Full wwPDB X-ray Structure Validation Report

Aug 7, 2020 – 01:44 PM BST

PDB ID	:	6YDX
Title	:	Insulin-regulated aminopeptidase complexed with a macrocyclic peptidic inhibitor
Authors	:	Mpakali, A.; Saridakis, E.; Giastas, P.; Stratikos, E.
Deposited on	:	2020-03-21
Resolution	:	3.20 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:

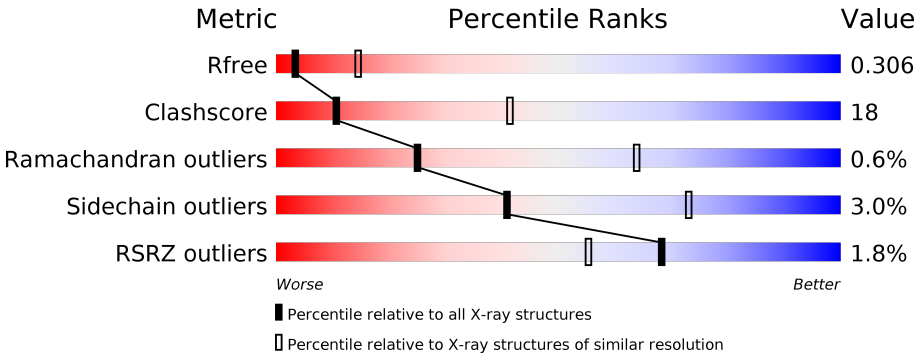
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	912	2% 55% 37% 6%
1	B	912	2% 58% 34% 6%
2	C	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%

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Mol	Chain	Length	Quality of chain
2	I	2	100%
3	D	3	67% 33%
3	H	3	33% 67%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 14298 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 Leucyl-cystinyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	856	Total	C	N	O	S	0	4	0
			6868	4448	1118	1276	26			
1	B	853	Total	C	N	O	S	0	0	0
			6827	4422	1113	1266	26			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	initiating methionine	UNP Q9UIQ6
A	125	GLY	-	expression tag	UNP Q9UIQ6
A	126	ILE	-	expression tag	UNP Q9UIQ6
A	127	LEU	-	expression tag	UNP Q9UIQ6
A	128	PRO	-	expression tag	UNP Q9UIQ6
A	129	SER	-	expression tag	UNP Q9UIQ6
A	130	PRO	-	expression tag	UNP Q9UIQ6
A	131	GLY	-	expression tag	UNP Q9UIQ6
A	132	ASN	-	expression tag	UNP Q9UIQ6
A	133	PRO	-	expression tag	UNP Q9UIQ6
A	134	ALA	-	expression tag	UNP Q9UIQ6
A	135	LEU	-	expression tag	UNP Q9UIQ6
A	136	LEU	-	expression tag	UNP Q9UIQ6
A	137	SER	-	expression tag	UNP Q9UIQ6
A	138	LEU	-	expression tag	UNP Q9UIQ6
A	139	VAL	-	expression tag	UNP Q9UIQ6
A	140	SER	-	expression tag	UNP Q9UIQ6
A	141	LEU	-	expression tag	UNP Q9UIQ6
A	142	LEU	-	expression tag	UNP Q9UIQ6
A	143	SER	-	expression tag	UNP Q9UIQ6
A	144	VAL	-	expression tag	UNP Q9UIQ6
A	145	LEU	-	expression tag	UNP Q9UIQ6
A	146	LEU	-	expression tag	UNP Q9UIQ6
A	147	MET	-	expression tag	UNP Q9UIQ6
A	148	GLY	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	149	CYS	-	expression tag	UNP Q9UIQ6
A	150	VAL	-	expression tag	UNP Q9UIQ6
A	151	ALA	-	expression tag	UNP Q9UIQ6
A	152	GLU	-	expression tag	UNP Q9UIQ6
A	153	THR	-	expression tag	UNP Q9UIQ6
A	154	GLY	-	expression tag	UNP Q9UIQ6
A	1026	ARG	-	expression tag	UNP Q9UIQ6
A	1027	THR	-	expression tag	UNP Q9UIQ6
A	1028	GLU	-	expression tag	UNP Q9UIQ6
A	1029	THR	-	expression tag	UNP Q9UIQ6
A	1030	SER	-	expression tag	UNP Q9UIQ6
A	1031	GLN	-	expression tag	UNP Q9UIQ6
A	1032	VAL	-	expression tag	UNP Q9UIQ6
A	1033	ALA	-	expression tag	UNP Q9UIQ6
A	1034	PRO	-	expression tag	UNP Q9UIQ6
A	1035	ALA	-	expression tag	UNP Q9UIQ6
B	124	MET	-	initiating methionine	UNP Q9UIQ6
B	125	GLY	-	expression tag	UNP Q9UIQ6
B	126	ILE	-	expression tag	UNP Q9UIQ6
B	127	LEU	-	expression tag	UNP Q9UIQ6
B	128	PRO	-	expression tag	UNP Q9UIQ6
B	129	SER	-	expression tag	UNP Q9UIQ6
B	130	PRO	-	expression tag	UNP Q9UIQ6
B	131	GLY	-	expression tag	UNP Q9UIQ6
B	132	ASN	-	expression tag	UNP Q9UIQ6
B	133	PRO	-	expression tag	UNP Q9UIQ6
B	134	ALA	-	expression tag	UNP Q9UIQ6
B	135	LEU	-	expression tag	UNP Q9UIQ6
B	136	LEU	-	expression tag	UNP Q9UIQ6
B	137	SER	-	expression tag	UNP Q9UIQ6
B	138	LEU	-	expression tag	UNP Q9UIQ6
B	139	VAL	-	expression tag	UNP Q9UIQ6
B	140	SER	-	expression tag	UNP Q9UIQ6
B	141	LEU	-	expression tag	UNP Q9UIQ6
B	142	LEU	-	expression tag	UNP Q9UIQ6
B	143	SER	-	expression tag	UNP Q9UIQ6
B	144	VAL	-	expression tag	UNP Q9UIQ6
B	145	LEU	-	expression tag	UNP Q9UIQ6
B	146	LEU	-	expression tag	UNP Q9UIQ6
B	147	MET	-	expression tag	UNP Q9UIQ6
B	148	GLY	-	expression tag	UNP Q9UIQ6
B	149	CYS	-	expression tag	UNP Q9UIQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	150	VAL	-	expression tag	UNP Q9UIQ6
B	151	ALA	-	expression tag	UNP Q9UIQ6
B	152	GLU	-	expression tag	UNP Q9UIQ6
B	153	THR	-	expression tag	UNP Q9UIQ6
B	154	GLY	-	expression tag	UNP Q9UIQ6
B	1026	ARG	-	expression tag	UNP Q9UIQ6
B	1027	THR	-	expression tag	UNP Q9UIQ6
B	1028	GLU	-	expression tag	UNP Q9UIQ6
B	1029	THR	-	expression tag	UNP Q9UIQ6
B	1030	SER	-	expression tag	UNP Q9UIQ6
B	1031	GLN	-	expression tag	UNP Q9UIQ6
B	1032	VAL	-	expression tag	UNP Q9UIQ6
B	1033	ALA	-	expression tag	UNP Q9UIQ6
B	1034	PRO	-	expression tag	UNP Q9UIQ6
B	1035	ALA	-	expression tag	UNP Q9UIQ6

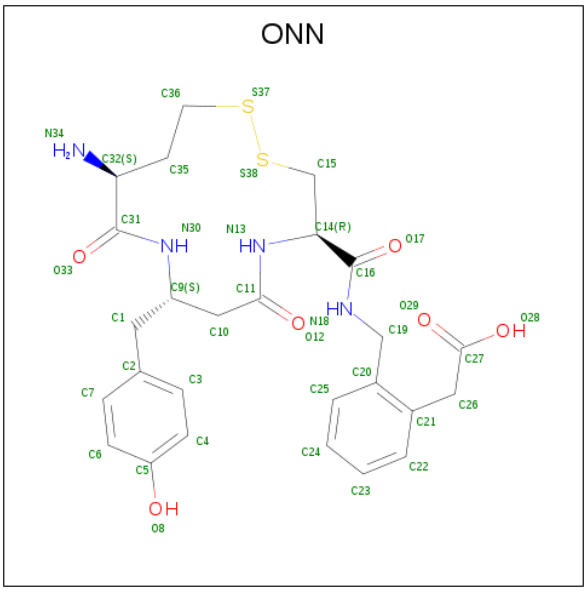
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	3	Total C N O 39 22 2 15	0	0	0
3	H	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is 2-[2-[[[(4 {R},8 {S},11 {S})-11-azanyl-8-[(4-hydroxyphenyl)methyl]-6,10-bis(oxidanylidene)-1,2-dithia-5,9-diazacyclotridec-4-yl]carbonylamino]methyl]phenyl]ethanoic acid (three-letter code: ONN) (formula: $C_{26}H_{32}N_4O_6S_2$) (labeled as "Ligand of Interest" by author).

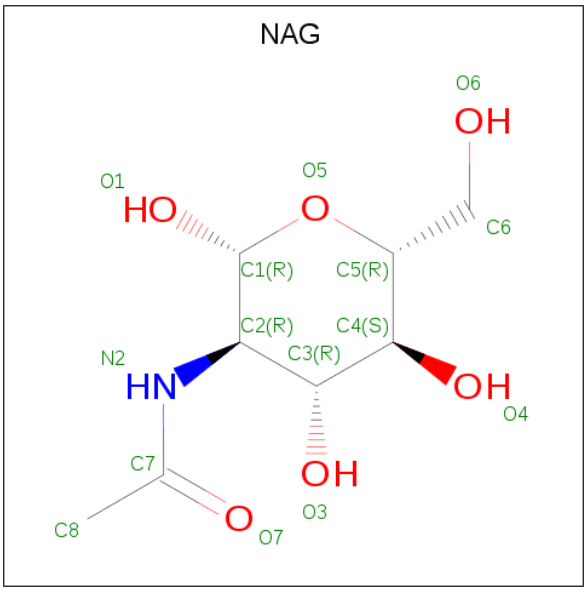


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 76 52 8 12 4	0	1
4	B	1	Total C N O S 76 52 8 12 4	0	1

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

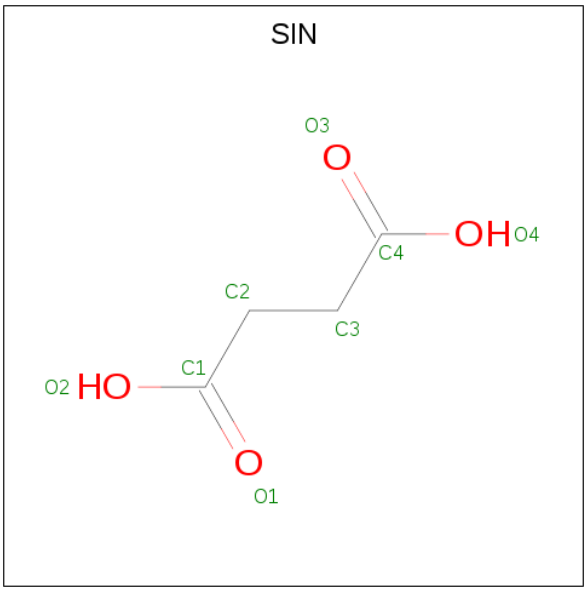
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Zn 1 1	0	0
5	A	1	Total Zn 1 1	0	0

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



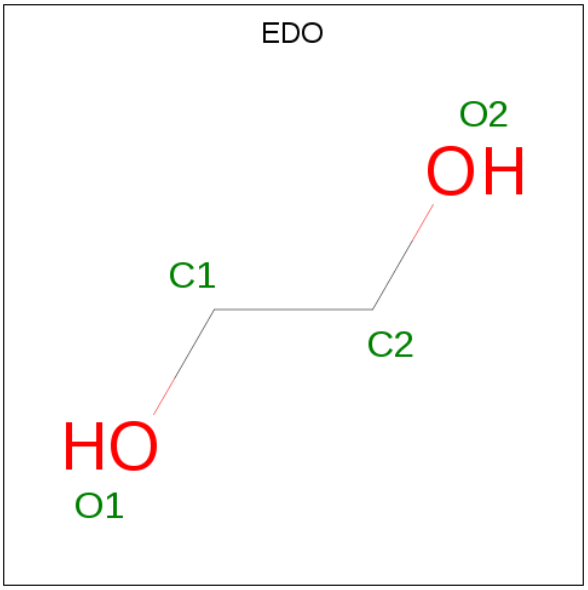
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total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

- Molecule 7 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 4 4	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

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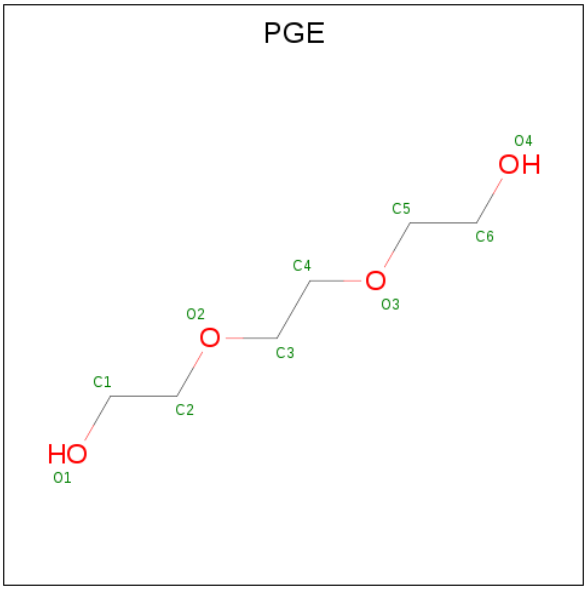
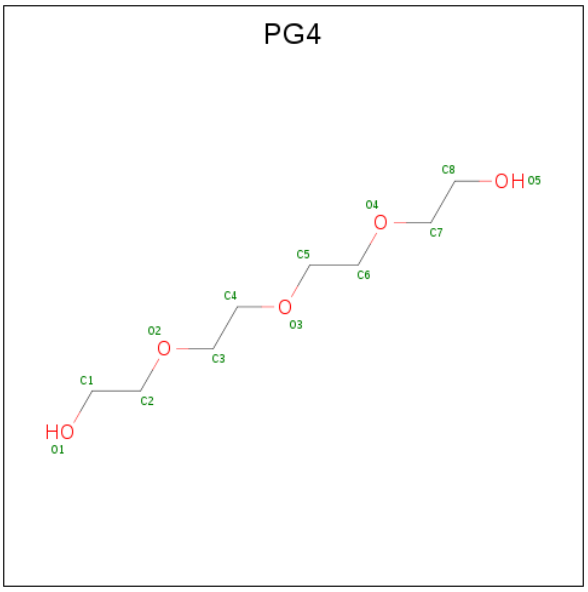
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



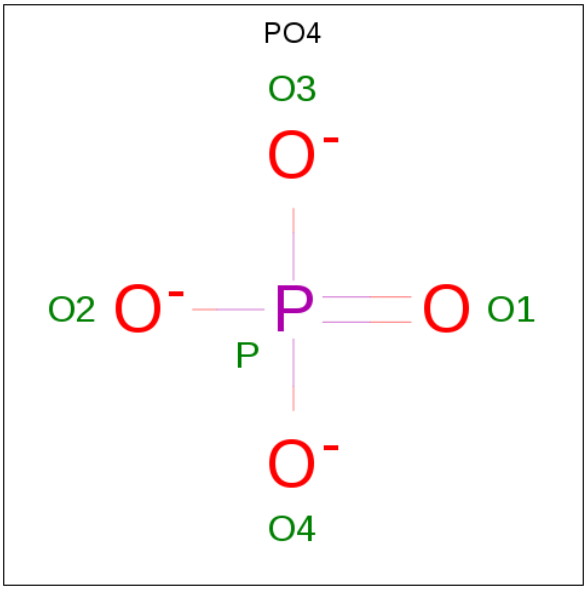
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 10 6 4	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



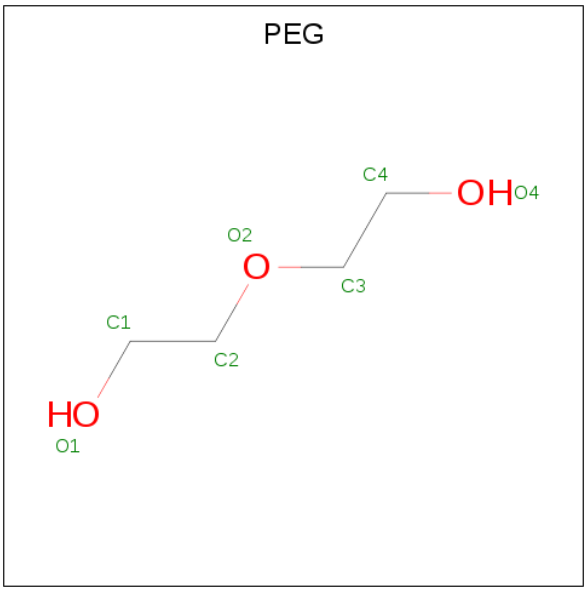
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 13 8 5	0	0

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O P 5 4 1	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 7 4 3	0	0

- Molecule 13 is water.

