B:407:PHE:CD2	1:B:431:VAL:HG22	2.48	0.48
1:B:628:PHE:HB3	1:B:632:GLN:HB2	1.96	0.48
1:A:129:TRP:CB	1:A:134:LEU:CD2	2.91	0.48
1:A:575:ASP:OD1	1:A:577:THR:N	2.34	0.48
1:B:233:HIS:O	1:B:233:HIS:CD2	2.67	0.48
1:B:372:PRO:HD2	1:B:396:ASN:O	2.13	0.48
1:B:263:THR:HG23	1:B:296:ALA:HB2	1.95	0.48
1:A:688:TYR:HB3	1:A:739:TRP:HD1	1.78	0.48
1:B:447:LYS:HE2	5:B:829:HOH:O	2.03	0.48
1:B:166:TRP:CZ2	1:B:168:GLY:HA3	2.49	0.48
3:E:1:NAG:H61	3:E:3:NAG:C7	2.44	0.48
1:A:697:ASN:CG	5:A:857:HOH:O	2.51	0.48
1:A:163:PRO:O	5:A:910:HOH:O	2.20	0.48
1:A:617:GLN:CB	5:A:808:HOH:O	2.62	0.48
1:A:689:LYS:HD2	1:A:742:GLN:NE2	2.29	0.48
1:B:129:TRP:HB3	1:B:134:LEU:HD21	1.95	0.48
1:B:290:ILE:N	1:B:290:ILE:HD13	2.28	0.48
1:A:350:LEU:N	1:A:350:LEU:HD12	2.29	0.48
1:A:628:PHE:HB3	1:A:632:GLN:HB2	1.95	0.48
1:A:366:ALA:HB3	1:A:468:PHE:CE1	2.48	0.47
1:A:218:HIS:ND1	1:A:510:ALA:HB3	2.29	0.47
1:B:143:LEU:CD2	1:B:270:MET:CG	2.87	0.47
1:B:247:ARG:NE	5:B:62:HOH:O	2.43	0.47
1:B:685:ALA:HB2	1:B:710:LYS:O	2.14	0.47
1:A:290:ILE:HD13	1:A:290:ILE:N	2.29	0.47
1:A:622:LEU:CD2	1:A:622:LEU:O	2.62	0.47
1:B:570:THR:HG21	1:B:605:ALA:HA	1.96	0.47
1:B:672:GLN:CG	1:B:674:PHE:CZ	2.92	0.47
1:A:177:ASN:O	1:A:180:MET:HB2	2.13	0.47
1:A:208:SER:O	1:A:254:LYS:HD3	2.14	0.47
1:B:493:TYR:CZ	5:B:845:HOH:O	2.65	0.47
1:A:270:MET:HE3	1:A:281:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HH21	1:A:759:GLU:HB2	1.78	0.47
1:B:237:ALA:N	1:B:238:PRO:CD	2.78	0.47
1:A:702:VAL:CG2	1:A:703:SER:N	2.77	0.47
1:B:500:ASP:OD2	1:B:564:ARG:HD2	2.15	0.47
1:A:357:ARG:NH2	1:A:474:ASP:OD2	2.45	0.47
1:B:326:ASN:C	1:B:326:ASN:HD22	2.18	0.47
1:A:367:PHE:N	1:B:526:LEU:O	2.44	0.47
3:G:1:NAG:O4	3:G:2:FUC:H5	2.14	0.47
1:B:129:TRP:CG	1:B:134:LEU:CD2	2.98	0.47
1:B:586:ASN:HD22	1:B:587:ASN:H	1.58	0.47
1:B:199:ASP:OD1	1:B:199:ASP:C	2.54	0.47
1:B:622:LEU:CD2	1:B:622:LEU:O	2.63	0.47
1:A:491:ARG:O	1:A:760:VAL:HG13	2.15	0.47
1:B:186:ILE:HD13	1:B:249:ARG:HB3	1.97	0.47
1:B:352:ASN:HD21	1:B:354:LEU:CB	2.27	0.47
1:A:399:VAL:CG1	1:A:419:LEU:HD13	2.44	0.46
1:A:689:LYS:HD3	5:A:862:HOH:O	2.14	0.46
1:B:393:ASN:N	1:B:394:PRO:CD	2.77	0.46
1:A:393:ASN:N	1:A:394:PRO:CD	2.78	0.46
1:A:218:HIS:HE1	1:A:532:ILE:O	1.98	0.46
1:A:129:TRP:HB3	1:A:134:LEU:HD21	1.96	0.46
1:A:500:ASP:OD2	1:A:564:ARG:HD2	2.14	0.46
1:A:615:THR:O	1:A:618:ASP:HB2	2.15	0.46
1:B:399:VAL:CG1	1:B:419:LEU:HD13	2.45	0.46
1:A:176:PHE:HA	1:A:180:MET:CE	2.46	0.46
1:B:177:ASN:O	1:B:180:MET:HB2	2.16	0.46
1:B:238:PRO:CD	5:B:106:HOH:O	2.53	0.46
1:B:345:ALA:CB	1:B:472:TYR:HE1	2.28	0.46
1:A:154:PHE:HE1	1:A:217:THR:HG23	1.81	0.46
1:B:678:VAL:O	1:B:678:VAL:HG13	2.15	0.46
1:A:411:MET:HE3	1:A:437:PHE:CD1	2.51	0.46
1:B:385:GLU:HG3	5:B:80:HOH:O	2.16	0.46
1:B:493:TYR:HE2	1:B:496:ILE:HG13	1.81	0.46
1:A:325:LEU:HA	1:A:486:ALA:CB	2.46	0.46
1:B:540:ALA:O	1:B:543:HIS:HB2	2.16	0.46
1:A:407:PHE:CD2	1:A:431:VAL:HG22	2.50	0.45
1:A:446:LYS:N	5:A:899:HOH:O	2.48	0.45
1:A:663:ILE:HD13	1:A:663:ILE:N	2.24	0.45
1:B:329:SER:HB2	1:B:332:ILE:HD12	1.97	0.45
1:B:493:TYR:CE2	1:B:495:GLY:HA3	2.50	0.45
1:B:491:ARG:O	1:B:760:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASN:HD22	1:A:587:ASN:H	1.63	0.45
1:A:229:LYS:CB	5:A:94:HOH:O	2.64	0.45
3:G:1:NAG:C6	3:G:3:NAG:O7	2.53	0.45
1:A:147:ILE:N	1:A:211:ASP:HB2	2.31	0.45
1:B:208:SER:O	1:B:254:LYS:HD3	2.16	0.45
1:B:685:ALA:N	5:B:988:HOH:O	2.50	0.45
1:A:578:ARG:CA	1:A:578:ARG:HE	2.29	0.45
1:B:310:LEU:O	5:B:102:HOH:O	2.21	0.45
1:B:350:LEU:N	1:B:350:LEU:HD12	2.31	0.45
1:A:570:THR:HG21	1:A:605:ALA:HA	1.97	0.45
1:A:390:GLN:NE2	3:E:3:NAG:N2	2.63	0.45
1:A:327:ASN:HA	5:A:951:HOH:O	2.16	0.45
1:A:727:ASP:OD1	1:A:731:SER:CB	2.60	0.45
1:A:157:ASP:CG	5:A:909:HOH:O	2.54	0.45
1:A:586:ASN:O	1:A:587:ASN:HB2	2.17	0.45
1:A:129:TRP:CG	1:A:134:LEU:CD2	2.99	0.45
1:B:156:ASP:OD1	1:B:182:ASN:HB2	2.17	0.45
1:A:198:ASN:HB2	5:A:799:HOH:O	2.16	0.45
1:A:481:VAL:O	1:A:584:SER:HB3	2.17	0.45
1:B:127:GLY:HA3	1:B:603:ASN:OD1	2.16	0.44
1:B:689:LYS:HD2	1:B:742:GLN:NE2	2.29	0.44
1:A:237:ALA:N	1:A:238:PRO:CD	2.80	0.44
1:A:574:LEU:HD23	1:A:580:PRO:HA	1.98	0.44
1:B:218:HIS:HE1	1:B:532:ILE:O	2.01	0.44
1:A:271:ASP:OD2	1:A:638:ARG:NH2	2.50	0.44
1:A:326:ASN:C	1:A:326:ASN:HD22	2.21	0.44
1:A:372:PRO:HD2	1:A:396:ASN:O	2.17	0.44
1:A:617:GLN:HB2	5:A:808:HOH:O	2.16	0.44
1:A:676:ARG:NH2	5:A:50:HOH:O	2.46	0.44
1:B:254:LYS:HE2	1:B:257:PHE:CD2	2.53	0.44
1:B:702:VAL:CG2	1:B:703:SER:N	2.78	0.44
1:A:314:SER:HB2	1:A:537:THR:HB	1.99	0.44
1:A:128:LEU:CD2	1:A:550:MET:HB3	2.48	0.44
1:A:703:SER:HA	1:A:704:PRO:C	2.38	0.44
1:A:129:TRP:CD2	1:A:134:LEU:HD22	2.52	0.44
1:A:379:LEU:HD12	1:A:380:SER:N	2.33	0.44
1:A:448:GLU:HA	1:A:451:GLN:HE21	1.83	0.44
1:B:218:HIS:CG	1:B:510:ALA:HB3	2.53	0.44
1:A:244:VAL:CG1	1:A:546:GLY:HA3	2.48	0.44
1:A:143:LEU:HD12	1:A:253:TYR:HB2	1.98	0.44