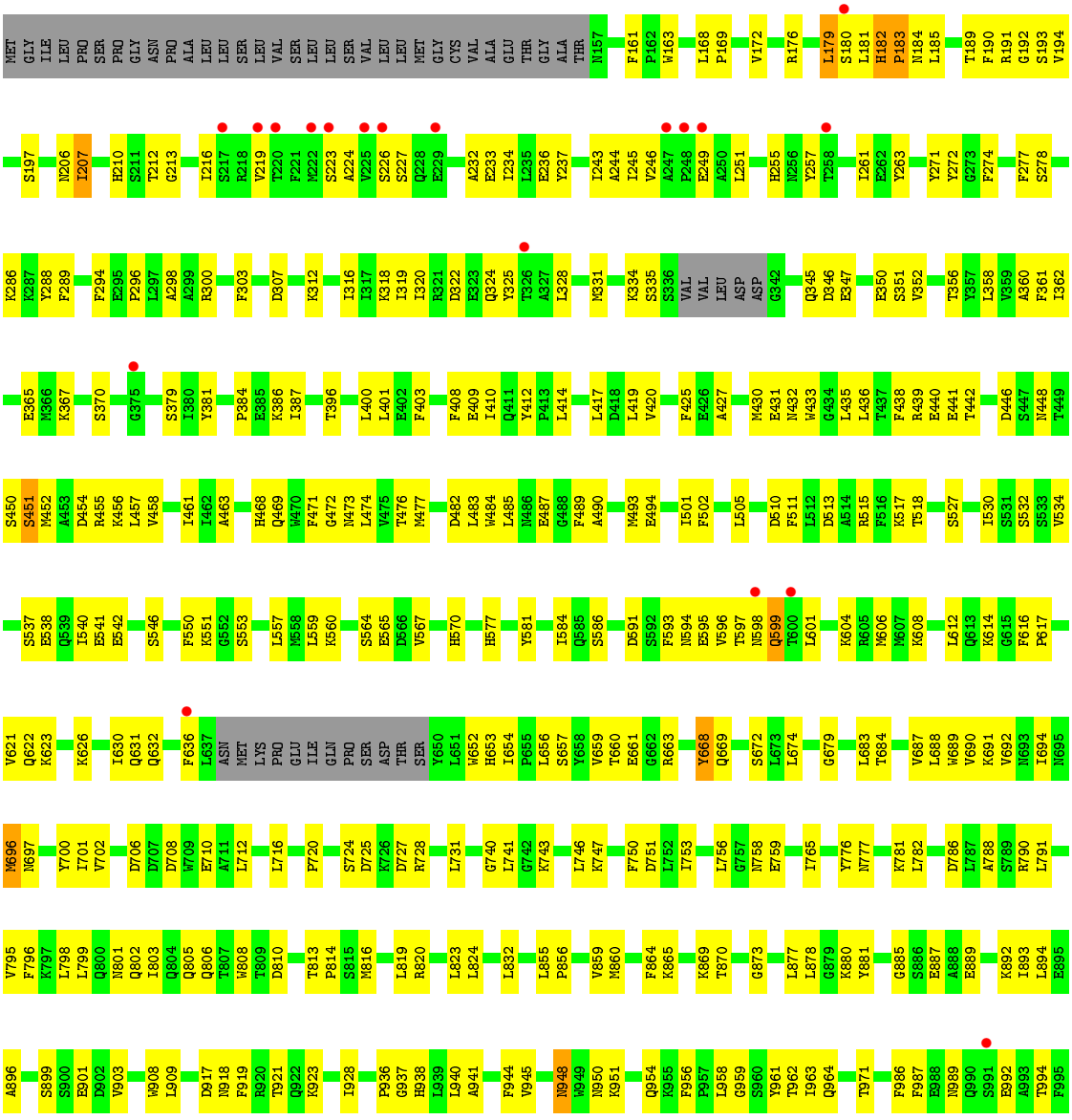
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	11	Total O 11 11	0	0
13	B	17	Total O 17 17	0	0

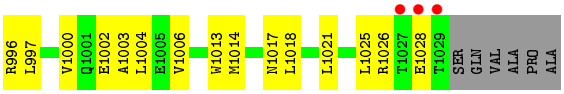
3 Residue-property plots (i)

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: Leucyl-cystinyl aminopeptidase

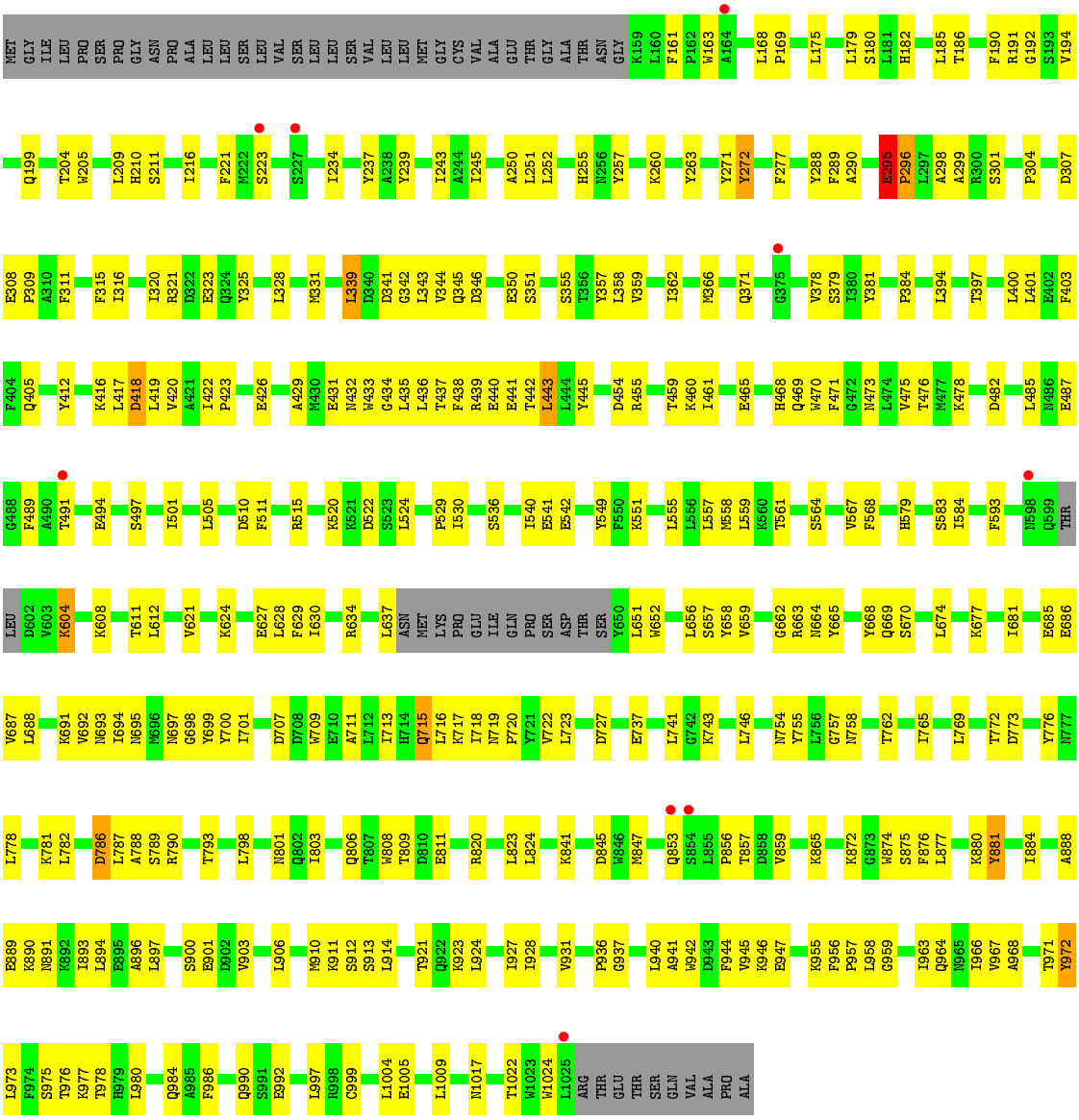
Chain A:





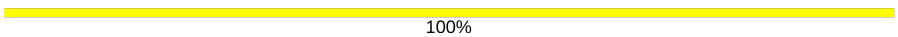
• Molecule 1: Leucyl-cystinyl aminopeptidase

Chain B:



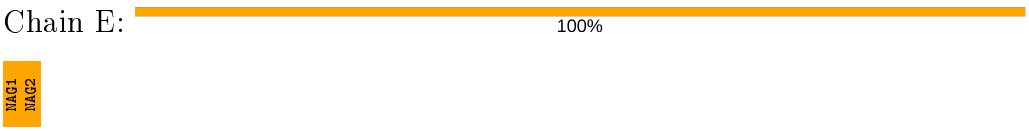
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain E:

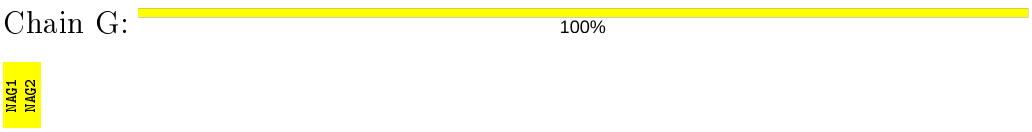


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

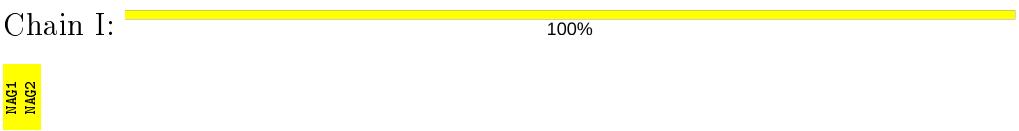
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



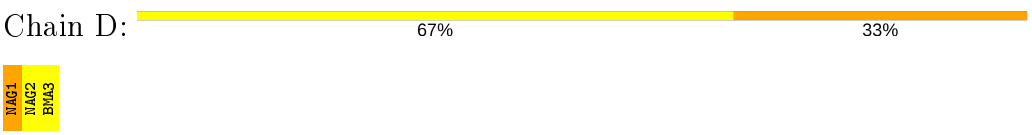
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain D:



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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.42Å 118.63Å 141.39Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	45.96 – 3.20 45.96 – 3.01	Depositor EDS
% Data completeness (in resolution range)	81.7 (45.96-3.20) 69.8 (45.96-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.277 , 0.314 0.271 , 0.306	Depositor DCC
R_{free} test set	1597 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	56.3	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	14298	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3379e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, PGE, ONN, NAG, PO4, EDO, PG4, BMA, PEG, SIN