1:A:236:TYR:CE1	1:A:469:GLN:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:VAL:CG2	1:B:735:GLY:N	2.81	0.44
1:A:524:ASN:N	1:A:524:ASN:HD22	2.15	0.43
1:B:129:TRP:CD2	1:B:134:LEU:HD22	2.52	0.43
1:B:192:ASN:ND2	1:B:207:ASN:OD1	2.51	0.43
1:A:123:ASN:ND2	1:A:125:SER:HB2	2.33	0.43
1:B:325:LEU:HA	1:B:486:ALA:CB	2.47	0.43
1:B:379:LEU:HD12	1:B:380:SER:N	2.33	0.43
1:A:352:ASN:HD21	1:A:354:LEU:H	1.64	0.43
1:A:329:SER:HB2	1:A:332:ILE:HD12	1.99	0.43
1:B:574:LEU:HD23	1:B:580:PRO:HA	2.00	0.43
1:A:488:GLY:HA3	1:A:498:LYS:O	2.18	0.43
1:A:685:ALA:HB2	1:A:710:LYS:O	2.18	0.43
1:A:718:TYR:CZ	1:A:739:TRP:CH2	3.07	0.43
1:B:176:PHE:HA	1:B:180:MET:CE	2.48	0.43
1:B:696:LYS:HE3	1:B:696:LYS:HB2	1.86	0.43
1:A:528:SER:O	5:A:880:HOH:O	2.21	0.43
1:A:692:LEU:HB3	1:A:700:ILE:HD11	2.00	0.43
1:B:271:ASP:OD2	1:B:638:ARG:NH2	2.52	0.43
1:A:555:HIS:CB	5:A:878:HOH:O	2.66	0.43
1:B:578:ARG:HE	1:B:578:ARG:HA	1.84	0.43
1:B:481:VAL:O	1:B:584:SER:HB3	2.19	0.43
4:F:1:NAG:H3	4:F:2:FUC:C5	2.48	0.43
1:A:201:THR:HG23	5:A:915:HOH:O	2.18	0.43
1:A:186:ILE:HD13	1:A:249:ARG:HB3	2.00	0.43
1:B:123:ASN:ND2	1:B:125:SER:HB2	2.34	0.43
1:B:154:PHE:HE1	1:B:217:THR:HG23	1.84	0.43
1:B:270:MET:HE3	1:B:281:ILE:HD13	2.01	0.43
1:B:518:ALA:HB2	1:B:529:THR:HG22	2.01	0.43
1:A:678:VAL:O	1:A:678:VAL:HG13	2.18	0.42
1:B:177:ASN:H	1:B:180:MET:HE1	1.82	0.42
1:B:663:ILE:CD1	1:B:663:ILE:H	2.26	0.42
1:B:236:TYR:CE1	1:B:469:GLN:HA	2.54	0.42
1:A:263:THR:O	1:A:266:LEU:HB3	2.18	0.42
1:A:447:LYS:N	5:A:899:HOH:O	2.26	0.42
1:A:192:ASN:ND2	1:A:207:ASN:OD1	2.53	0.42
1:A:352:ASN:HD21	1:A:354:LEU:HB2	1.85	0.42
1:B:615:THR:O	1:B:618:ASP:HB2	2.19	0.42
1:B:346:GLY:O	1:B:442:VAL:HG11	2.19	0.42
1:B:347:THR:HG21	1:B:355:LYS:HE3	2.02	0.42
1:B:411:MET:HE3	1:B:437:PHE:CD1	2.55	0.42
1:A:218:HIS:CG	1:A:510:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HD3	1:B:344:PHE:CZ	2.54	0.42
1:B:661:TYR:CD2	1:B:661:TYR:O	2.73	0.42
1:A:254:LYS:HE2	1:A:257:PHE:CD2	2.55	0.42
1:A:424:PHE:HB2	1:A:443:VAL:HG22	2.02	0.42
1:B:703:SER:HA	1:B:704:PRO:C	2.40	0.42
1:A:113:THR:HA	1:A:116:THR:HB	2.02	0.42
1:A:199:ASP:C	1:A:199:ASP:OD1	2.57	0.42
1:A:493:TYR:HE2	1:A:496:ILE:HG13	1.85	0.42
1:B:586:ASN:C	1:B:586:ASN:HD22	2.21	0.42
1:A:342:ARG:HD3	1:A:344:PHE:CZ	2.54	0.42
1:A:661:TYR:O	1:A:661:TYR:CD2	2.72	0.42
1:A:156:ASP:OD1	1:A:182:ASN:HB2	2.20	0.42
1:A:442:VAL:HG22	1:A:466:ILE:HD13	2.01	0.42
1:A:127:GLY:HA3	1:A:603:ASN:OD1	2.19	0.42
1:A:734:VAL:CG2	1:A:735:GLY:N	2.82	0.42
1:B:446:LYS:HA	5:B:901:HOH:O	2.18	0.42
1:B:575:ASP:OD1	1:B:575:ASP:C	2.58	0.42
1:A:390:GLN:NE2	3:E:3:NAG:HN2	2.17	0.42
1:A:399:VAL:HG12	1:A:419:LEU:HD13	2.02	0.41
1:A:668:THR:O	1:A:669:LEU:C	2.58	0.41
1:B:113:THR:HA	1:B:116:THR:HB	2.02	0.41
1:B:177:ASN:N	1:B:180:MET:HE2	2.33	0.41
1:B:237:ALA:N	1:B:471:THR:HG21	2.32	0.41
1:B:718:TYR:CZ	1:B:739:TRP:CH2	3.07	0.41
1:B:390:GLN:HE22	3:H:3:NAG:HN2	1.69	0.41
1:B:442:VAL:HG22	1:B:466:ILE:HD13	2.02	0.41
1:B:460:VAL:O	1:B:461:THR:CB	2.60	0.41
1:B:394:PRO:HA	1:B:397:THR:HG23	2.03	0.41
1:A:242:ARG:HD3	1:A:242:ARG:N	2.36	0.41
1:A:270:MET:CE	1:A:281:ILE:HD13	2.51	0.41
1:A:626:LEU:HD23	1:A:628:PHE:CE1	2.55	0.41
1:A:702:VAL:CG2	1:A:703:SER:H	2.32	0.41
1:A:262:PHE:CE2	5:A:799:HOH:O	2.57	0.41
1:A:416:ARG:HD2	5:A:938:HOH:O	2.20	0.41
1:A:586:ASN:HD22	1:A:586:ASN:C	2.22	0.41
1:B:737:ILE:O	1:B:737:ILE:HG23	2.21	0.41
1:B:244:VAL:CG1	1:B:546:GLY:HA3	2.50	0.41
1:B:330:PRO:HB3	1:B:496:ILE:HD12	2.03	0.41
1:B:582:LYS:HD2	1:B:587:ASN:O	2.21	0.41
1:B:626:LEU:HD23	1:B:628:PHE:CE1	2.56	0.41
1:A:385:GLU:CG	1:A:413:ILE:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ASN:ND2	1:A:525:ILE:HG13	2.36	0.40
1:A:582:LYS:HD2	1:A:587:ASN:O	2.22	0.40
1:B:237:ALA:N	1:B:238:PRO:HD3	2.37	0.40
1:B:668:THR:O	1:B:669:LEU:C	2.59	0.40
1:A:362:PHE:CE2	1:A:366:ALA:HB2	2.56	0.40
1:A:371:SER:HA	1:A:372:PRO:HD3	1.91	0.40
1:B:488:GLY:HA3	1:B:498:LYS:O	2.22	0.40
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.95	0.40
1:A:376:ASN:HB2	5:A:829:HOH:O	2.20	0.40
1:A:737:ILE:HG23	1:A:737:ILE:O	2.20	0.40
1:B:191:PHE:HA	5:B:825:HOH:O	2.21	0.40
1:B:292:LEU:HG	5:B:913:HOH:O	2.21	0.40
1:B:428:ASP:HA	1:B:429:PRO:HD2	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:3:NAG:O3	5:A:820:HOH:O[6_555]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	632/649 (97%)	597 (94%)	32 (5%)	3 (0%)	29 48
1	B	625/649 (96%)	589 (94%)	34 (5%)	2 (0%)	41 61
All	All	1257/1298 (97%)	1186 (94%)	66 (5%)	5 (0%)	34 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	638	ARG
1	B	653	ASN
1	A	380	SER
1	A	461	THR
1	B	461	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	528/533 (99%)	482 (91%)	46 (9%)	10 20
1	B	525/533 (98%)	480 (91%)	45 (9%)	10 20
All	All	1053/1066 (99%)	962 (91%)	91 (9%)	10 20