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	0.40	0/7047	0.69	5/9566 (0.1%)
1	B	0.40	1/6994 (0.0%)	0.70	3/9498 (0.0%)
All	All	0.40	1/14041 (0.0%)	0.70	8/19064 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	881	TYR	CD1-CE1	-5.92	1.30	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	GLU	C-N-CD	-9.98	98.65	120.60
1	A	408	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	A	408	PHE	CB-CG-CD1	6.53	125.37	120.80
1	B	400	LEU	CB-CG-CD2	-6.10	100.63	111.00
1	A	207	ILE	CG1-CB-CG2	-6.05	98.10	111.40
1	B	857	THR	CA-CB-CG2	-5.76	104.33	112.40
1	A	179	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	1004	LEU	CB-CG-CD1	-5.14	102.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	295	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6868	0	6703	261	0
1	B	6827	0	6664	240	0
2	C	28	0	25	1	0
2	E	28	0	25	3	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
3	D	39	0	34	2	0
3	H	39	0	34	3	0
4	A	76	0	0	3	0
4	B	76	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	70	0	64	6	0
6	B	70	0	65	0	0
7	A	8	0	4	0	0
8	A	8	0	12	1	0
8	B	12	0	18	0	0
9	A	10	0	14	0	0
10	A	13	0	18	0	0
11	A	5	0	0	0	0
12	B	7	0	10	1	0
13	A	11	0	0	0	0
13	B	17	0	0	1	0
All	All	14298	0	13765	517	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (517) 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:B:168:LEU:HD13	1:B:210:HIS:CE1	1.81	1.15
1:B:695:ASN:N	1:B:727:ASP:OD1	1.83	1.11
1:A:482:ASP:HB3	1:A:485:LEU:HD12	1.37	1.07
1:A:207:ILE:HG22	1:A:245:ILE:HB	1.47	0.97
1:B:717:LYS:HE2	1:B:754:ASN:HB2	1.47	0.96
1:A:621:VAL:HG21	1:A:692:VAL:HG21	1.46	0.96
1:A:172:VAL:HG11	1:A:207:ILE:HG13	1.46	0.95
1:A:236:GLU:HG3	1:A:243:ILE:HG22	1.49	0.93
1:B:741:LEU:HD11	1:B:743:LYS:HG2	1.51	0.92
1:A:971:THR:HG21	1:A:1003:ALA:HB1	1.55	0.88
1:B:877:LEU:HD22	1:B:893:ILE:HG23	1.57	0.86
1:B:621:VAL:HG21	1:B:692:VAL:HG21	1.57	0.85
1:B:168:LEU:CD1	1:B:210:HIS:CE1	2.59	0.85
1:A:616:PHE:HE2	1:A:701:ILE:HG13	1.42	0.84
1:A:216:ILE:HD12	1:A:261:ILE:HD11	1.62	0.82
1:A:781:LYS:HD2	1:A:938:HIS:CG	2.15	0.81
1:A:855:LEU:HD23	1:A:860:MET:HG2	1.62	0.79
1:B:628:LEU:HD11	1:B:681:ILE:HB	1.65	0.78
1:B:659:VAL:HG12	1:B:691:LYS:HB3	1.65	0.77
1:B:401:LEU:O	1:B:405:GLN:HG3	1.85	0.77
1:B:185:LEU:HD21	1:B:290:ALA:HB2	1.65	0.77
1:B:662:GLY:HA2	1:B:687:VAL:HA	1.65	0.76
1:B:634:ARG:HD3	1:B:652:TRP:HH2	1.51	0.75
1:B:252:LEU:HB2	1:B:255:HIS:ND1	2.02	0.75
1:A:511:PHE:HE2	1:A:557:LEU:HD22	1.52	0.74
1:A:441:GLU:HG3	1:A:887:GLU:CG	2.17	0.74
1:B:911:LYS:HD2	1:B:914:LEU:HD23	1.70	0.73
1:A:472:GLY:O	1:A:476:THR:HB	1.89	0.73
1:A:806:GLN:HE21	1:A:823:LEU:HD12	1.54	0.73
1:B:194:VAL:HG21	1:B:304:PRO:HD2	1.71	0.73
1:A:570:HIS:HB3	1:A:596:VAL:HG21	1.70	0.73
1:A:179:LEU:HD22	1:A:181:LEU:HD23	1.72	0.71
1:A:616:PHE:CE2	1:A:701:ILE:HG13	2.26	0.71
1:A:901:GLU:HG2	1:A:936:PRO:HG3	1.72	0.71
1:B:416:LYS:HD2	1:B:418:ASP:OD2	1.91	0.71
1:B:482:ASP:HB3	1:B:485:LEU:HD12	1.71	0.71
1:A:865:LYS:O	1:A:869:LYS:HE3	1.90	0.71
1:B:959:GLY:H	1:B:963:ILE:HD11	1.55	0.70
1:B:781:LYS:HE2	1:B:973:LEU:HD13	1.73	0.70
1:A:455:ARG:HH12	1:A:505:LEU:HD21	1.56	0.70
1:B:429:ALA:HB2	1:B:461:ILE:HD11	1.72	0.70
1:B:564:SER:HB2	1:B:567:VAL:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HD13	1:A:263:TYR:HB3	1.75	0.68
1:A:410:ILE:HD12	1:A:410:ILE:H	1.58	0.68
1:A:441:GLU:HG3	1:A:887:GLU:HG3	1.75	0.68
1:B:782:LEU:HD11	1:B:975:SER:HB2	1.75	0.68
1:A:961:TYR:HA	1:A:964:GLN:HG2	1.76	0.67
1:A:877:LEU:HD22	1:A:893:ILE:HG23	1.74	0.67
1:A:530:ILE:HG23	1:A:551:LYS:HD3	1.77	0.67
1:B:856:PRO:HG2	1:B:859:VAL:HG22	1.77	0.67
1:A:593:PHE:O	1:A:597:THR:HG22	1.95	0.67
1:B:986:PHE:O	1:B:990:GLN:NE2	2.28	0.67
1:A:756:LEU:O	1:A:802:GLN:NE2	2.28	0.66
1:A:223:SER:HB2	1:A:257:TYR:HA	1.77	0.66
1:A:959:GLY:H	1:A:963:ILE:HD11	1.60	0.66
1:B:903:VAL:HG23	1:B:940:LEU:HD22	1.77	0.66
1:A:606:MET:HG3	1:A:653:HIS:HB2	1.78	0.66
1:A:765:ILE:HD12	1:A:819:LEU:HD11	1.78	0.65
1:A:881:TYR:OH	1:A:923:LYS:HE2	1.96	0.65
1:B:693:ASN:HB2	1:B:700:TYR:CE2	2.32	0.65
1:B:366:MET:HA	1:B:384:PRO:HD3	1.78	0.65
1:B:403:PHE:HE2	1:B:497:SER:HA	1.60	0.65
1:B:637:LEU:HD22	1:B:1009:LEU:HD13	1.78	0.65
1:B:362:ILE:HG12	1:B:435:LEU:HD21	1.77	0.65
1:A:206:ASN:OD1	1:A:246:VAL:HG12	1.95	0.65
1:B:419:LEU:HG	1:B:438:PHE:HE2	1.60	0.65
1:A:659:VAL:HG13	1:A:669:GLN:HG2	1.79	0.64
4:B:1101[A]:ONN:N18	4:B:1101[A]:ONN:O12	2.30	0.64
1:A:599:GLN:HB2	1:A:601:LEU:HD23	1.79	0.64
1:A:741:LEU:HD11	1:A:743:LYS:HG2	1.78	0.64
1:B:316:ILE:HG12	1:B:350:GLU:HG3	1.79	0.64
1:B:894:LEU:CD2	1:B:923:LYS:HD3	2.27	0.64
1:B:769:LEU:HA	1:B:772:THR:HG22	1.78	0.64
1:B:478:LYS:HE3	1:B:583:SER:HB2	1.80	0.64
1:A:294:PHE:HA	1:A:298:ALA:HB3	1.77	0.64
1:A:179:LEU:CD2	1:A:181:LEU:HD23	2.28	0.64
1:B:288:TYR:HB2	1:B:325:TYR:OH	1.98	0.64
1:B:656:LEU:HD12	1:B:656:LEU:N	2.13	0.64
1:B:331:MET:HG2	1:B:351:SER:HB3	1.80	0.63
1:A:992:GLU:O	1:A:996:ARG:HG2	1.99	0.63
1:A:403:PHE:HB2	1:A:501:ILE:HD12	1.80	0.63
1:A:956:PHE:HB2	1:A:963:ILE:HG23	1.80	0.63
1:B:701:ILE:CD1	1:B:737:GLU:HG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:THR:HG22	1:A:690:VAL:HG12	1.81	0.63
1:B:182:HIS:HB3	1:B:191:ARG:HB2	1.80	0.63
1:B:511:PHE:HE2	1:B:557:LEU:HD22	1.63	0.63
1:A:251:LEU:H	1:A:251:LEU:HD12	1.64	0.63
1:A:318:LYS:HG2	1:A:347:GLU:HB3	1.81	0.62
1:B:491:THR:HA	1:B:494:GLU:HG2	1.82	0.62
1:B:803:ILE:HG12	1:B:823:LEU:HB3	1.81	0.62
1:B:320:ILE:HG12	1:B:345:GLN:HG3	1.81	0.62
1:A:441:GLU:HG3	1:A:887:GLU:HG2	1.81	0.62
1:A:511:PHE:CE2	1:A:557:LEU:HD22	2.34	0.62
1:B:455:ARG:HH12	1:B:505:LEU:HD21	1.64	0.62
1:A:255:HIS:HA	6:A:1106:NAG:H82	1.81	0.62
1:A:219:VAL:HB	1:A:234:ILE:HD11	1.82	0.62
1:A:917:ASP:O	1:A:919:PHE:N	2.28	0.62
1:A:691:LYS:HE2	1:A:731:LEU:HG	1.82	0.61
1:B:628:LEU:CD1	1:B:681:ILE:HB	2.31	0.61
1:A:210:HIS:HB3	1:A:300:ARG:HG2	1.83	0.61
1:A:781:LYS:HD2	1:A:938:HIS:CD2	2.35	0.61
1:B:628:LEU:HD13	1:B:630:ILE:HD11	1.83	0.60
1:B:955:LYS:HE3	1:B:955:LYS:HA	1.82	0.60
1:A:692:VAL:HB	1:A:702:VAL:HG11	1.83	0.60
1:B:419:LEU:HD11	1:B:436:LEU:HD22	1.82	0.60
1:A:786:ASP:O	1:A:790:ARG:HG3	2.00	0.60
1:B:976:THR:HG22	1:B:978:THR:H	1.65	0.60
1:A:455:ARG:NH1	1:A:505:LEU:HD21	2.16	0.60
1:B:624:LYS:HE3	1:B:629:PHE:HB2	1.83	0.60
1:B:455:ARG:HG2	1:B:455:ARG:HH11	1.66	0.60
1:A:360:ALA:HB2	1:A:432:ASN:ND2	2.17	0.59
1:B:881:TYR:OH	1:B:923:LYS:HE3	2.02	0.59
1:A:810:ASP:N	1:A:820:ARG:HH22	2.00	0.59
1:A:928:ILE:HD13	1:A:945:VAL:HG22	1.82	0.59
1:A:185:LEU:HD13	1:A:288:TYR:CB	2.33	0.59
1:A:439:ARG:HD3	1:A:441:GLU:OE1	2.03	0.59
1:A:654:ILE:HG23	1:A:700:TYR:CE2	2.38	0.59
1:B:161:PHE:CD1	1:B:237:TYR:HB2	2.38	0.59
1:B:746:LEU:HD22	1:B:1017:ASN:HB3	1.83	0.59
1:A:271:TYR:HE2	1:A:921:THR:HB	1.67	0.58
1:A:484:TRP:CD2	1:A:530:ILE:HD12	2.38	0.58
1:A:457:LEU:O	1:A:461:ILE:HG13	2.03	0.58
1:A:690:VAL:O	1:A:712:LEU:HD21	2.03	0.58
1:A:889:GLU:O	1:A:893:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LEU:HD11	1:A:674:LEU:HB2	1.85	0.58
1:B:937:GLY:HA2	1:B:940:LEU:HB3	1.84	0.58
1:B:378:VAL:HG22	1:B:417:LEU:HB3	1.86	0.58
1:A:791:LEU:O	1:A:795:VAL:HG23	2.04	0.58
1:B:180:SER:O	1:B:192:GLY:HA2	2.02	0.58
1:A:312:LYS:NZ	1:A:474:LEU:O	2.36	0.58
1:B:460:LYS:HG2	1:B:494:GLU:OE1	2.04	0.58
1:A:212:THR:HG21	8:A:1118:EDO:H11	1.86	0.57
1:A:484:TRP:CE2	1:A:530:ILE:HD12	2.39	0.57
1:A:608:LYS:HD2	1:A:612:LEU:HD13	1.85	0.57
1:A:207:ILE:CG2	1:A:245:ILE:HB	2.29	0.57
1:A:420:VAL:O	1:A:438:PHE:HB2	2.03	0.57
1:A:352:VAL:HB	1:A:581:TYR:HE2	1.70	0.57
1:A:776:TYR:CD2	1:A:788:ALA:HB1	2.40	0.56
1:A:750:PHE:CZ	1:A:791:LEU:HD11	2.40	0.56
1:B:394:LEU:O	1:B:397:THR:HG22	2.04	0.56
1:A:894:LEU:CD2	1:A:923:LYS:HD3	2.36	0.56
1:B:558:MET:CG	1:B:698:GLY:HA2	2.35	0.56
1:A:184:ASN:N	1:A:189:THR:O	2.36	0.56
1:A:370:SER:HB3	1:A:379:SER:HA	1.86	0.56
1:A:271:TYR:CE2	1:A:921:THR:HB	2.39	0.56
1:A:485:LEU:HD11	1:A:586:SER:HA	1.87	0.56
1:B:1005:GLU:O	1:B:1009:LEU:HG	2.06	0.56
1:B:271:TYR:HE2	1:B:921:THR:HB	1.70	0.56
1:A:790:ARG:HB3	1:A:1025:LEU:HD22	1.86	0.56
1:A:185:LEU:HD13	1:A:288:TYR:HB3	1.87	0.56
1:A:515:ARG:CZ	1:A:696:MET:HG2	2.36	0.56
1:A:1014:MET:O	1:A:1018:LEU:HB3	2.06	0.56
1:A:335:SER:CB	1:A:346:ASP:HA	2.36	0.56
1:B:530:ILE:HG21	1:B:551:LYS:HB3	1.87	0.56
1:B:716:LEU:O	1:B:720:PRO:HG3	2.05	0.56
1:A:409:GLU:HG2	1:A:409:GLU:O	2.05	0.55
1:B:476:THR:O	1:B:584:ILE:N	2.35	0.55
1:A:971:THR:CG2	1:A:1003:ALA:HB1	2.33	0.55
1:A:419:LEU:HD11	1:A:436:LEU:HD22	1.88	0.55
1:A:630:ILE:O	1:A:679:GLY:N	2.40	0.55
1:B:295:GLU:OE1	1:B:357:TYR:CD1	2.59	0.55
1:B:487:GLU:HB3	1:B:549:TYR:CE2	2.42	0.55
1:A:223:SER:CB	1:A:257:TYR:HA	2.35	0.55
1:B:343:LEU:O	1:B:344:VAL:HG23	2.06	0.55
1:B:659:VAL:HG23	1:B:669:GLN:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:NAG:H82	2:E:1:NAG:O3	2.07	0.55
1:A:753:ILE:HG13	1:A:753:ILE:O	2.07	0.55
1:A:436:LEU:HD11	1:A:469:GLN:NE2	2.21	0.55
1:A:322:ASP:HB3	1:A:325:TYR:HE2	1.72	0.55
1:A:224:ALA:HB3	1:A:227:SER:HB2	1.89	0.54
2:F:1:NAG:H3	2:F:1:NAG:O7	2.08	0.54
1:B:776:TYR:CD1	1:B:788:ALA:HB1	2.42	0.54
1:B:884:ILE:HD11	1:B:890:LYS:HG3	1.88	0.54
1:B:894:LEU:HD23	1:B:923:LYS:HD3	1.89	0.54
1:B:911:LYS:HG2	13:B:1210:HOH:O	2.06	0.54
1:B:163:TRP:CE2	1:B:169:PRO:HD3	2.43	0.54
1:B:455:ARG:NH1	1:B:505:LEU:HD21	2.22	0.54
1:A:1021:LEU:O	1:A:1025:LEU:HB2	2.07	0.54
1:A:753:ILE:O	1:A:798:LEU:HD21	2.08	0.54
1:A:617:PRO:HG2	1:A:700:TYR:HB3	1.90	0.54
1:B:906:LEU:HD22	1:B:931:VAL:HG22	1.90	0.54
1:B:277:PHE:CE1	1:B:289:PHE:HB3	2.42	0.54
1:B:894:LEU:O	1:B:894:LEU:HD12	2.08	0.54
1:B:928:ILE:HD12	1:B:966:ILE:HD13	1.89	0.54
1:A:527:SER:O	1:A:614:LYS:HD2	2.07	0.54
1:B:476:THR:O	1:B:583:SER:HA	2.07	0.54
1:B:175:LEU:HD11	1:B:199:GLN:HB2	1.90	0.53
1:B:321:ARG:NE	1:B:346:ASP:OD2	2.33	0.53
1:B:315:PHE:CE2	1:B:359:VAL:HG21	2.42	0.53
1:A:180:SER:HA	1:A:318:LYS:O	2.08	0.53
1:A:799:LEU:O	1:A:803:ILE:HG13	2.08	0.53
1:A:903:VAL:HG23	1:A:940:LEU:HD22	1.89	0.53
1:A:747:LYS:O	1:A:751:ASP:N	2.37	0.53
1:A:958:LEU:HG	1:A:997:LEU:HD21	1.90	0.53
1:B:216:ILE:HD12	1:B:234:ILE:HD13	1.90	0.53
1:B:992:GLU:HA	1:B:992:GLU:OE1	2.08	0.53
1:A:684:THR:HG22	2:E:2:NAG:H61	1.89	0.53
1:A:319:ILE:O	1:A:346:ASP:N	2.40	0.53
1:A:454:ASP:O	1:A:458:VAL:HG13	2.08	0.53
1:A:799:LEU:HD23	1:A:802:GLN:NE2	2.23	0.53
1:B:271:TYR:CE2	1:B:921:THR:HB	2.44	0.53
3:D:1:NAG:H61	3:D:2:NAG:HN2	1.74	0.53
1:A:194:VAL:HG23	1:A:263:TYR:HE2	1.74	0.53
1:B:186:THR:HG21	3:H:2:NAG:C7	2.39	0.53
1:A:777:ASN:O	1:A:781:LYS:HG2	2.09	0.53
1:B:557:LEU:O	1:B:561:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASP:H	1:A:820:ARG:HH22	1.57	0.52
1:A:168:LEU:HG	1:A:210:HIS:CE1	2.44	0.52
1:B:478:LYS:CE	1:B:583:SER:HB2	2.39	0.52
1:B:786:ASP:O	1:B:790:ARG:HG3	2.09	0.52
6:A:1112:NAG:H82	6:A:1112:NAG:O3	2.09	0.52
1:A:324:GLN:OE1	1:A:324:GLN:HA	2.08	0.52
1:B:237:TYR:CE1	1:B:239:TYR:HD2	2.28	0.52
1:B:168:LEU:HD13	1:B:210:HIS:HE1	1.61	0.52
1:A:433:TRP:CH2	1:A:474:LEU:HA	2.45	0.52
1:A:756:LEU:HD22	1:A:798:LEU:HD23	1.92	0.52
1:A:630:ILE:HD13	1:A:656:LEU:HD13	1.92	0.52
1:A:994:THR:HA	1:A:997:LEU:HD13	1.91	0.52
1:B:790:ARG:O	1:B:793:THR:HG22	2.10	0.52
1:A:442:THR:HG23	1:A:461:ILE:HD12	1.92	0.52
1:B:323:GLU:HG3	1:B:342:GLY:O	2.09	0.52
1:A:316:ILE:HG22	1:A:350:GLU:HA	1.93	0.51
1:B:455:ARG:NH1	1:B:455:ARG:HG2	2.25	0.51
1:B:713:ILE:O	1:B:717:LYS:HG3	2.10	0.51
1:A:370:SER:OG	6:A:1112:NAG:H83	2.10	0.51
1:A:937:GLY:HA2	1:A:940:LEU:HB3	1.91	0.51
1:B:903:VAL:HA	1:B:906:LEU:HD12	1.92	0.51
6:A:1115:NAG:O3	6:A:1115:NAG:H82	2.10	0.51
1:A:278:SER:HB2	1:A:286:LYS:HD2	1.91	0.51
1:A:564:SER:HB3	1:A:567:VAL:HG23	1.93	0.51
1:A:163:TRP:CE2	1:A:169:PRO:HD3	2.46	0.51
1:A:657:SER:OG	1:A:694:ILE:HG12	2.09	0.51
1:B:234:ILE:HG22	1:B:245:ILE:HG13	1.93	0.51
1:B:891:ASN:ND2	1:B:923:LYS:NZ	2.59	0.51
1:B:722:VAL:HG23	1:B:723:LEU:HD12	1.91	0.51
1:B:358:LEU:HD22	1:B:432:ASN:HA	1.92	0.51
1:A:944:PHE:O	1:A:948:ASN:HB2	2.11	0.50
1:A:604:LYS:O	1:A:608:LYS:HG2	2.11	0.50
1:B:658:TYR:CZ	1:B:670:SER:HB3	2.46	0.50
1:B:856:PRO:HG2	1:B:859:VAL:CG2	2.41	0.50
1:A:808:TRP:HB3	1:A:859:VAL:HG11	1.93	0.50
1:B:709:TRP:O	1:B:713:ILE:HG13	2.12	0.50
1:A:856:PRO:O	1:A:860:MET:HG3	2.11	0.50
1:B:698:GLY:HA3	1:B:700:TYR:CE1	2.47	0.50
1:B:758:ASN:ND2	1:B:758:ASN:O	2.44	0.50
3:H:2:NAG:O3	3:H:2:NAG:O7	2.28	0.50
1:A:471:PHE:HE2	1:A:493:MET:HG3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:ARG:HG2	1:B:686:GLU:O	2.12	0.50
1:B:716:LEU:HD21	1:B:723:LEU:HD22	1.94	0.50
6:A:1106:NAG:O3	6:A:1106:NAG:O7	2.24	0.50
1:A:328:LEU:HB2	1:A:362:ILE:HG12	1.93	0.50
1:A:441:GLU:CG	1:A:887:GLU:HG3	2.40	0.50
1:A:622:GLN:OE1	1:A:631:GLN:NE2	2.45	0.50
1:A:956:PHE:HB2	1:A:963:ILE:CG2	2.42	0.50
1:B:163:TRP:CH2	1:B:169:PRO:HB3	2.47	0.50
1:A:176[B]:ARG:HH12	1:A:350:GLU:CB	2.25	0.49
1:A:461:ILE:HG12	4:A:1101[B]:ONN:C6	2.42	0.49
1:A:483:LEU:HD21	1:A:487:GLU:HG3	1.94	0.49
1:A:864:PHE:CE2	1:A:893:ILE:HG12	2.47	0.49
1:A:864:PHE:HB3	1:A:896:ALA:HB2	1.95	0.49
1:A:656:LEU:N	1:A:672:SER:O	2.45	0.49
1:B:223:SER:HB3	1:B:257:TYR:CD2	2.47	0.49
1:A:172:VAL:HG11	1:A:207:ILE:CG1	2.32	0.49
1:B:403:PHE:HB2	1:B:501:ILE:HD11	1.94	0.49
1:B:956:PHE:HB2	1:B:963:ILE:HG23	1.95	0.49
1:A:183:PRO:HB3	1:A:190:PHE:HB3	1.95	0.49
1:B:542:GLU:CD	1:B:997:LEU:HD22	2.33	0.49
1:A:358:LEU:HD11	1:A:473:ASN:HA	1.93	0.49
1:A:182:HIS:HB2	1:A:320:ILE:HD13	1.93	0.49
1:A:362:ILE:HG23	1:A:435:LEU:HD21	1.93	0.49
1:B:475:VAL:HG22	1:B:579:HIS:O	2.12	0.49
1:A:194:VAL:HG21	1:A:303:PHE:HB2	1.95	0.48
1:B:651:LEU:HD11	1:B:677:LYS:HB2	1.95	0.48
1:B:628:LEU:HD12	1:B:628:LEU:O	2.13	0.48
1:A:442:THR:CG2	1:A:461:ILE:HD12	2.43	0.48
1:A:741:LEU:HD11	1:A:743:LYS:HE3	1.95	0.48
1:B:185:LEU:HD13	1:B:288:TYR:HB3	1.96	0.48
1:A:515:ARG:NH2	1:A:696:MET:HG2	2.28	0.48
1:A:724:SER:HB2	1:A:727:ASP:H	1.78	0.48
1:B:947:GLU:OE1	1:B:947:GLU:HA	2.14	0.48
1:A:182:HIS:N	1:A:191:ARG:O	2.43	0.48
1:A:542:GLU:OE2	1:A:997:LEU:HG	2.14	0.48
1:B:194:VAL:O	1:B:260:LYS:HA	2.13	0.48
1:B:468:HIS:HA	1:B:471:PHE:O	2.13	0.48
1:B:746:LEU:HB3	1:B:1024:TRP:HH2	1.79	0.48
1:A:987:PHE:CD2	1:A:1000:VAL:HG13	2.49	0.47
4:A:1101[B]:ONN:C11	4:A:1101[B]:ONN:N18	2.77	0.47
1:A:456:LYS:HD3	1:A:510:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ILE:CG2	1:A:551:LYS:HD3	2.42	0.47
1:B:328:LEU:HD11	1:B:381:TYR:CD2	2.49	0.47
1:B:718:ILE:HG13	1:B:719:ASN:H	1.79	0.47
1:A:660:THR:HG22	1:A:690:VAL:CG1	2.44	0.47
1:B:416:LYS:HB3	1:B:416:LYS:HE3	1.66	0.47
1:B:889:GLU:O	1:B:893:ILE:HG13	2.14	0.47
3:H:3:BMA:O6	3:H:3:BMA:O4	2.22	0.47
1:A:219:VAL:HG13	1:A:232:ALA:HB3	1.95	0.47
1:A:396:THR:HG23	1:A:502:PHE:CZ	2.48	0.47
1:A:706:ASP:O	1:A:710:GLU:HG2	2.14	0.47
1:B:781:LYS:HD3	1:B:781:LYS:N	2.29	0.47
4:A:1101[B]:ONN:O12	4:A:1101[B]:ONN:N18	2.48	0.47
1:A:632:GLN:OE1	1:A:652:TRP:HE3	1.97	0.47
1:A:438:PHE:HD2	1:A:442:THR:HG22	1.80	0.47
1:A:386:LYS:HE3	1:A:885:GLY:O	2.14	0.47
1:B:321:ARG:HH21	1:B:321:ARG:HG3	1.79	0.47
1:B:485:LEU:HD13	1:B:584:ILE:CD1	2.45	0.47
1:B:522:ASP:OD2	1:B:551:LYS:HE3	2.15	0.47
1:A:591:ASP:O	1:A:595:GLU:N	2.45	0.47
1:A:810:ASP:H	1:A:820:ARG:NH2	2.13	0.47
1:B:272:TYR:CD2	1:B:298:ALA:HB2	2.50	0.47
1:A:532:SER:O	1:A:534:VAL:HG23	2.13	0.47
3:D:1:NAG:H3	3:D:1:NAG:H83	1.97	0.47
1:B:379:SER:HB3	1:B:418:ASP:OD1	2.15	0.46
1:A:233:GLU:HB3	1:A:246:VAL:CG2	2.45	0.46
1:A:559:LEU:HD23	1:A:593:PHE:CE1	2.50	0.46
1:A:728:ARG:NH1	1:A:759:GLU:OE1	2.49	0.46
1:B:778:LEU:HD23	1:B:973:LEU:HD23	1.97	0.46
1:A:1028:GLU:OE1	1:A:1028:GLU:N	2.37	0.46
1:A:400:LEU:HD13	1:A:463:ALA:HA	1.97	0.46
1:A:741:LEU:O	1:A:741:LEU:HD12	2.16	0.46
1:A:328:LEU:HD11	1:A:381:TYR:CE2	2.51	0.46
1:A:1021:LEU:CD2	1:A:1025:LEU:HD12	2.44	0.46
1:A:401:LEU:HD22	1:A:417:LEU:HD23	1.97	0.46
1:A:860:MET:HB2	1:A:892:LYS:HE2	1.96	0.46
1:B:442:THR:HB	1:B:461:ILE:HD13	1.98	0.46
1:A:277:PHE:CE1	1:A:289:PHE:HB3	2.50	0.46
1:A:430:MET:HE3	1:A:431:GLU:H	1.80	0.46
1:A:660:THR:OG1	1:A:668:TYR:CD2	2.69	0.46
1:A:427:ALA:O	1:A:439:ARG:HG3	2.15	0.46
1:B:210:HIS:HB2	1:B:307:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:TYR:CE1	1:B:688:LEU:HD11	2.51	0.46
1:B:923:LYS:O	1:B:927:ILE:HG13	2.16	0.46
1:A:716:LEU:O	1:A:720:PRO:HG3	2.16	0.45
1:B:237:TYR:CE1	1:B:239:TYR:CD2	3.04	0.45
1:B:426:GLU:OE2	1:B:439:ARG:NH2	2.48	0.45
1:B:762:THR:HA	1:B:765:ILE:HG22	1.97	0.45
1:B:776:TYR:CE1	1:B:788:ALA:HB1	2.52	0.45
1:A:320:ILE:HA	1:A:345:GLN:HA	1.97	0.45
1:A:692:VAL:HG12	1:A:702:VAL:HG21	1.98	0.45
1:A:750:PHE:CD1	1:A:753:ILE:HD11	2.50	0.45
1:B:296:PRO:HG2	1:B:541:GLU:OE1	2.16	0.45
1:A:213:GLY:O	6:A:1116:NAG:H62	2.16	0.45
1:B:438:PHE:CE1	1:B:465:GLU:HG3	2.51	0.45
1:B:968:ALA:O	1:B:972:TYR:HB3	2.16	0.45
1:A:331:MET:HG2	1:A:351:SER:OG	2.16	0.45
1:A:436:LEU:HB3	1:A:438:PHE:HE1	1.81	0.45
1:A:617:PRO:HB3	1:A:652:TRP:CE3	2.51	0.45
1:A:623:LYS:HB3	1:A:708:ASP:OD2	2.16	0.45
1:B:381:TYR:CB	1:B:420:VAL:HG23	2.47	0.45
1:B:694:ILE:HG23	1:B:727:ASP:OD2	2.17	0.45
1:A:485:LEU:HD13	1:A:584:ILE:HD12	1.97	0.45
1:B:482:ASP:HB3	1:B:485:LEU:CD1	2.42	0.45
1:B:977:LYS:HE3	1:B:980:LEU:HD23	1.99	0.45
1:A:446:ASP:O	1:A:450:SER:HB3	2.17	0.45
1:A:550:PHE:HA	1:A:553:SER:HB3	1.99	0.45
1:A:617:PRO:HD3	1:A:652:TRP:CD2	2.52	0.45
12:B:1118:PEG:H41	12:B:1118:PEG:H21	1.42	0.45
1:B:662:GLY:HA3	1:B:685:GLU:OE2	2.18	0.45
1:B:295:GLU:HG3	1:B:296:PRO:HD3	1.98	0.44
1:B:487:GLU:HB3	1:B:549:TYR:CD2	2.52	0.44
1:B:339:LEU:HA	1:B:339:LEU:HD12	1.71	0.44
1:B:976:THR:HG22	1:B:978:THR:N	2.31	0.44
1:A:750:PHE:CE1	1:A:753:ILE:HD11	2.53	0.44
1:B:808:TRP:CZ2	1:B:824:LEU:HD22	2.52	0.44
1:A:941:ALA:O	1:A:945:VAL:HG23	2.17	0.44
1:B:339:LEU:HD23	1:B:343:LEU:HD23	1.98	0.44
1:A:318:LYS:HA	1:A:347:GLU:HA	1.99	0.44
1:A:384:PRO:O	1:A:387:ILE:HG12	2.18	0.44
1:A:808:TRP:CZ3	1:A:824:LEU:HD13	2.53	0.44
1:B:272:TYR:OH	1:B:296:PRO:HB2	2.18	0.44
1:B:715:GLN:OE1	1:B:722:VAL:HG21	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:LYS:HD3	1:B:880:LYS:HA	1.78	0.44
1:B:901:GLU:HA	1:B:936:PRO:HG3	1.98	0.44
1:B:542:GLU:OE2	1:B:997:LEU:HD22	2.18	0.44
1:B:657:SER:O	1:B:693:ASN:N	2.50	0.44
1:B:841:LYS:HD3	1:B:841:LYS:HA	1.71	0.44
1:A:185:LEU:HD13	1:A:288:TYR:HB2	2.00	0.44
1:B:211:SER:HB3	1:B:243:ILE:HG23	2.00	0.44
1:B:524:LEU:HB3	1:B:1005:GLU:OE1	2.18	0.44
1:A:451:SER:OG	1:A:452:MET:N	2.51	0.44
1:A:986:PHE:O	1:A:989:ASN:HB2	2.17	0.44
1:B:381:TYR:HB2	1:B:420:VAL:HG23	2.00	0.44
1:B:685:GLU:O	1:B:687:VAL:HG13	2.18	0.44
1:B:941:ALA:O	1:B:945:VAL:HG23	2.18	0.44
1:A:307:ASP:HA	1:A:356:THR:HG21	2.00	0.44
1:A:412:TYR:CE2	1:A:414:LEU:HB2	2.53	0.44
1:A:513:ASP:O	1:A:517:LYS:HD3	2.18	0.44
1:B:182:HIS:O	1:B:190:PHE:HA	2.18	0.44
1:A:518:THR:OG1	1:A:546:SER:HB3	2.18	0.43
1:A:663:ARG:HG2	1:A:688:LEU:HD21	2.00	0.43
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.87	0.43
1:A:880:LYS:HA	1:A:880:LYS:HE2	2.00	0.43
1:A:950:ASN:O	1:A:954:GLN:HG3	2.17	0.43
1:B:967:VAL:O	1:B:971:THR:HG23	2.18	0.43
1:B:422:ILE:HD11	1:B:437:THR:HB	2.00	0.43
1:B:469:GLN:O	1:B:473:ASN:HB2	2.18	0.43
1:B:568:PHE:CE1	1:B:593:PHE:HZ	2.36	0.43
1:B:956:PHE:HA	1:B:957:PRO:HD3	1.76	0.43
1:A:515:ARG:NH2	1:A:557:LEU:HD23	2.33	0.43
1:A:223:SER:HB3	1:A:257:TYR:CD2	2.53	0.43
1:A:720:PRO:HG2	1:A:758:ASN:HB2	2.00	0.43
1:A:870:THR:HG22	1:A:873:GLY:H	1.82	0.43
4:B:1101[B]:ONN:N18	4:B:1101[B]:ONN:C11	2.80	0.43
1:A:661:GLU:HB2	1:A:689:TRP:CZ2	2.53	0.43
1:A:724:SER:HB2	1:A:727:ASP:HB2	2.00	0.43
1:B:811:GLU:O	1:B:820:ARG:NH2	2.51	0.43
1:B:204:THR:O	1:B:251:LEU:HB2	2.19	0.43
1:B:608:LYS:HG2	1:B:612:LEU:HD12	2.01	0.43
1:B:634:ARG:CD	1:B:652:TRP:HH2	2.27	0.43
1:A:181:LEU:HA	1:A:192:GLY:HA2	2.01	0.43
1:A:216:ILE:HD13	1:A:263:TYR:CB	2.48	0.43
1:A:335:SER:CB	1:A:347:GLU:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:LEU:O	1:A:878:LEU:HD12	2.19	0.43
1:B:787:LEU:HD11	1:B:1022:THR:HA	2.01	0.43
1:B:634:ARG:HD3	1:B:652:TRP:CH2	2.42	0.43
1:A:1013:TRP:HH2	1:A:1021:LEU:HD12	1.83	0.43
1:A:796:PHE:HB2	1:A:832:LEU:HD13	2.01	0.43
1:B:445:TYR:CE2	1:B:455:ARG:HB2	2.54	0.43
1:B:656:LEU:HD11	1:B:674:LEU:CB	2.49	0.43
1:A:168:LEU:HA	1:A:169:PRO:HD2	1.86	0.43
1:A:320:ILE:HG12	1:A:345:GLN:HB2	2.01	0.43
1:A:367:LYS:CB	1:A:387:ILE:HG21	2.49	0.43
1:A:511:PHE:HE1	1:A:553:SER:HG	1.66	0.43
1:A:801:ASN:O	1:A:805:GLN:HG2	2.19	0.43
1:B:299:ALA:HB3	1:B:307:ASP:OD2	2.19	0.43
1:B:707:ASP:O	1:B:711:ALA:N	2.48	0.43
1:B:765:ILE:HD11	1:B:823:LEU:HD21	2.01	0.43
1:A:410:ILE:HG13	1:A:577:HIS:CE1	2.55	0.42
1:A:756:LEU:HD22	1:A:798:LEU:CD2	2.48	0.42
1:B:530:ILE:HD11	1:B:611:THR:HG22	2.01	0.42
1:B:847:MET:HE3	1:B:872:LYS:HG2	2.01	0.42
1:B:847:MET:HG3	1:B:876:PHE:CG	2.54	0.42
1:A:538:GLU:O	1:A:542:GLU:HG3	2.19	0.42
1:B:656:LEU:N	1:B:656:LEU:CD1	2.81	0.42
1:B:694:ILE:O	1:B:697:ASN:ND2	2.50	0.42
1:B:715:GLN:O	1:B:718:ILE:HG13	2.19	0.42
1:B:762:THR:O	1:B:765:ILE:HG22	2.20	0.42
1:B:806:GLN:OE1	1:B:820:ARG:HA	2.19	0.42
2:E:2:NAG:H82	2:E:2:NAG:O3	2.19	0.42
1:B:263:TYR:CE1	1:B:304:PRO:HD3	2.54	0.42
1:B:179:LEU:HD12	1:B:194:VAL:HG22	2.02	0.42
1:B:308:GLU:HB2	1:B:311:PHE:CD2	2.54	0.42
1:B:423:PRO:HA	1:B:440:GLU:HG3	2.01	0.42
1:B:624:LYS:O	1:B:627:GLU:HG2	2.20	0.42
1:B:403:PHE:CG	1:B:501:ILE:HD11	2.54	0.42
1:B:924:LEU:HD12	1:B:924:LEU:O	2.19	0.42
1:A:469:GLN:OE1	1:A:469:GLN:HA	2.20	0.42
1:B:328:LEU:HB2	1:B:362:ILE:HB	2.02	0.42
1:A:660:THR:HB	1:A:687:VAL:HG11	2.00	0.42
1:B:205:TRP:CH2	1:B:250:ALA:HB2	2.54	0.42
1:B:469:GLN:HB2	1:B:470:TRP:CE3	2.55	0.42
1:A:560:LYS:HE3	1:A:565:GLU:HG3	2.01	0.42
1:B:168:LEU:HD21	1:B:209:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLY:HA2	1:B:798:LEU:O	2.20	0.42
1:B:685:GLU:OE1	1:B:685:GLU:N	2.53	0.42
1:B:809:THR:HB	1:B:811:GLU:HG3	2.02	0.42
1:B:957:PRO:O	1:B:958:LEU:HB3	2.20	0.42
1:A:322:ASP:OD1	2:C:1:NAG:N2	2.53	0.42
1:A:534:VAL:HG12	1:A:540:ILE:HG13	2.02	0.42
1:A:776:TYR:CE2	1:A:788:ALA:HB1	2.55	0.42
1:B:309:PRO:O	1:B:355:SER:HB3	2.20	0.42
1:A:746:LEU:HD22	1:A:1017:ASN:HB3	2.01	0.41
1:B:559:LEU:HA	1:B:559:LEU:HD12	1.83	0.41
1:A:806:GLN:HA	1:A:806:GLN:OE1	2.19	0.41
4:B:1101[B]:ONN:C19	4:B:1101[B]:ONN:C27	2.98	0.41
1:B:431:GLU:OE1	1:B:468:HIS:CG	2.74	0.41
1:B:454:ASP:OD2	1:B:888:ALA:HB1	2.19	0.41
1:B:459:THR:HG21	1:B:505:LEU:CD2	2.50	0.41
1:B:551:LYS:HG2	1:B:555:LEU:HD13	2.00	0.41
1:B:604:LYS:HA	1:B:604:LYS:HD3	1.87	0.41
1:A:490:ALA:O	1:A:494:GLU:N	2.51	0.41
1:A:813:THR:O	1:A:816:MET:N	2.53	0.41
1:B:419:LEU:HG	1:B:438:PHE:CE2	2.49	0.41
1:B:438:PHE:CD2	1:B:443:LEU:HG	2.55	0.41
1:B:551:LYS:HG3	1:B:699:TYR:CZ	2.55	0.41
1:B:942:TRP:CE2	1:B:946:LYS:HD2	2.56	0.41
1:A:403:PHE:HB2	1:A:501:ILE:CD1	2.49	0.41
1:A:440:GLU:HG3	1:A:887:GLU:HG2	2.02	0.41
1:A:948:ASN:HD22	1:A:948:ASN:HA	1.64	0.41
1:B:321:ARG:NH2	1:B:321:ARG:HG3	2.36	0.41
1:A:365:GLU:O	1:A:384:PRO:HD3	2.20	0.41
1:A:725:ASP:N	1:A:725:ASP:OD1	2.45	0.41
1:A:741:LEU:HD12	1:A:741:LEU:C	2.40	0.41
1:A:476:THR:OG1	1:A:477:MET:N	2.53	0.41
1:B:665:TYR:HE1	1:B:688:LEU:HD11	1.85	0.41
1:A:951:LYS:HB3	1:A:951:LYS:HE3	1.89	0.41
1:A:865:LYS:HD3	1:A:899:SER:CB	2.51	0.41
1:B:439:ARG:NH1	1:B:441:GLU:OE1	2.54	0.41
1:B:663:ARG:NH2	1:B:686:GLU:HB3	2.36	0.41
1:B:881:TYR:CD1	1:B:881:TYR:C	2.93	0.41
1:B:161:PHE:CE1	1:B:237:TYR:HB2	2.55	0.41
1:B:964:GLN:HG3	1:B:999:CYS:HB2	2.03	0.41
1:A:185:LEU:HA	1:A:185:LEU:HD23	1.86	0.41
1:A:468:HIS:HA	1:A:471:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:GLU:O	1:A:1006:VAL:HG23	2.21	0.41
1:A:740:GLY:HA2	1:A:1013:TRP:CD1	2.56	0.41
1:B:536:SER:O	1:B:540:ILE:HG13	2.21	0.41
1:A:360:ALA:HB1	1:A:435:LEU:HD23	2.02	0.40
1:A:908:TRP:CE3	1:A:909:LEU:HD23	2.56	0.40
1:B:984:GLN:HG2	1:B:1004:LEU:HD11	2.03	0.40
1:B:515:ARG:NH2	1:B:557:LEU:HD23	2.37	0.40
1:B:630:ILE:HG21	1:B:656:LEU:HD21	2.02	0.40
1:B:845:ASP:HB3	1:B:853:GLN:OE1	2.21	0.40
1:B:874:TRP:CE2	1:B:897:LEU:HD22	2.55	0.40
1:B:914:LEU:HA	1:B:924:LEU:HD22	2.01	0.40
1:B:168:LEU:CD1	1:B:210:HIS:NE2	2.82	0.40
1:B:321:ARG:NH2	1:B:325:TYR:O	2.54	0.40
1:B:769:LEU:O	1:B:773:ASP:N	2.45	0.40
1:A:537:SER:O	1:A:541:GLU:HG2	2.22	0.40
1:A:626:LYS:O	1:A:683:LEU:HB2	2.22	0.40
1:B:865:LYS:HG2	1:B:896:ALA:HA	2.03	0.40
1:B:910:MET:HB3	1:B:944:PHE:CE2	2.56	0.40
1:A:161:PHE:HE1	1:A:244:ALA:N	2.20	0.40
1:A:616:PHE:CD1	1:A:616:PHE:N	2.88	0.40
1:A:746:LEU:HD21	1:A:1021:LEU:HG	2.04	0.40
1:A:956:PHE:CD1	1:A:962:THR:HG21	2.57	0.40
1:B:412:TYR:OH	1:B:434:GLY:HA2	2.21	0.40
1:B:743:LYS:HA	1:B:743:LYS:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	854/912 (94%)	811 (95%)	36 (4%)	7 (1%)	19 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	847/912 (93%)	813 (96%)	30 (4%)	4 (0%)	29 67
All	All	1701/1824 (93%)	1624 (96%)	66 (4%)	11 (1%)	25 64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	PRO
1	B	664	ASN
1	A	697	ASN
1	A	425	PHE
1	A	918	ASN
1	A	249	GLU
1	A	183	PRO
1	B	339	LEU
1	B	295	GLU
1	A	814	PRO
1	A	296	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	742/813 (91%)	722 (97%)	20 (3%)	44 75
1	B	738/813 (91%)	714 (97%)	24 (3%)	38 71
All	All	1480/1626 (91%)	1436 (97%)	44 (3%)	41 73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	193	SER
1	A	197	SER
1	A	226	SER
1	A	237	TYR