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	128	LEU
1	A	138	VAL
1	A	140	VAL
1	A	143	LEU
1	A	144	ASP
1	A	164	LYS
1	A	184	LYS
1	A	185	LEU
1	A	201	THR
1	A	223	THR
1	A	242	ARG
1	A	266	LEU
1	A	278	VAL
1	A	290	ILE
1	A	326	ASN
1	A	352	ASN
1	A	368	VAL
1	A	391	VAL

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Mol	Chain	Res	Type
1	A	395	GLU
1	A	397	THR
1	A	414	ILE
1	A	437	PHE
1	A	442	VAL
1	A	460	VAL
1	A	471	THR
1	A	500	ASP
1	A	502	LEU
1	A	524	ASN
1	A	539	MET
1	A	586	ASN
1	A	622	LEU
1	A	624	CYS
1	A	634	LYS
1	A	638	ARG
1	A	645	CYS
1	A	663	ILE
1	A	668	THR
1	A	679	THR
1	A	687	THR
1	A	721	THR
1	A	722	ILE
1	A	732	ARG
1	A	734	VAL
1	A	739	TRP
1	A	740	VAL
1	B	116	THR
1	B	128	LEU
1	B	138	VAL
1	B	140	VAL
1	B	143	LEU
1	B	164	LYS
1	B	184	LYS
1	B	185	LEU
1	B	201	THR
1	B	223	THR
1	B	242	ARG
1	B	266	LEU
1	B	278	VAL
1	B	290	ILE
1	B	326	ASN

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	368	VAL
1	B	391	VAL
1	B	395	GLU
1	B	397	THR
1	B	414	ILE
1	B	437	PHE
1	B	442	VAL
1	B	460	VAL
1	B	471	THR
1	B	500	ASP
1	B	502	LEU
1	B	524	ASN
1	B	539	MET
1	B	586	ASN
1	B	622	LEU
1	B	624	CYS
1	B	634	LYS
1	B	638	ARG
1	B	645	CYS
1	B	663	ILE
1	B	668	THR
1	B	679	THR
1	B	687	THR
1	B	721	THR
1	B	722	ILE
1	B	732	ARG
1	B	734	VAL
1	B	739	TRP
1	B	740	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	136	GLN
1	A	175	GLN
1	A	218	HIS
1	A	272	GLN
1	A	326	ASN
1	A	352	ASN
1	A	390	GLN

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Mol	Chain	Res	Type
1	A	451	GLN
1	A	524	ASN
1	A	555	HIS
1	A	586	ASN
1	A	617	GLN
1	B	123	ASN
1	B	136	GLN
1	B	175	GLN
1	B	218	HIS
1	B	326	ASN
1	B	352	ASN
1	B	390	GLN
1	B	451	GLN
1	B	524	ASN
1	B	555	HIS
1	B	586	ASN
1	B	617	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	1.13	1 (7%)	17,19,21	1.67	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	2	2	14,14,15	0.83	0	17,19,21	2.03	5 (29%)
3	NAG	D	1	1,3	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
3	FUC	D	2	3	10,10,11	0.77	0	14,14,16	1.35	2 (14%)
3	NAG	D	3	3	14,14,15	0.56	0	17,19,21	1.27	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.44	0	17,19,21	8.80	6 (35%)
3	FUC	E	2	3	10,10,11	0.71	0	14,14,16	0.61	0
3	NAG	E	3	3	14,14,15	0.57	0	17,19,21	0.60	0
4	NAG	F	1	1,4	14,14,15	0.45	0	17,19,21	0.87	0
4	FUC	F	2	4	10,10,11	0.60	0	14,14,16	0.96	0
3	NAG	G	1	1,3	14,14,15	0.56	0	17,19,21	0.66	0
3	FUC	G	2	3	10,10,11	0.72	0	14,14,16	0.62	0
3	NAG	G	3	3	14,14,15	0.58	0	17,19,21	0.66	0
3	NAG	H	1	1,3	14,14,15	0.53	0	17,19,21	2.12	3 (17%)
3	FUC	H	2	3	10,10,11	0.64	0	14,14,16	0.55	0
3	NAG	H	3	3	14,14,15	0.55	0	17,19,21	0.77	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	1/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	1/6/23/26	0/1/1/1
4	NAG	F	1	1,4	1/1/5/7	2/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	G	2	3	-	-	0/1/1/1
3	NAG	G	3	3	-	5/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.35	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	O7-C7-C8	-18.45	87.78	122.06
3	E	1	NAG	C8-C7-N2	18.10	146.75	116.10
3	E	1	NAG	O5-C1-C2	-17.15	84.21	111.29
3	E	1	NAG	C1-O5-C5	13.40	130.35	112.19
3	E	1	NAG	C4-C3-C2	-9.86	96.57	111.02
3	E	1	NAG	O3-C3-C2	8.55	127.16	109.47
3	H	1	NAG	C1-O5-C5	6.04	120.37	112.19
3	H	1	NAG	C4-C3-C2	-5.18	103.43	111.02
2	C	2	NAG	C4-C3-C2	-4.47	104.46	111.02
2	C	1	NAG	C4-C3-C2	-4.12	104.98	111.02
2	C	2	NAG	O5-C1-C2	-3.92	105.10	111.29
2	C	2	NAG	C1-C2-N2	3.23	116.00	110.49
3	D	3	NAG	C4-C3-C2	-3.21	106.31	111.02
3	D	2	FUC	C1-C2-C3	2.98	113.33	109.67
3	D	1	NAG	O5-C1-C2	-2.96	106.61	111.29
3	D	3	NAG	O5-C1-C2	-2.83	106.82	111.29
2	C	2	NAG	C1-O5-C5	2.63	115.76	112.19
3	D	2	FUC	C3-C4-C5	2.54	113.72	109.77
2	C	1	NAG	O4-C4-C3	-2.39	104.81	110.35
2	C	1	NAG	C2-N2-C7	-2.29	119.64	122.90
2	C	1	NAG	C3-C4-C5	-2.28	106.17	110.24
3	H	3	NAG	C2-N2-C7	-2.20	119.76	122.90
2	C	2	NAG	C2-N2-C7	-2.20	119.77	122.90
3	H	1	NAG	O5-C5-C4	2.15	116.06	110.83
2	C	1	NAG	O6-C6-C5	-2.14	103.96	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	NAG	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
3	G	3	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	G	3	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	G	3	NAG	O7-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	H	1	NAG	O5-C5-C6-O6
3	G	3	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	D	3	NAG	C1-C2-N2-C7
3	G	3	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	D	1	NAG	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7

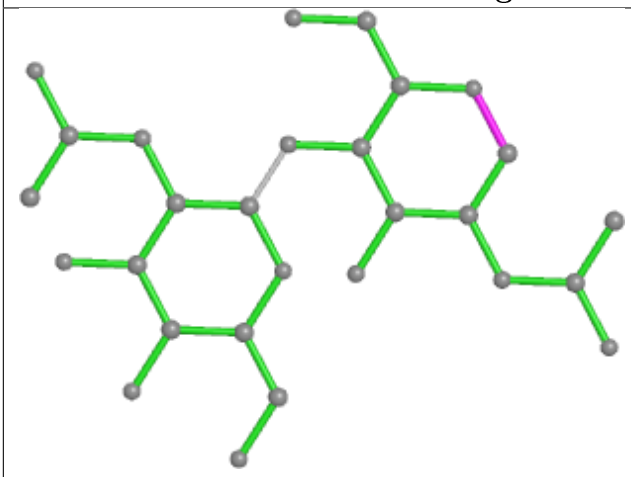
There are no ring outliers.

13 monomers are involved in 29 short contacts:

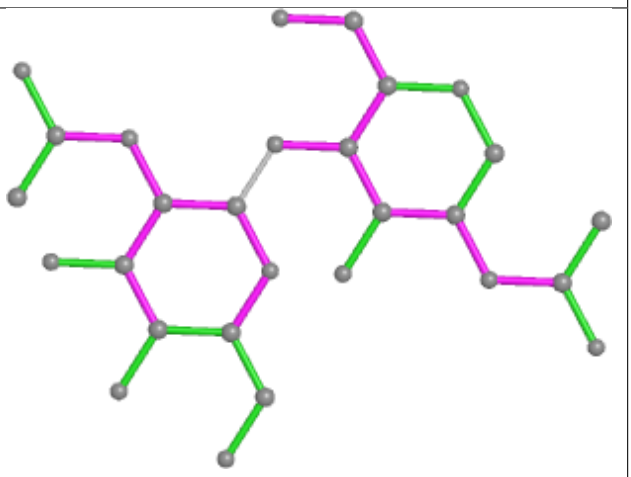
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	FUC	4	0
4	F	1	NAG	3	0
3	G	3	NAG	12	1
3	E	3	NAG	5	0
3	E	2	FUC	1	0
4	F	2	FUC	2	0
3	H	3	NAG	1	0
3	D	3	NAG	1	0
2	C	2	NAG	1	0
3	E	1	NAG	4	0
3	G	1	NAG	9	0
3	D	1	NAG	1	0
2	C	1	NAG	2	0