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Mol	Chain	Res	Type
1	A	272	TYR
1	A	274	PHE
1	A	334	LYS
1	A	361	PHE
1	A	448	ASN
1	A	451	SER
1	A	489	PHE
1	A	594	ASN
1	A	598	ASN
1	A	599	GLN
1	A	636	PHE
1	A	668	TYR
1	A	696	MET
1	A	948	ASN
1	A	1026	ARG
1	B	221	PHE
1	B	272	TYR
1	B	301	SER
1	B	341	ASP
1	B	371	GLN
1	B	418	ASP
1	B	433	TRP
1	B	443	LEU
1	B	489	PHE
1	B	510	ASP
1	B	520	LYS
1	B	529	PRO
1	B	604	LYS
1	B	668	TYR
1	B	715	GLN
1	B	755	TYR
1	B	786	ASP
1	B	789	SER
1	B	801	ASN
1	B	875	SER
1	B	900	SER
1	B	912	SER
1	B	913	SER
1	B	972	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	733	ASN
1	A	948	ASN
1	B	324	GLN
1	B	777	ASN
1	B	891	ASN
1	B	990	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	0.34	0	17,19,21	0.61	0
2	NAG	C	2	2	14,14,15	2.16	2 (14%)	17,19,21	1.74	3 (17%)
3	NAG	D	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	1.64	3 (17%)
3	NAG	D	2	3	14,14,15	0.16	0	17,19,21	0.62	0
3	BMA	D	3	3	11,11,12	1.17	2 (18%)	15,15,17	1.08	1 (6%)
2	NAG	E	1	1,2	14,14,15	1.83	2 (14%)	17,19,21	1.33	2 (11%)
2	NAG	E	2	2	14,14,15	0.84	2 (14%)	17,19,21	1.00	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.38	0	17,19,21	0.93	1 (5%)
2	NAG	F	2	2	14,14,15	0.91	1 (7%)	17,19,21	0.80	0
2	NAG	G	1	1,2	14,14,15	0.94	2 (14%)	17,19,21	1.18	1 (5%)
2	NAG	G	2	2	14,14,15	0.94	1 (7%)	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	H	1	1,3	14,14,15	1.25	1 (7%)	17,19,21	1.90	4 (23%)
3	NAG	H	2	3	14,14,15	0.68	1 (7%)	17,19,21	1.19	1 (5%)
3	BMA	H	3	3	11,11,12	0.91	1 (9%)	15,15,17	1.66	5 (33%)
2	NAG	I	1	1,2	14,14,15	1.26	1 (7%)	17,19,21	2.19	5 (29%)
2	NAG	I	2	2	14,14,15	1.17	1 (7%)	17,19,21	2.65	2 (11%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	7.61	1.55	1.43
2	E	1	NAG	O5-C1	5.81	1.53	1.43
3	H	1	NAG	O5-C1	-4.31	1.36	1.43
2	I	2	NAG	O5-C1	4.00	1.50	1.43
2	E	1	NAG	C1-C2	3.46	1.57	1.52
2	G	2	NAG	O5-C1	3.44	1.49	1.43
3	D	1	NAG	O5-C1	3.39	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-3.05	1.38	1.43
2	F	2	NAG	O5-C1	-2.87	1.39	1.43
2	G	1	NAG	O5-C1	2.58	1.47	1.43
3	H	3	BMA	C1-C2	2.40	1.57	1.52
3	H	2	NAG	O5-C1	-2.36	1.39	1.43
2	G	1	NAG	C1-C2	2.28	1.55	1.52
3	D	3	BMA	O5-C5	2.16	1.47	1.43
2	C	2	NAG	C1-C2	2.14	1.55	1.52
2	E	2	NAG	C1-C2	2.07	1.55	1.52
3	D	3	BMA	C2-C3	-2.05	1.49	1.52
2	E	2	NAG	O5-C1	2.02	1.46	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C2-N2-C7	9.50	136.43	122.90
2	I	1	NAG	C2-N2-C7	5.68	130.99	122.90
3	H	1	NAG	O4-C4-C5	-5.40	95.89	109.30
3	D	1	NAG	C2-N2-C7	4.70	129.60	122.90
2	C	2	NAG	C2-N2-C7	4.34	129.09	122.90
2	G	1	NAG	O4-C4-C3	-4.25	100.52	110.35
2	C	2	NAG	C1-C2-N2	4.13	117.55	110.49
3	H	2	NAG	C1-O5-C5	4.00	117.61	112.19
2	I	1	NAG	O4-C4-C3	3.75	119.01	110.35
3	H	1	NAG	C1-O5-C5	-3.66	107.23	112.19
2	E	1	NAG	O4-C4-C3	-3.53	102.18	110.35
3	H	3	BMA	C1-C2-C3	3.53	114.00	109.67
2	I	2	NAG	C1-O5-C5	3.40	116.80	112.19
2	I	1	NAG	O3-C3-C2	3.26	116.21	109.47
3	H	1	NAG	C3-C4-C5	2.89	115.39	110.24
3	D	1	NAG	C1-C2-N2	2.76	115.21	110.49
2	F	1	NAG	C2-N2-C7	2.66	126.69	122.90
2	C	2	NAG	C1-O5-C5	2.62	115.74	112.19
3	H	3	BMA	O5-C5-C4	-2.61	104.48	110.83
2	I	1	NAG	C1-O5-C5	2.55	115.65	112.19
2	I	1	NAG	C1-C2-N2	-2.54	106.14	110.49
3	D	3	BMA	O2-C2-C3	-2.54	105.05	110.14
3	H	3	BMA	O5-C1-C2	2.50	114.63	110.77
3	H	1	NAG	O4-C4-C3	-2.49	104.60	110.35
3	D	1	NAG	C1-O5-C5	2.40	115.44	112.19
3	H	3	BMA	O5-C5-C6	2.38	110.94	107.20
2	E	1	NAG	O5-C5-C6	2.08	110.46	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	3	BMA	O2-C2-C3	-2.05	106.03	110.14
2	E	2	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (30) torsion outliers are listed below:

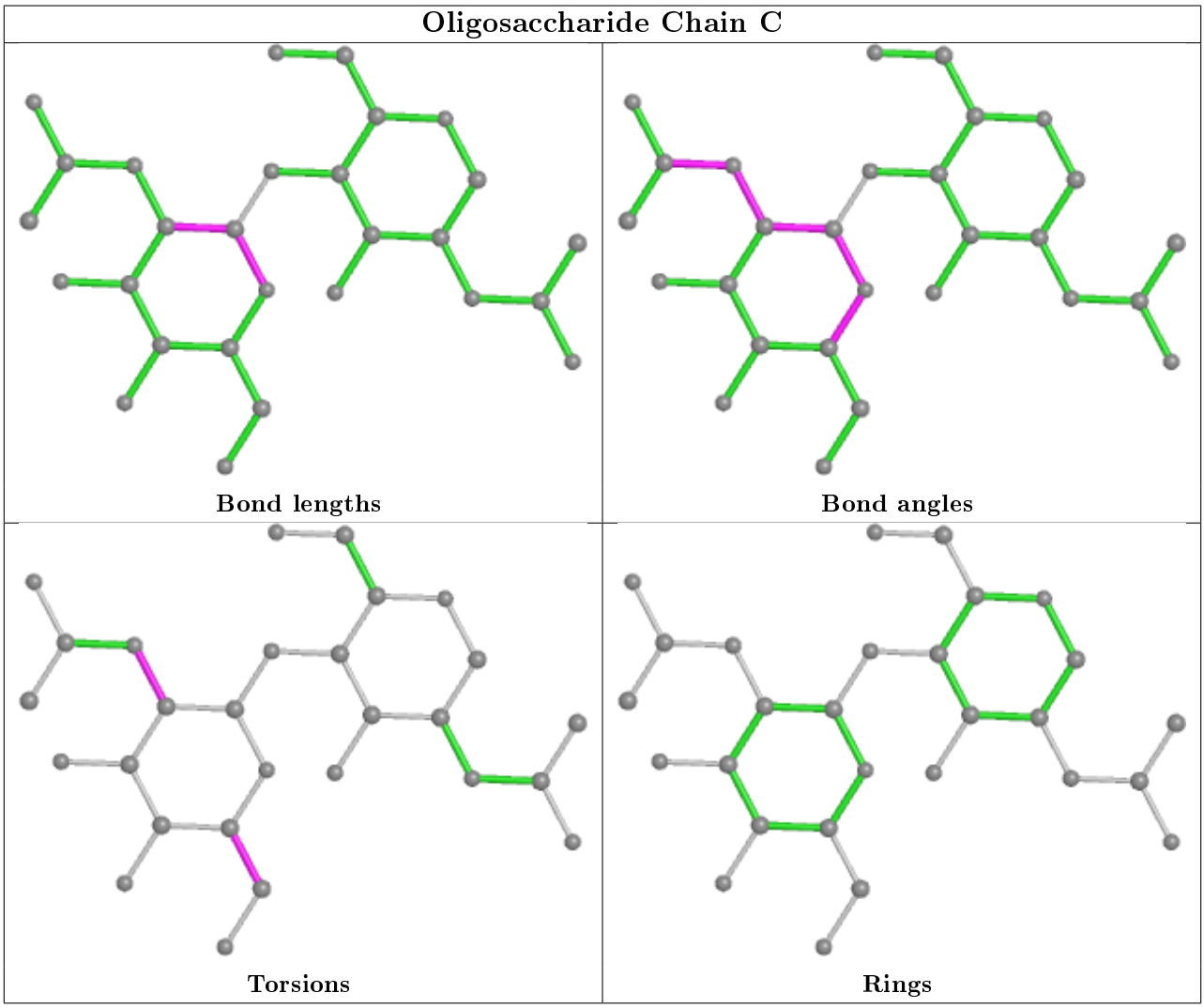
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2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