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

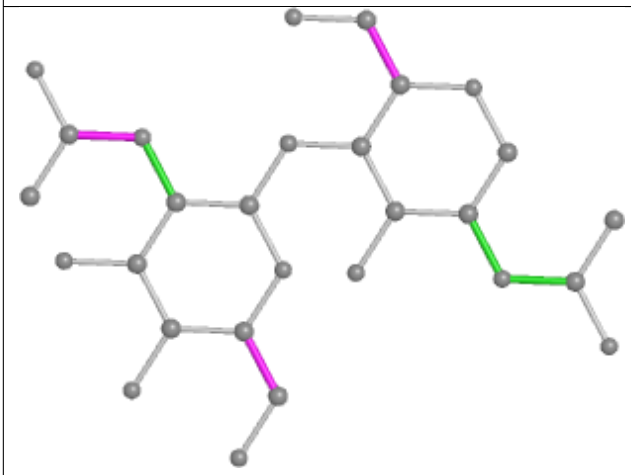
Oligosaccharide Chain C



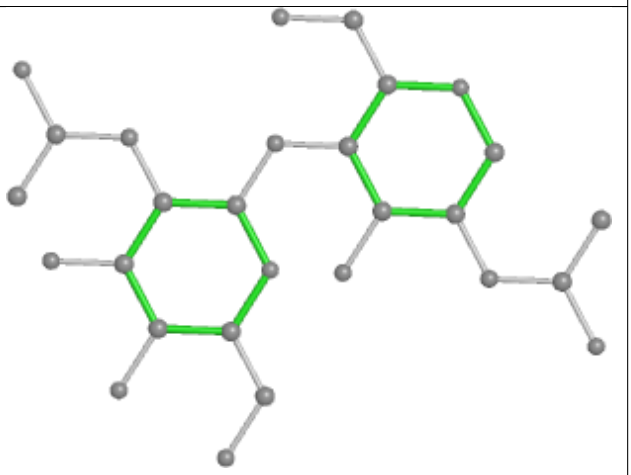
Bond lengths



Bond angles

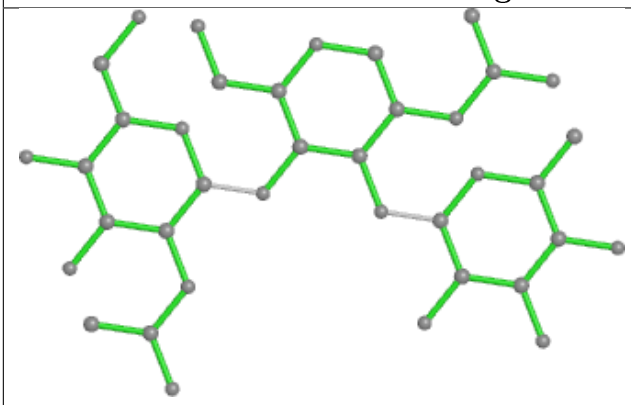


Torsions

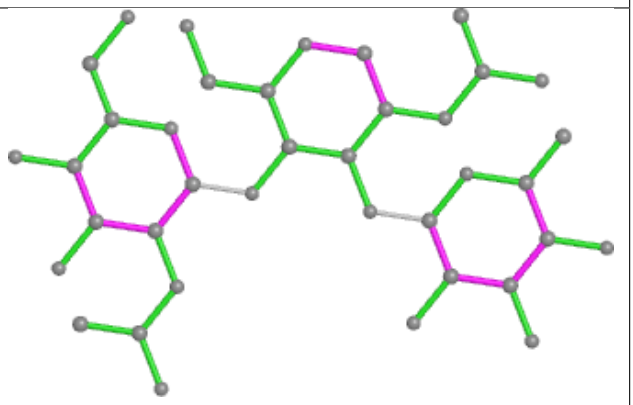


Rings

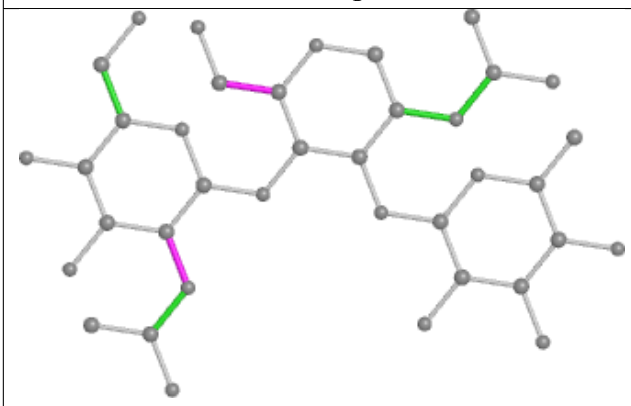
Oligosaccharide Chain D



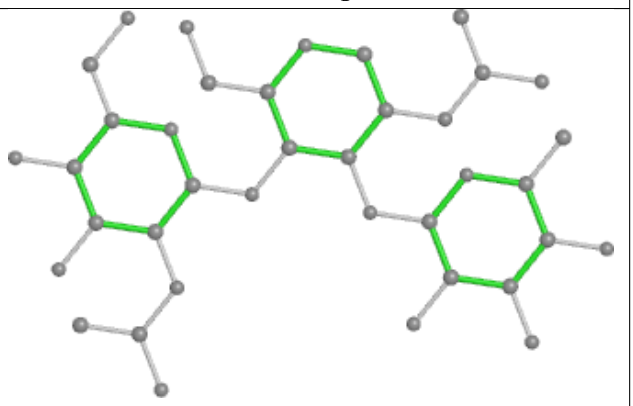
Bond lengths



Bond angles

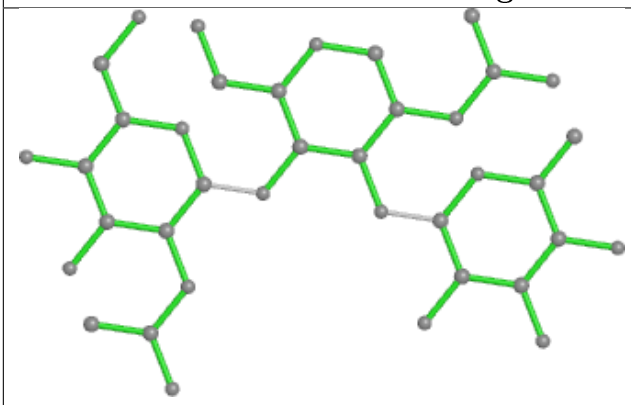


Torsions

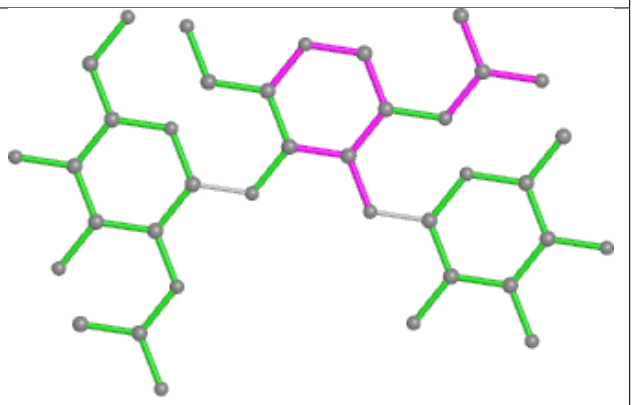


Rings

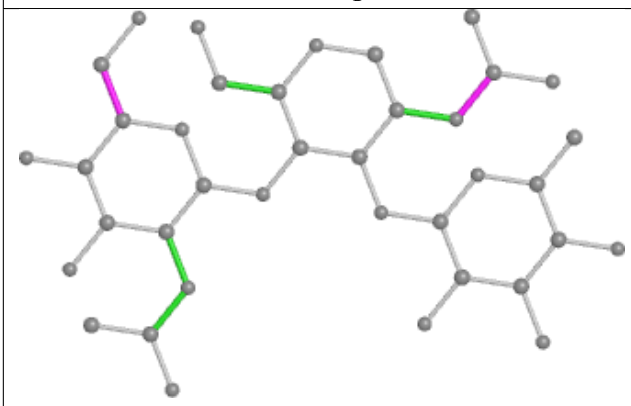
Oligosaccharide Chain E



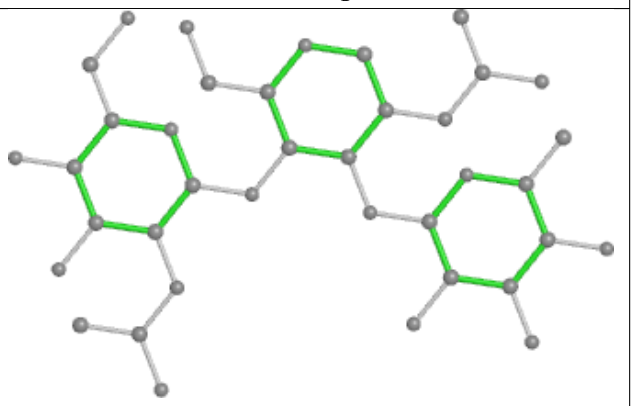
Bond lengths



Bond angles

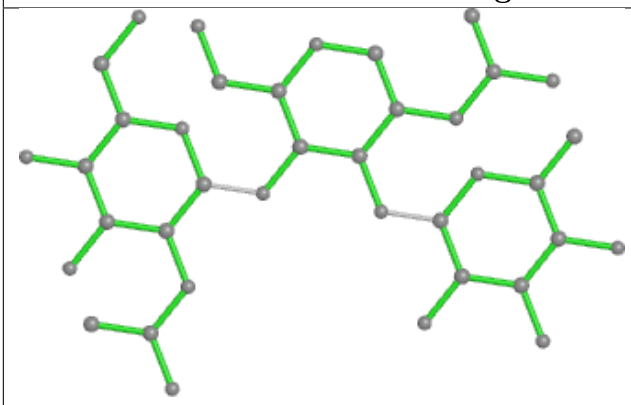


Torsions

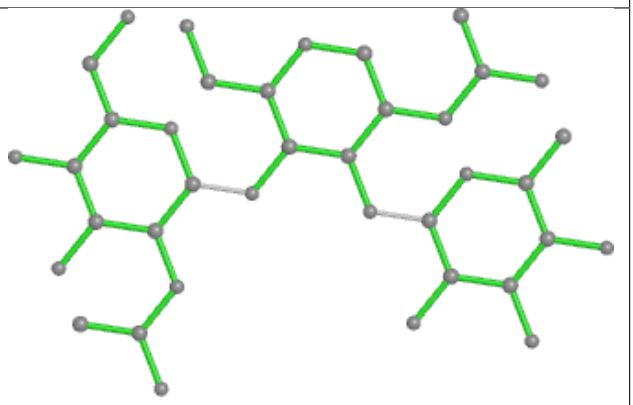


Rings

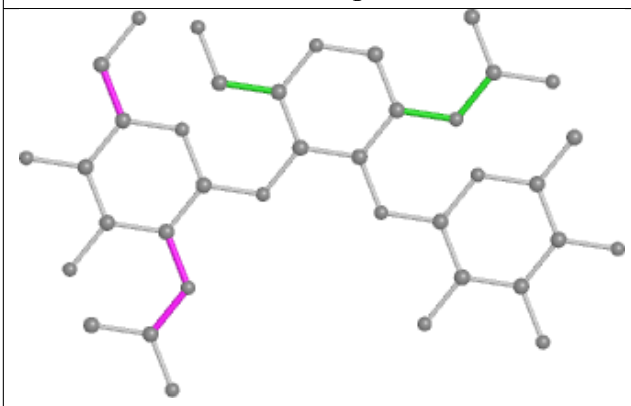
Oligosaccharide Chain G



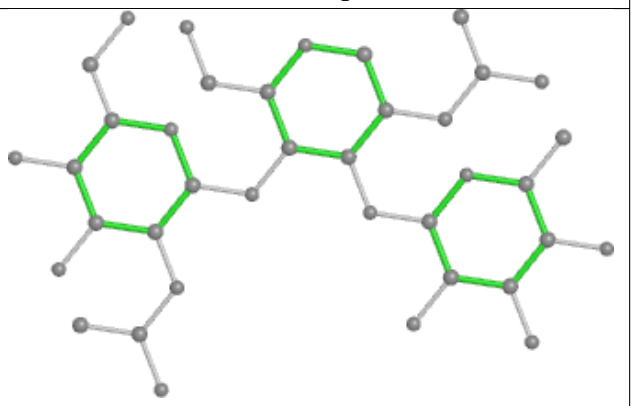
Bond lengths



Bond angles

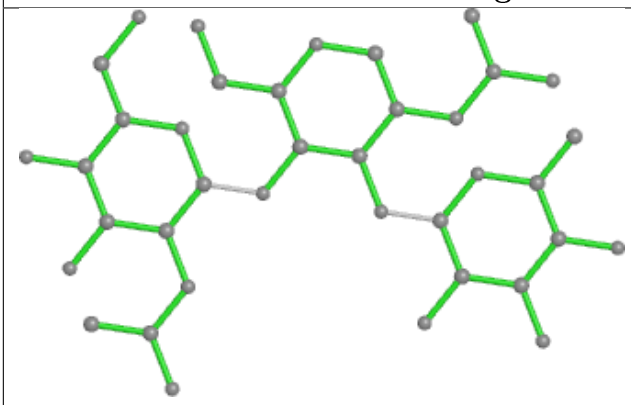


Torsions

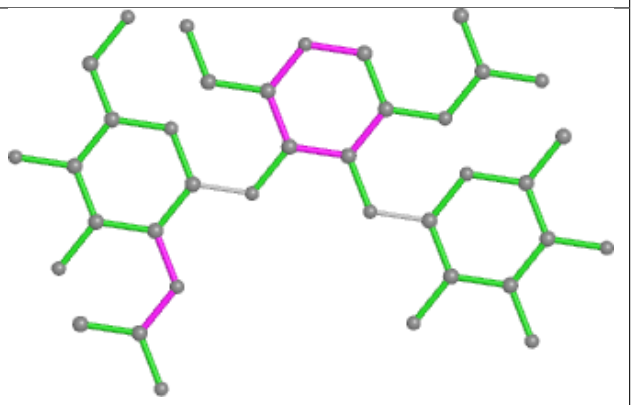


Rings

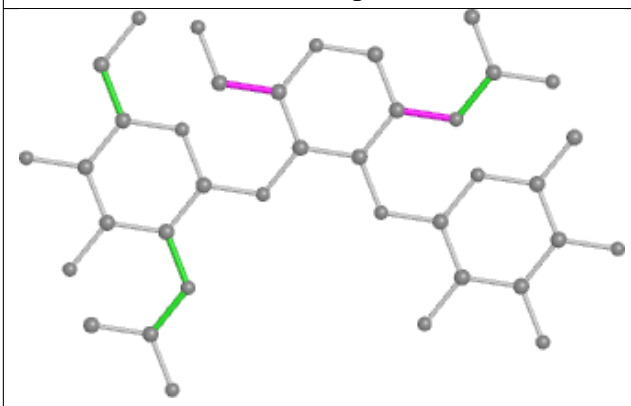
Oligosaccharide Chain H



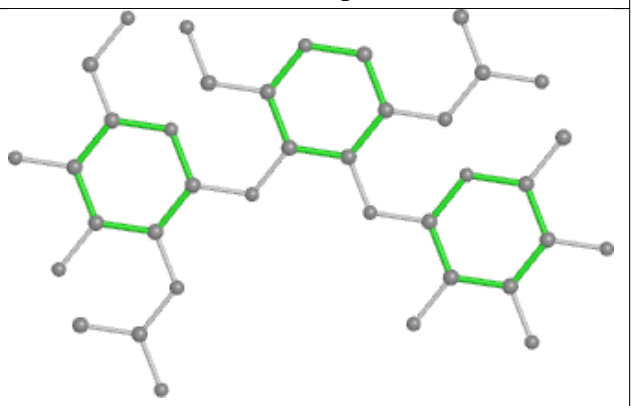
Bond lengths



Bond angles

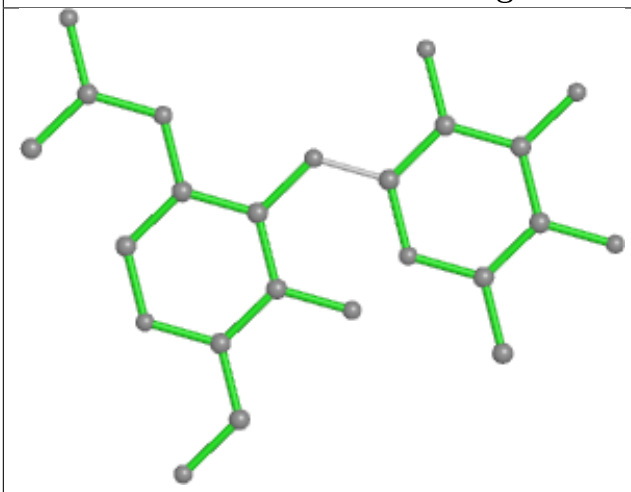


Torsions

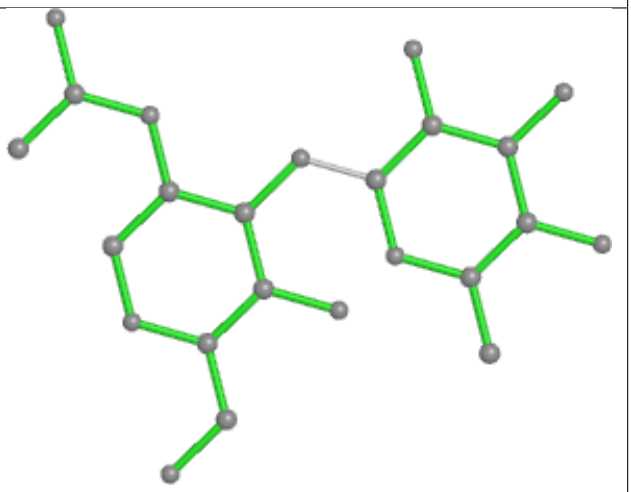


Rings

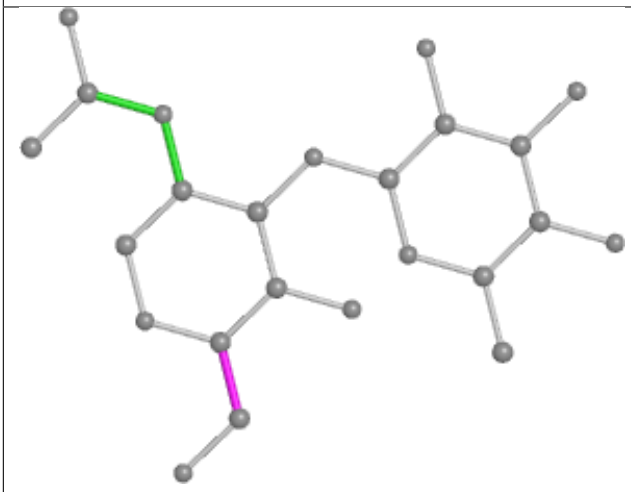
Oligosaccharide Chain F



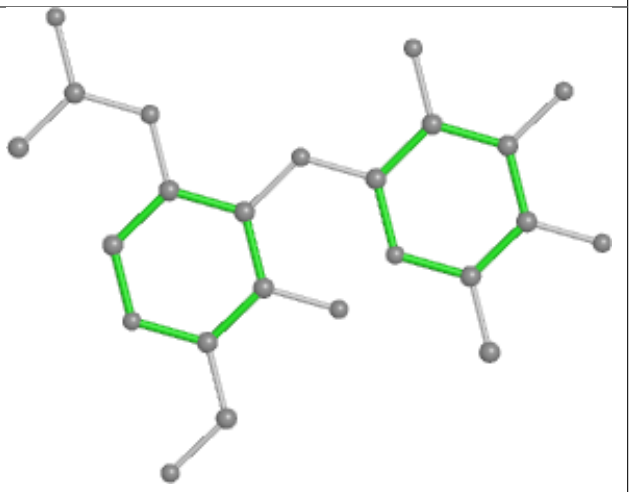
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	642/649 (98%)	0.11	28 (4%)	34	37	33, 48, 65, 79	0
1	B	639/649 (98%)	0.09	18 (2%)	53	56	33, 48, 65, 79	0
All	All	1281/1298 (98%)	0.10	46 (3%)	42	46	33, 48, 65, 79	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	667	PHE	5.2
1	A	460	VAL	4.7
1	B	745	ASN	4.7
1	A	665	GLY	3.9
1	A	405	GLY	3.9
1	A	725	ILE	3.6
1	B	664	GLU	3.3
1	A	668	THR	3.3
1	A	723	ARG	3.3
1	A	643	HIS	3.2
1	A	461	THR	3.2
1	B	423	ILE	3.1
1	A	663	ILE	3.1
1	A	669	LEU	3.0
1	A	666	ASN	3.0
1	A	664	GLU	2.8
1	A	645	CYS	2.7
1	B	578	ARG	2.7
1	B	460	VAL	2.7
1	A	710	LYS	2.7
1	B	743	ASN	2.6
1	A	392	GLU	2.6
1	A	630	GLU	2.5
1	A	739	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	722	ILE	2.5
1	B	422	ALA	2.4
1	B	386	GLU	2.4
1	B	666	ASN	2.4
1	A	474	ASP	2.3
1	A	422	ALA	2.3
1	B	645	CYS	2.3
1	A	685	ALA	2.2
1	A	427	GLU	2.2
1	B	164	LYS	2.2
1	B	648	PRO	2.2
1	B	742	GLN	2.1
1	A	144	ASP	2.1
1	B	399	VAL	2.1
1	A	458	ASN	2.1
1	B	400	ILE	2.1
1	A	386	GLU	2.1
1	A	627	ASN	2.1
1	B	711	ASN	2.1
1	B	710	LYS	2.1
1	A	649	SER	2.0
1	A	634	LYS	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	F	1	14/15	0.71	0.33	66,72,75,76	0
2	NAG	C	2	14/15	0.74	0.41	14,16,19,20	14
4	FUC	F	2	10/11	0.78	0.52	76,78,78,78	0
3	NAG	G	3	14/15	0.79	0.34	55,55,57,58	0
3	NAG	D	3	14/15	0.84	0.27	53,56,57,57	0
3	NAG	G	1	14/15	0.85	0.17	51,53,54,55	0