There are no ring outliers.

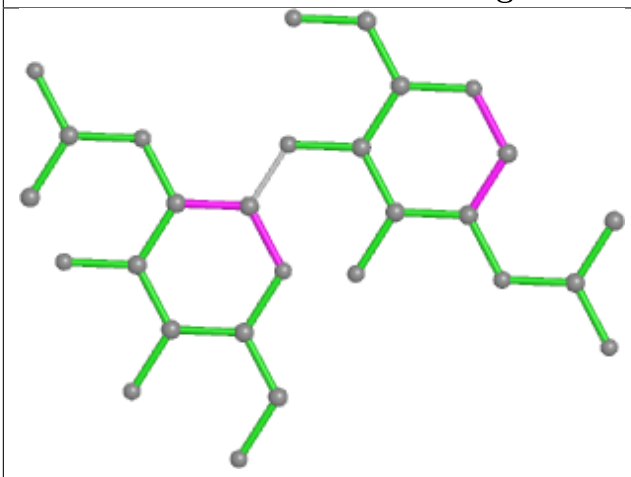
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
2	C	1	NAG	1	0
3	D	1	NAG	2	0
2	E	1	NAG	1	0
2	F	1	NAG	1	0
3	D	2	NAG	1	0
3	H	3	BMA	1	0
3	H	2	NAG	2	0

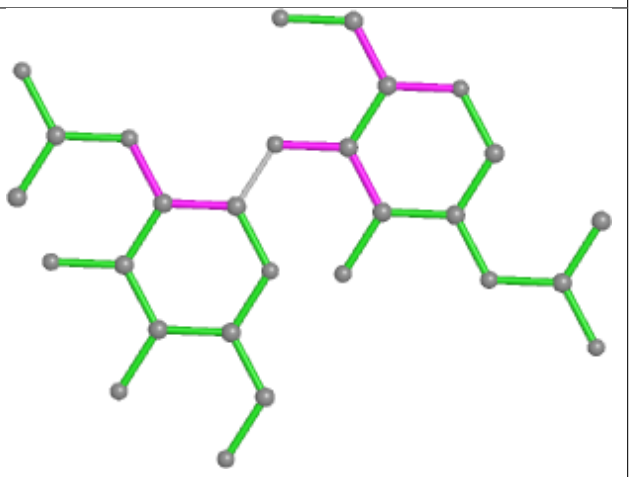
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