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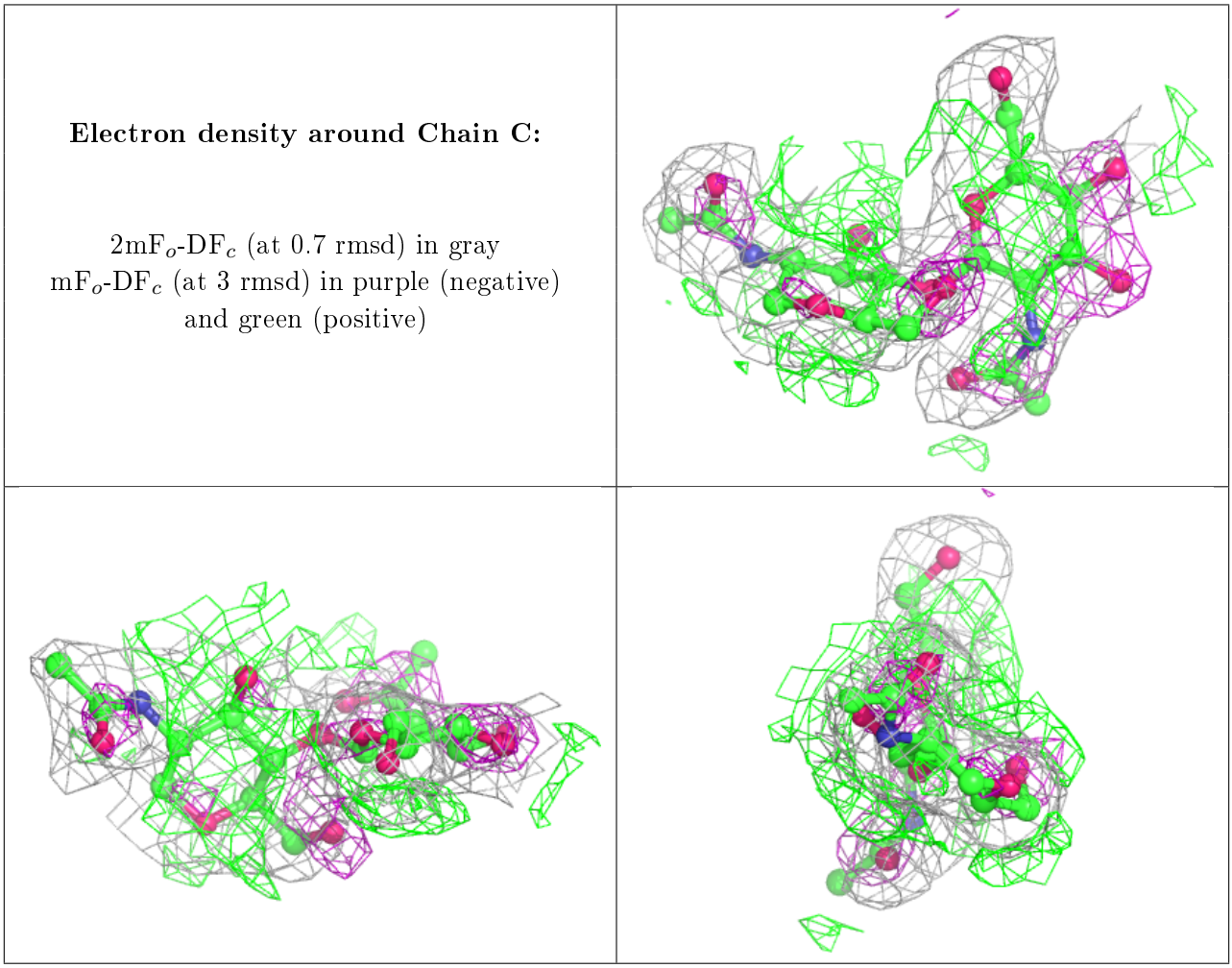
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	1	14/15	0.85	0.27	13,14,16,18	14
3	NAG	H	1	14/15	0.86	0.14	60,62,64,64	0
3	NAG	E	3	14/15	0.89	0.24	78,78,79,79	0
3	FUC	G	2	10/11	0.90	0.20	54,54,55,55	0
3	NAG	E	1	14/15	0.90	0.14	75,76,78,78	0
3	NAG	H	3	14/15	0.92	0.21	65,66,66,67	0
3	NAG	D	1	14/15	0.93	0.20	51,53,55,55	0
3	FUC	H	2	10/11	0.93	0.30	64,65,65,66	0
3	FUC	E	2	10/11	0.94	0.32	79,79,79,79	0
3	FUC	D	2	10/11	0.94	0.17	57,58,59,59	0

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

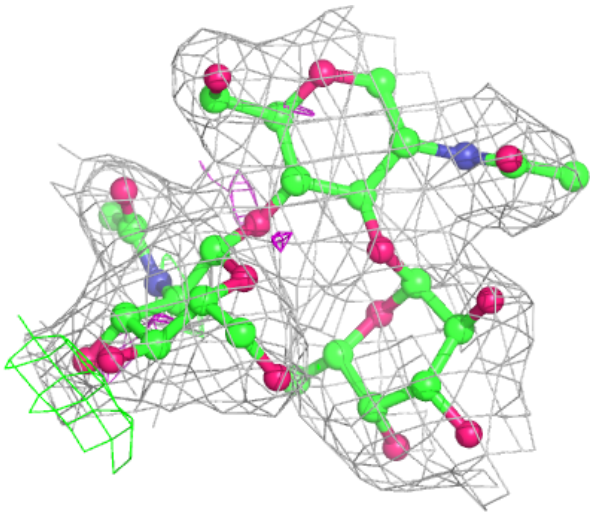
Electron density around Chain C:

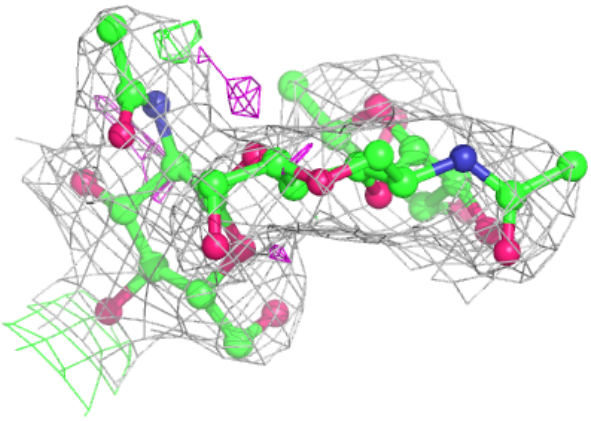
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

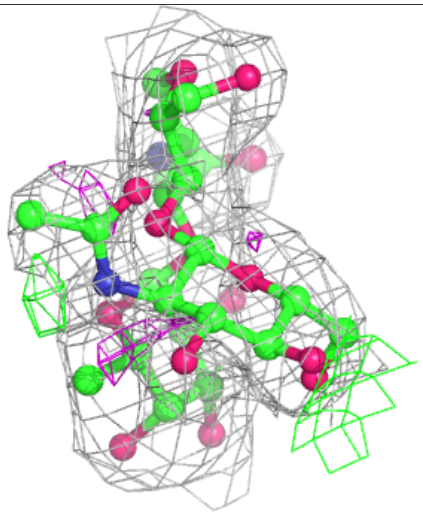


Electron density around Chain D:

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

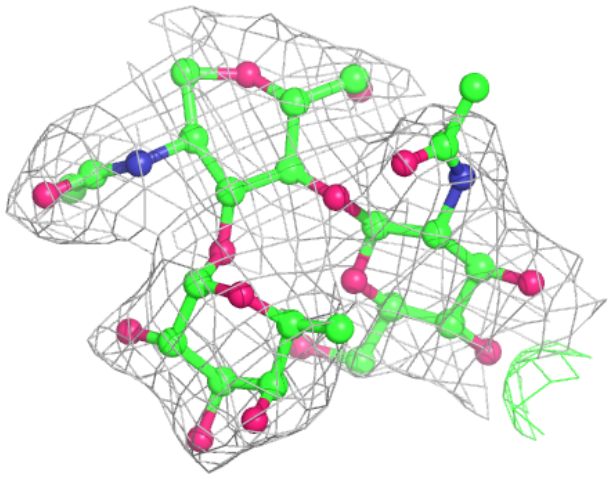


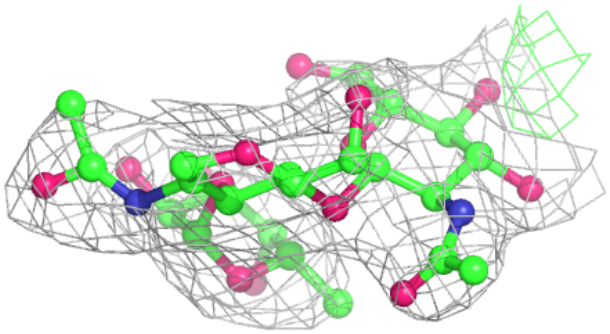


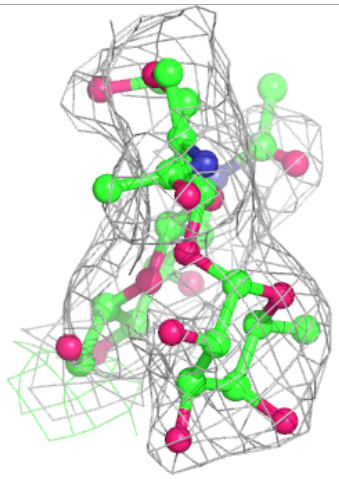


Electron density around Chain E:

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

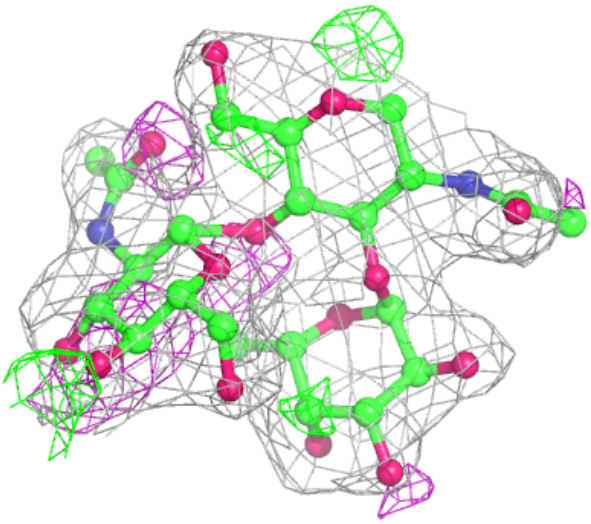


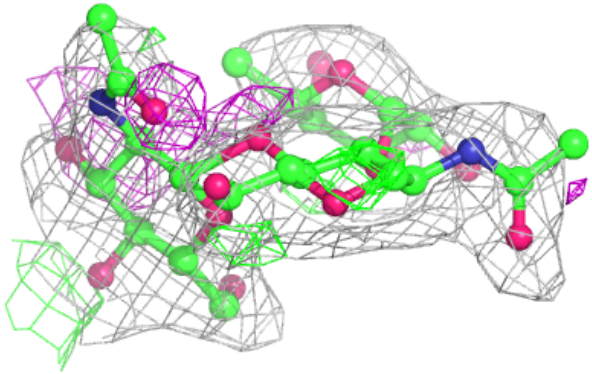




Electron density around Chain G:

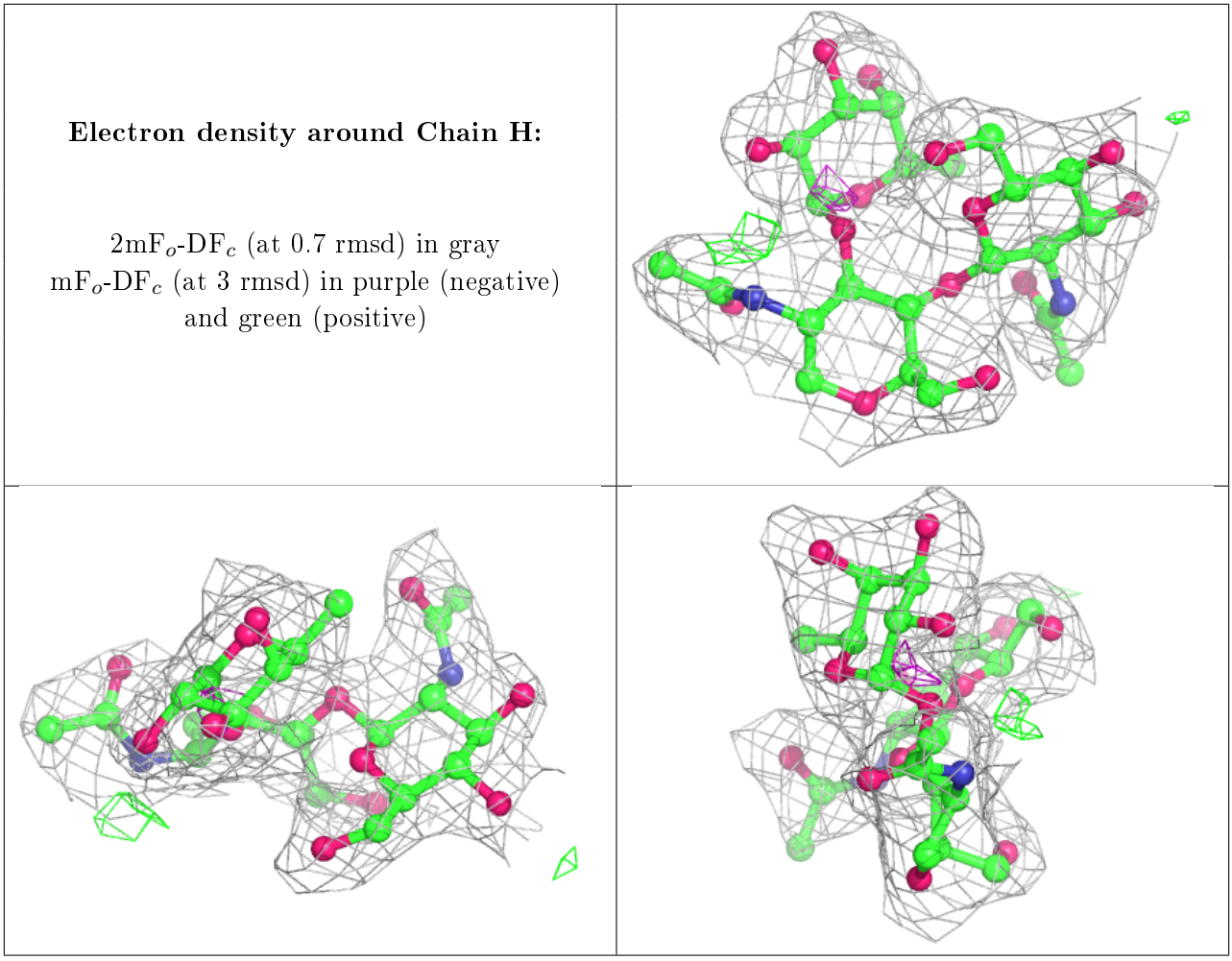
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





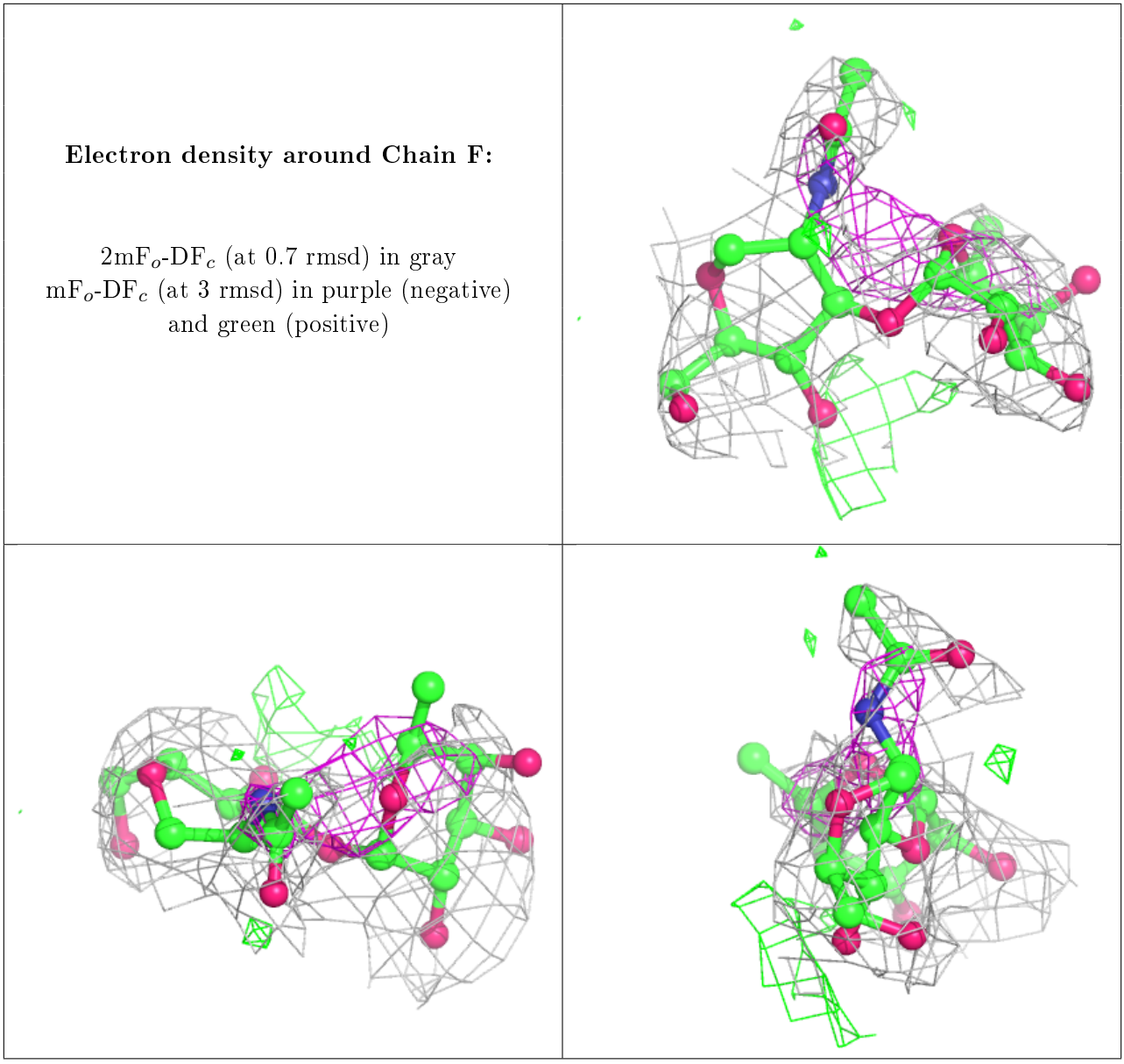
Electron density around Chain H:

$2mF_o$-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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.