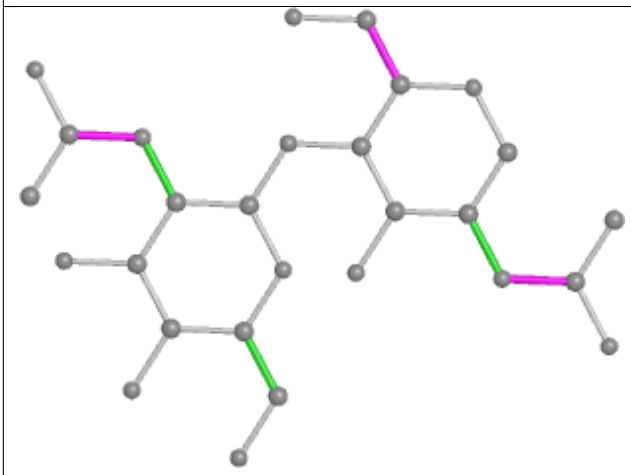
Oligosaccharide Chain E



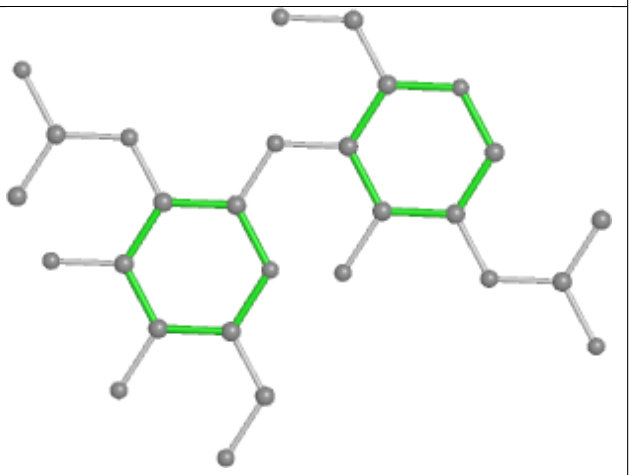
Bond lengths



Bond angles

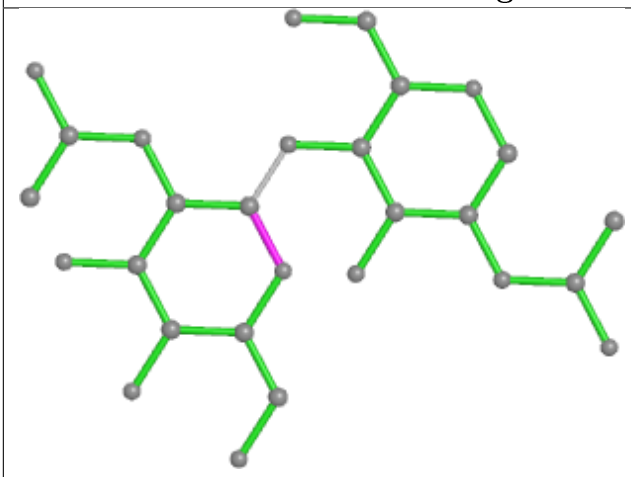


Torsions

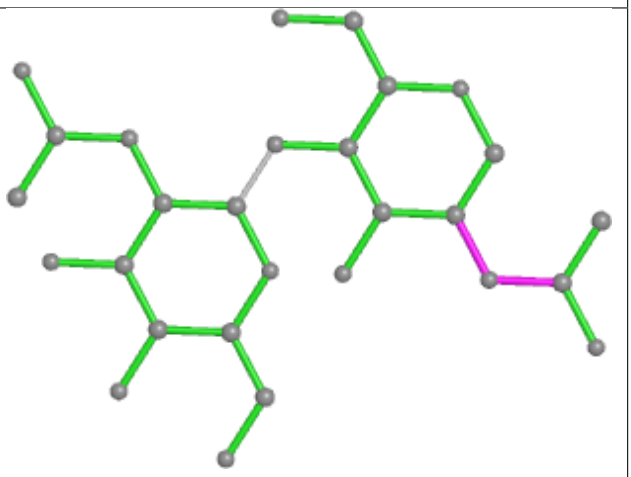


Rings

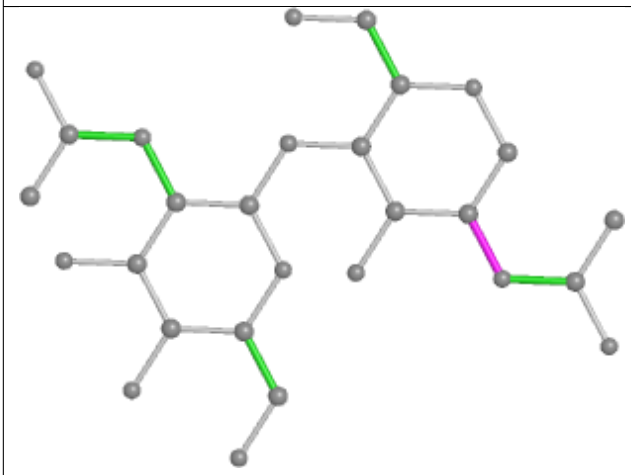
Oligosaccharide Chain F



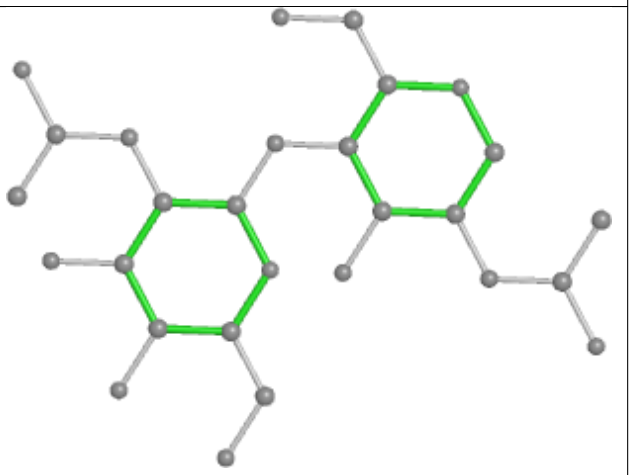
Bond lengths



Bond angles

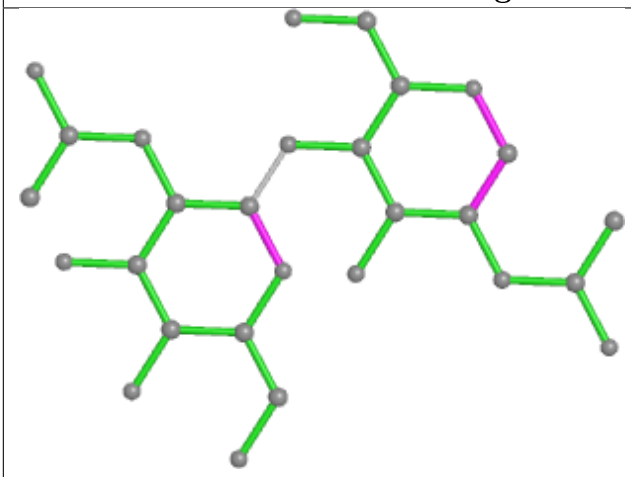


Torsions

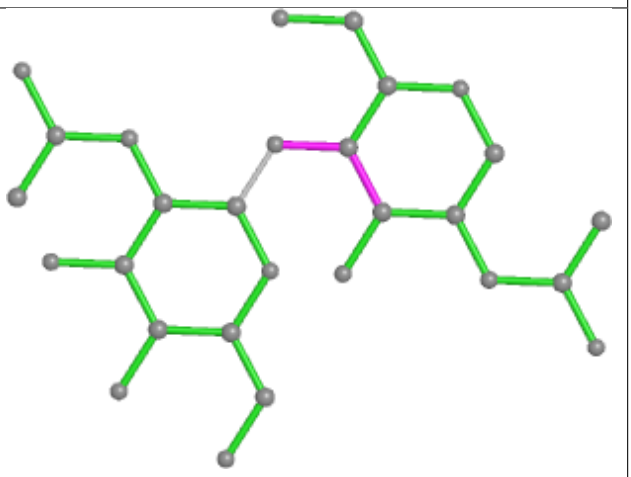


Rings

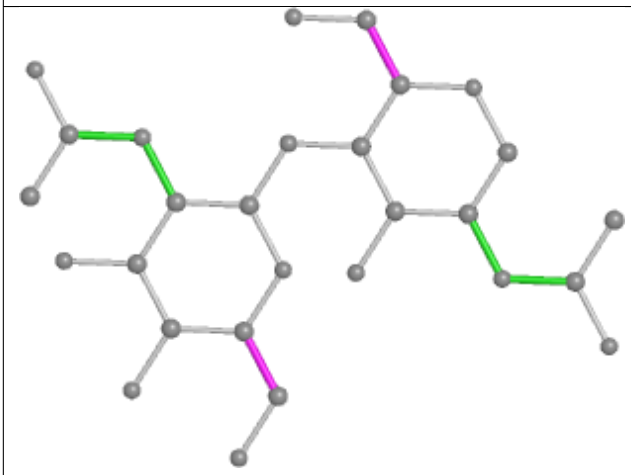
Oligosaccharide Chain G



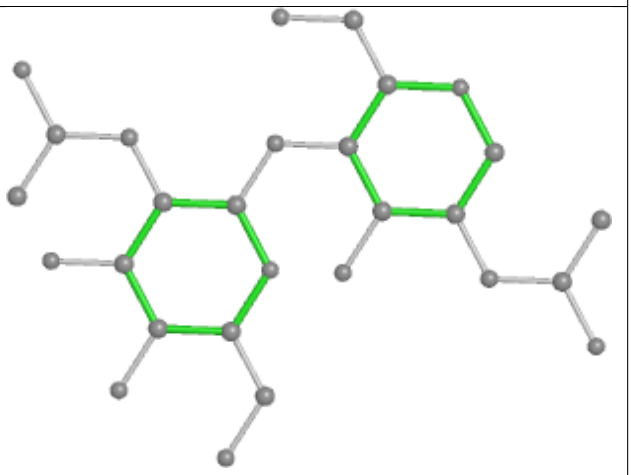
Bond lengths



Bond angles

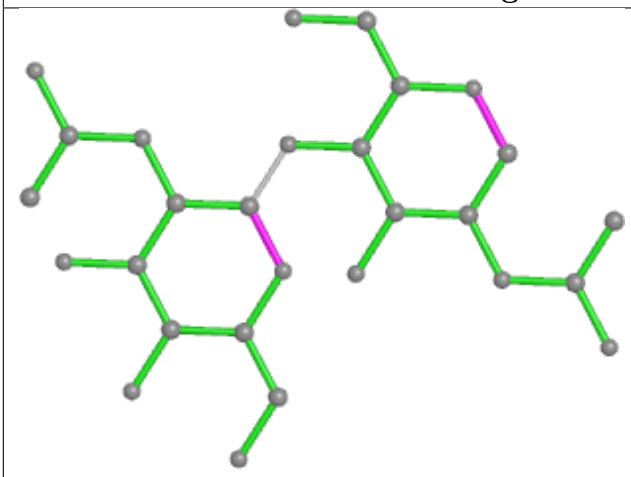


Torsions

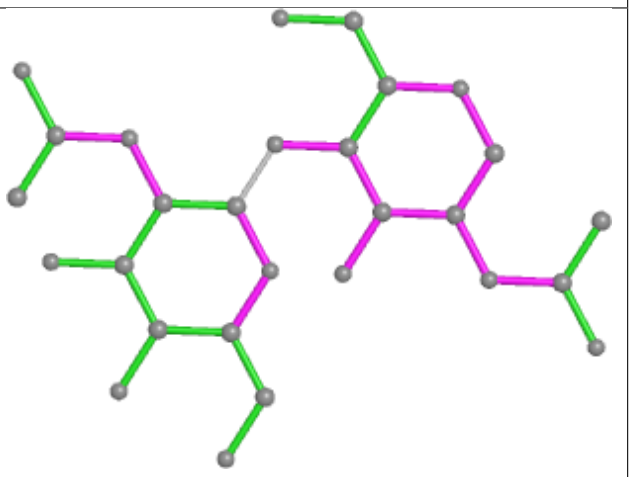


Rings

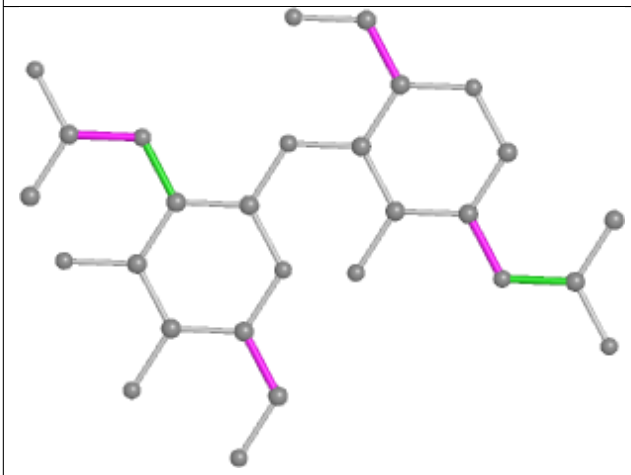
Oligosaccharide Chain I



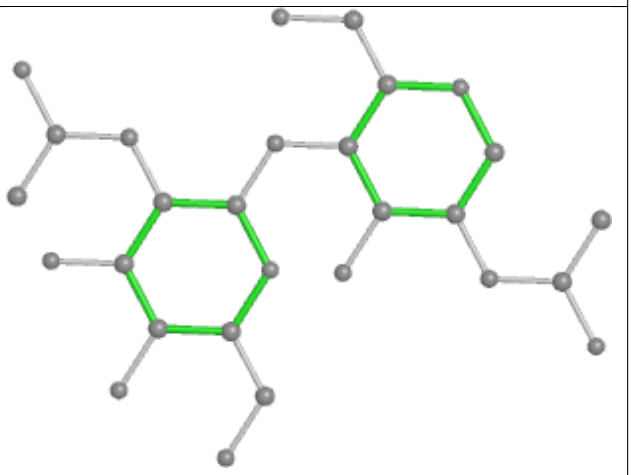
Bond lengths



Bond angles

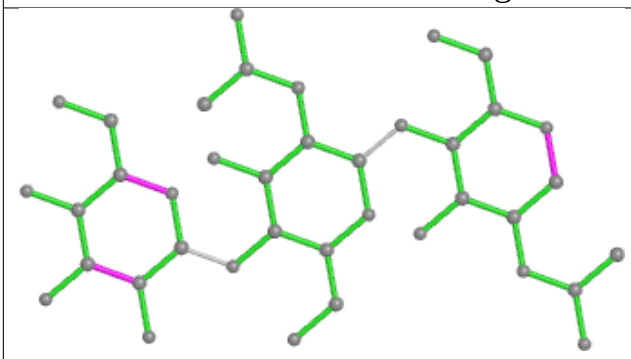


Torsions

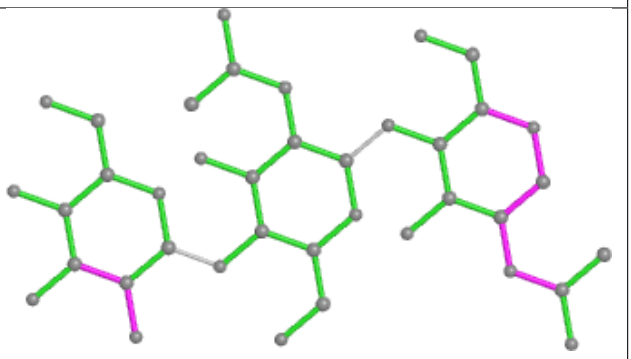


Rings

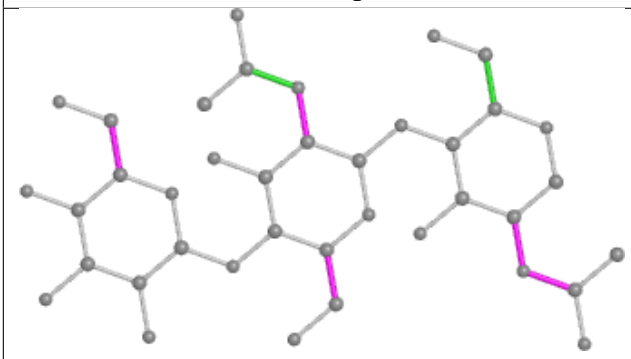
Oligosaccharide Chain D



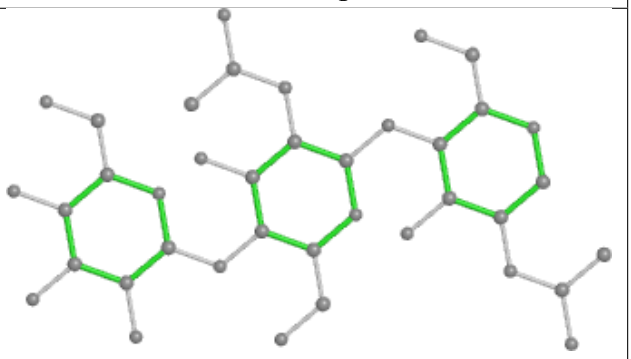
Bond lengths



Bond angles

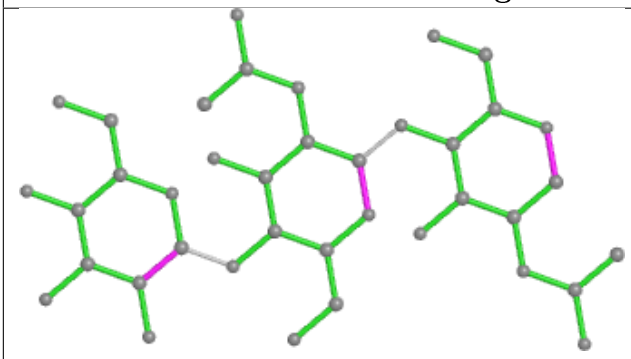


Torsions

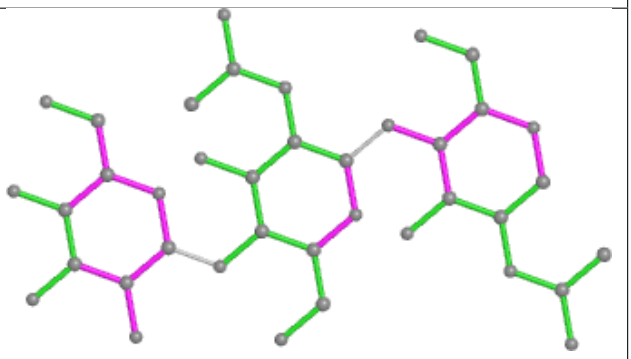


Rings

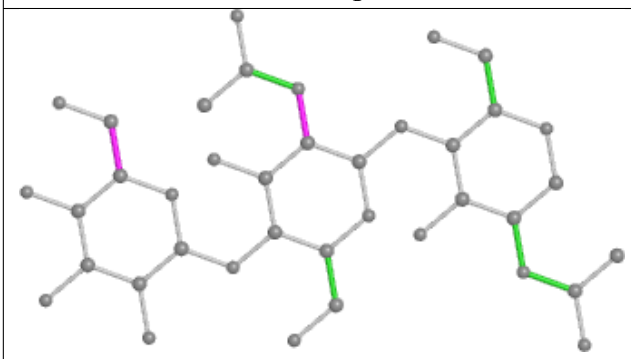
Oligosaccharide Chain H



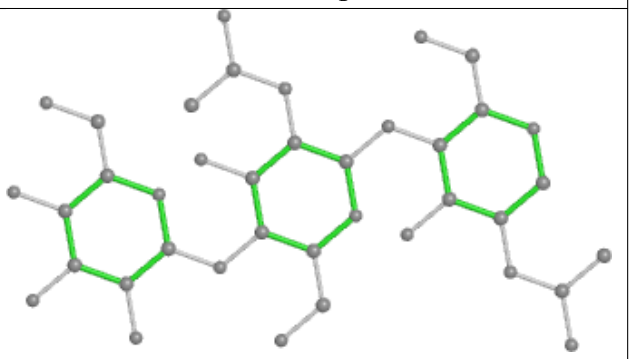
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PEG	B	1118	-	6,6,6	0.48	0	5,5,5	0.38	0
6	NAG	B	1106	1	14,14,15	1.55	1 (7%)	17,19,21	1.61	3 (17%)
4	ONN	A	1101[A]	5	37,40,40	2.96	12 (32%)	49,53,53	1.81	12 (24%)
4	ONN	A	1101[B]	5	37,40,40	2.94	12 (32%)	49,53,53	2.02	11 (22%)
10	PG4	A	1121	-	12,12,12	0.53	0	11,11,11	0.26	0
6	NAG	B	1110	1	14,14,15	0.43	0	17,19,21	0.66	0
6	NAG	A	1112	1	14,14,15	1.86	2 (14%)	17,19,21	1.31	2 (11%)
6	NAG	B	1113	1	14,14,15	0.44	0	17,19,21	0.67	0
6	NAG	A	1106	1	14,14,15	0.74	0	17,19,21	1.26	2 (11%)
4	ONN	B	1101[B]	5	37,40,40	2.95	12 (32%)	49,53,53	1.85	9 (18%)
4	ONN	B	1101[A]	5	37,40,40	2.92	11 (29%)	49,53,53	1.72	11 (22%)
8	EDO	B	1117	-	3,3,3	0.51	0	2,2,2	0.22	0
7	SIN	A	1117	-	1,7,7	0.11	0	2,8,8	1.59	1 (50%)
6	NAG	A	1116	1	14,14,15	1.95	2 (14%)	17,19,21	2.54	4 (23%)
8	EDO	A	1119	-	3,3,3	0.54	0	2,2,2	0.26	0
8	EDO	A	1118	-	3,3,3	0.39	0	2,2,2	0.70	0
8	EDO	B	1115	-	3,3,3	0.51	0	2,2,2	0.28	0
6	NAG	A	1105	1	14,14,15	0.90	1 (7%)	17,19,21	0.67	0
11	PO4	A	1122	-	4,4,4	0.87	0	6,6,6	0.61	0
6	NAG	B	1114	1	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
6	NAG	A	1115	1	14,14,15	1.66	2 (14%)	17,19,21	1.14	2 (11%)
6	NAG	B	1105	1	14,14,15	0.88	1 (7%)	17,19,21	1.30	2 (11%)
9	PGE	A	1120	-	9,9,9	0.55	0	8,8,8	0.60	0
8	EDO	B	1116	-	3,3,3	0.46	0	2,2,2	0.35	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
12	PEG	B	1118	-	-	2/4/4/4	-
6	NAG	B	1106	1	-	1/6/23/26	0/1/1/1
4	ONN	A	1101[A]	5	-	18/39/41/41	0/2/3/3
4	ONN	A	1101[B]	5	-	13/39/41/41	0/2/3/3
10	PG4	A	1121	-	-	8/10/10/10	-
6	NAG	B	1110	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1112	1	-	3/6/23/26	0/1/1/1
6	NAG	B	1113	1	-	3/6/23/26	0/1/1/1
6	NAG	A	1106	1	-	3/6/23/26	0/1/1/1
4	ONN	B	1101[B]	5	-	19/39/41/41	0/2/3/3
4	ONN	B	1101[A]	5	-	13/39/41/41	0/2/3/3
8	EDO	B	1117	-	-	1/1/1/1	-
7	SIN	A	1117	-	-	0/1/5/5	-
6	NAG	A	1116	1	-	1/6/23/26	0/1/1/1
8	EDO	A	1119	-	-	0/1/1/1	-
8	EDO	A	1118	-	-	0/1/1/1	-
8	EDO	B	1115	-	-	0/1/1/1	-
6	NAG	A	1105	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1114	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1115	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1105	1	-	0/6/23/26	0/1/1/1
9	PGE	A	1120	-	-	6/7/7/7	-
8	EDO	B	1116	-	-	0/1/1/1	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101[B]	ONN	C7-C6	7.97	1.53	1.38
4	A	1101[B]	ONN	C7-C6	7.88	1.53	1.38
4	A	1101[A]	ONN	C7-C6	7.86	1.53	1.38
4	B	1101[A]	ONN	C7-C6	7.69	1.52	1.38
4	B	1101[A]	ONN	C4-C5	7.52	1.53	1.38
4	B	1101[B]	ONN	C4-C5	7.36	1.53	1.38
4	A	1101[B]	ONN	C4-C5	7.30	1.52	1.38
4	A	1101[A]	ONN	C4-C5	7.29	1.52	1.38
4	A	1101[B]	ONN	C3-C2	6.73	1.53	1.38
4	B	1101[A]	ONN	C3-C2	6.72	1.53	1.38
4	A	1101[A]	ONN	C3-C2	6.65	1.53	1.38
4	B	1101[B]	ONN	C3-C2	6.62	1.53	1.38
4	B	1101[B]	ONN	C11-N13	6.46	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1116	NAG	O5-C1	-6.37	1.33	1.43
4	B	1101[A]	ONN	C16-N18	6.08	1.46	1.33
4	A	1101[A]	ONN	C31-N30	6.01	1.47	1.34
4	A	1101[A]	ONN	C16-N18	5.99	1.46	1.33
4	A	1101[B]	ONN	C16-N18	5.95	1.46	1.33
4	A	1101[A]	ONN	C11-N13	5.87	1.46	1.34
4	B	1101[B]	ONN	C31-N30	5.66	1.46	1.34
4	A	1101[B]	ONN	C31-N30	5.65	1.46	1.34
4	B	1101[A]	ONN	C11-N13	5.60	1.46	1.34
6	A	1115	NAG	O5-C1	5.55	1.52	1.43
4	A	1101[B]	ONN	C11-N13	5.53	1.45	1.34
6	B	1106	NAG	O5-C1	5.50	1.52	1.43
4	B	1101[A]	ONN	C31-N30	5.37	1.45	1.34
4	B	1101[B]	ONN	C16-N18	5.30	1.45	1.33
6	A	1112	NAG	C1-C2	5.07	1.59	1.52
6	A	1112	NAG	O5-C1	4.42	1.50	1.43
4	B	1101[B]	ONN	C3-C4	-3.77	1.31	1.38
4	A	1101[B]	ONN	C6-C5	-3.76	1.31	1.38
4	A	1101[A]	ONN	C3-C4	-3.76	1.31	1.38
4	B	1101[A]	ONN	C3-C4	-3.75	1.31	1.38
4	A	1101[B]	ONN	C3-C4	-3.72	1.32	1.38
4	B	1101[A]	ONN	C6-C5	-3.68	1.31	1.38
4	A	1101[A]	ONN	C6-C5	-3.62	1.32	1.38
4	B	1101[B]	ONN	C6-C5	-3.52	1.32	1.38
4	A	1101[A]	ONN	C7-C2	-3.19	1.32	1.38
6	B	1105	NAG	O5-C1	3.16	1.48	1.43
4	A	1101[B]	ONN	C7-C2	-3.03	1.32	1.38
4	B	1101[B]	ONN	C7-C2	-2.80	1.32	1.38
6	A	1105	NAG	O5-C1	-2.69	1.39	1.43
4	A	1101[B]	ONN	O17-C16	-2.68	1.18	1.23
4	B	1101[A]	ONN	C7-C2	-2.68	1.33	1.38
4	B	1101[A]	ONN	O17-C16	-2.64	1.18	1.23
6	A	1115	NAG	C1-C2	2.61	1.56	1.52
4	B	1101[A]	ONN	O33-C31	-2.49	1.18	1.23
4	B	1101[B]	ONN	O33-C31	-2.37	1.18	1.23
4	A	1101[B]	ONN	O12-C11	-2.35	1.18	1.23
6	A	1116	NAG	C3-C2	2.33	1.57	1.52
4	A	1101[A]	ONN	O17-C16	-2.29	1.18	1.23
4	A	1101[A]	ONN	O33-C31	-2.28	1.18	1.23
4	A	1101[B]	ONN	O33-C31	-2.28	1.18	1.23
4	A	1101[A]	ONN	O12-C11	-2.22	1.18	1.23
4	B	1101[B]	ONN	O12-C11	-2.19	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101[B]	ONN	O17-C16	-2.15	1.19	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1101[B]	ONN	C10-C9-N30	-7.75	101.14	110.11
6	A	1116	NAG	C1-C2-N2	-6.83	98.82	110.49
4	A	1101[B]	ONN	C9-C10-C11	-6.60	103.14	112.44
4	B	1101[A]	ONN	C10-C9-N30	-6.60	102.47	110.11
4	A	1101[B]	ONN	C10-C9-N30	-5.92	103.25	110.11
6	A	1116	NAG	C2-N2-C7	5.41	130.60	122.90
4	A	1101[A]	ONN	C9-C10-C11	-4.95	105.47	112.44
4	B	1101[B]	ONN	C9-C10-C11	-4.34	106.33	112.44
4	A	1101[B]	ONN	C9-N30-C31	4.26	129.99	123.20
4	A	1101[A]	ONN	C14-C16-N18	4.18	124.98	116.54
6	B	1106	NAG	C1-C2-N2	4.08	117.46	110.49
4	A	1101[B]	ONN	C10-C11-N13	4.02	121.59	116.33
4	A	1101[A]	ONN	C9-N30-C31	4.00	129.57	123.20
4	A	1101[B]	ONN	C20-C19-N18	-3.93	104.74	113.03
4	B	1101[B]	ONN	C9-N30-C31	3.74	129.16	123.20
4	B	1101[A]	ONN	C1-C9-C10	-3.43	105.16	111.04
4	B	1101[A]	ONN	C26-C21-C20	-3.43	118.38	122.48
6	B	1105	NAG	C1-O5-C5	3.40	116.79	112.19
4	B	1101[B]	ONN	O12-C11-C10	-3.36	116.57	121.50
6	A	1112	NAG	C2-N2-C7	3.12	127.35	122.90
4	A	1101[B]	ONN	O12-C11-C10	-3.12	116.93	121.50
4	A	1101[A]	ONN	C14-N13-C11	3.07	129.54	121.65
6	B	1114	NAG	C1-C2-N2	3.04	115.69	110.49
4	B	1101[A]	ONN	C19-C20-C21	-3.03	118.13	122.72
6	B	1106	NAG	C1-O5-C5	3.03	116.30	112.19
4	B	1101[A]	ONN	C15-S38-S37	3.02	111.64	103.82
6	A	1106	NAG	O4-C4-C3	-2.99	103.43	110.35
4	A	1101[A]	ONN	C19-C20-C21	-2.92	118.31	122.72
6	A	1116	NAG	O3-C3-C4	-2.90	103.64	110.35
4	A	1101[A]	ONN	C15-S38-S37	2.88	111.28	103.82
4	B	1101[B]	ONN	C1-C9-N30	2.85	115.86	110.39
4	B	1101[A]	ONN	C32-C31-N30	2.77	119.99	116.15
4	B	1101[B]	ONN	C10-C11-N13	2.76	119.94	116.33
4	A	1101[A]	ONN	O17-C16-N18	-2.74	117.11	122.99
4	A	1101[A]	ONN	C19-N18-C16	2.70	126.23	122.34
6	A	1116	NAG	C1-O5-C5	2.67	115.82	112.19
4	B	1101[A]	ONN	C16-C14-N13	-2.65	103.95	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1101[A]	ONN	C19-N18-C16	2.62	126.10	122.34
4	B	1101[B]	ONN	C15-S38-S37	2.55	110.44	103.82
4	A	1101[B]	ONN	C1-C9-N30	2.54	115.27	110.39
4	A	1101[B]	ONN	C15-S38-S37	2.53	110.36	103.82
6	A	1112	NAG	C1-O5-C5	2.50	115.58	112.19
4	B	1101[B]	ONN	C26-C21-C20	2.42	125.38	122.48
4	A	1101[A]	ONN	C32-C31-N30	2.41	119.50	116.15
4	A	1101[A]	ONN	C26-C21-C20	-2.39	119.62	122.48
4	A	1101[B]	ONN	C14-C16-N18	2.36	121.30	116.54
4	A	1101[A]	ONN	C2-C1-C9	-2.23	108.71	113.78
6	A	1115	NAG	O4-C4-C3	-2.23	105.19	110.35
4	A	1101[A]	ONN	C1-C9-N30	2.23	114.67	110.39
4	B	1101[B]	ONN	C19-N18-C16	-2.21	119.16	122.34
6	B	1105	NAG	C3-C4-C5	-2.21	106.30	110.24
4	A	1101[B]	ONN	C15-C14-N13	2.20	116.95	111.00
4	B	1101[A]	ONN	C20-C19-N18	-2.19	108.41	113.03
6	B	1114	NAG	C1-O5-C5	2.19	115.16	112.19
6	A	1106	NAG	O3-C3-C4	-2.13	105.43	110.35
6	B	1106	NAG	O3-C3-C4	2.11	115.23	110.35
6	A	1115	NAG	C2-N2-C7	2.09	125.89	122.90
4	A	1101[B]	ONN	C35-C32-C31	-2.06	106.39	110.85
7	A	1117	SIN	C2-C3-C4	-2.05	109.24	112.67
4	B	1101[A]	ONN	O17-C16-C14	-2.02	116.19	120.45
4	B	1101[A]	ONN	C9-N30-C31	2.01	126.41	123.20

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101[A]	ONN	C16-C14-C15-S38
4	A	1101[A]	ONN	N13-C14-C15-S38
4	A	1101[A]	ONN	C16-C14-N13-C11
4	A	1101[A]	ONN	N30-C31-C32-C35
4	A	1101[A]	ONN	O33-C31-C32-C35
4	A	1101[A]	ONN	C31-C32-C35-C36
4	A	1101[A]	ONN	N34-C32-C35-C36
4	A	1101[A]	ONN	C35-C36-S37-S38
4	A	1101[A]	ONN	C1-C9-N30-C31
4	A	1101[B]	ONN	C16-C14-C15-S38
4	A	1101[B]	ONN	N13-C14-C15-S38
4	A	1101[B]	ONN	N30-C31-C32-C35
4	A	1101[B]	ONN	N30-C31-C32-N34

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Mol	Chain	Res	Type	Atoms
4	A	1101[B]	ONN	O33-C31-C32-C35
4	A	1101[B]	ONN	C31-C32-C35-C36
4	A	1101[B]	ONN	N34-C32-C35-C36
4	A	1101[B]	ONN	C1-C9-N30-C31
4	B	1101[B]	ONN	C16-C14-C15-S38
4	B	1101[B]	ONN	N13-C14-C15-S38
4	B	1101[B]	ONN	C11-C10-C9-C1
4	B	1101[B]	ONN	C11-C10-C9-N30
4	B	1101[B]	ONN	C22-C21-C26-C27
4	B	1101[B]	ONN	N30-C31-C32-C35
4	B	1101[B]	ONN	N30-C31-C32-N34
4	B	1101[B]	ONN	O33-C31-C32-C35
4	B	1101[B]	ONN	O33-C31-C32-N34
4	B	1101[B]	ONN	N34-C32-C35-C36
4	B	1101[B]	ONN	C35-C36-S37-S38
4	B	1101[B]	ONN	C1-C9-N30-C31
4	B	1101[A]	ONN	C14-C15-S38-S37
4	B	1101[A]	ONN	N30-C31-C32-C35
4	B	1101[A]	ONN	O33-C31-C32-C35
4	B	1101[A]	ONN	C1-C9-N30-C31
6	A	1116	NAG	C3-C2-N2-C7
4	B	1101[B]	ONN	C16-C14-N13-C11
4	B	1101[A]	ONN	C20-C19-N18-C16
12	B	1118	PEG	C4-C3-O2-C2
6	A	1106	NAG	C1-C2-N2-C7
6	B	1110	NAG	O5-C5-C6-O6
6	A	1115	NAG	O5-C5-C6-O6
4	A	1101[A]	ONN	O17-C16-N18-C19
4	A	1101[A]	ONN	C36-S37-S38-C15
4	A	1101[A]	ONN	C14-C16-N18-C19
6	B	1113	NAG	O5-C5-C6-O6
4	B	1101[B]	ONN	C20-C21-C26-C27
6	B	1113	NAG	C4-C5-C6-O6
10	A	1121	PG4	C3-C4-O3-C5
6	A	1112	NAG	C8-C7-N2-C2
6	A	1112	NAG	O7-C7-N2-C2
6	A	1115	NAG	C8-C7-N2-C2
6	A	1115	NAG	O7-C7-N2-C2
6	A	1115	NAG	C4-C5-C6-O6
10	A	1121	PG4	O3-C5-C6-O4
4	A	1101[B]	ONN	C32-C35-C36-S37
4	B	1101[A]	ONN	C32-C35-C36-S37

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Mol	Chain	Res	Type	Atoms
6	B	1110	NAG	C4-C5-C6-O6
4	A	1101[B]	ONN	C36-S37-S38-C15
4	B	1101[B]	ONN	C36-S37-S38-C15
4	B	1101[A]	ONN	C36-S37-S38-C15
6	B	1114	NAG	O5-C5-C6-O6
6	A	1106	NAG	O5-C5-C6-O6
9	A	1120	PGE	O1-C1-C2-O2
9	A	1120	PGE	O3-C5-C6-O4
4	B	1101[A]	ONN	C35-C36-S37-S38
6	A	1112	NAG	O5-C5-C6-O6
12	B	1118	PEG	O2-C3-C4-O4
10	A	1121	PG4	O4-C7-C8-O5
4	A	1101[B]	ONN	O33-C31-C32-N34
4	A	1101[A]	ONN	C9-C10-C11-N13
4	B	1101[B]	ONN	C32-C35-C36-S37
4	B	1101[B]	ONN	C31-C32-C35-C36
4	B	1101[A]	ONN	C31-C32-C35-C36
4	A	1101[A]	ONN	C9-C10-C11-O12
8	B	1117	EDO	O1-C1-C2-O2
6	B	1114	NAG	C4-C5-C6-O6
4	B	1101[A]	ONN	N13-C14-C16-O17
10	A	1121	PG4	C4-C3-O2-C2
9	A	1120	PGE	C3-C4-O3-C5
10	A	1121	PG4	C1-C2-O2-C3
10	A	1121	PG4	C6-C5-O3-C4
4	B	1101[A]	ONN	N34-C32-C35-C36
9	A	1120	PGE	C6-C5-O3-C4
4	B	1101[B]	ONN	C9-C10-C11-N13
10	A	1121	PG4	C8-C7-O4-C6
4	B	1101[A]	ONN	N13-C14-C16-N18
4	A	1101[A]	ONN	O33-C31-C32-N34
6	B	1106	NAG	O5-C5-C6-O6
6	B	1113	NAG	C3-C2-N2-C7
6	A	1106	NAG	C3-C2-N2-C7
4	A	1101[A]	ONN	C22-C21-C26-C27
4	B	1101[A]	ONN	C22-C21-C26-C27
4	B	1101[B]	ONN	C9-C10-C11-O12
9	A	1120	PGE	C1-C2-O2-C3
4	A	1101[A]	ONN	N30-C31-C32-N34
4	A	1101[B]	ONN	C2-C1-C9-C10
9	A	1120	PGE	C4-C3-O2-C2
10	A	1121	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	A	1101[A]	ONN	N18-C19-C20-C25
4	A	1101[B]	ONN	C15-C14-N13-C11

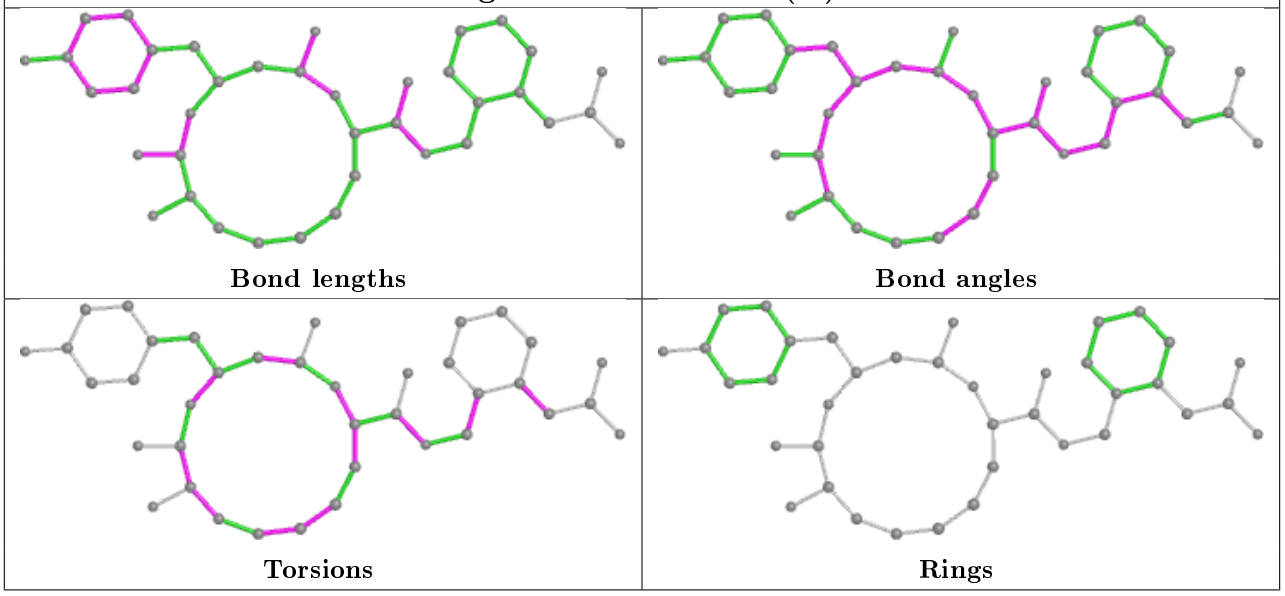
There are no ring outliers.

9 monomers are involved in 14 short contacts:

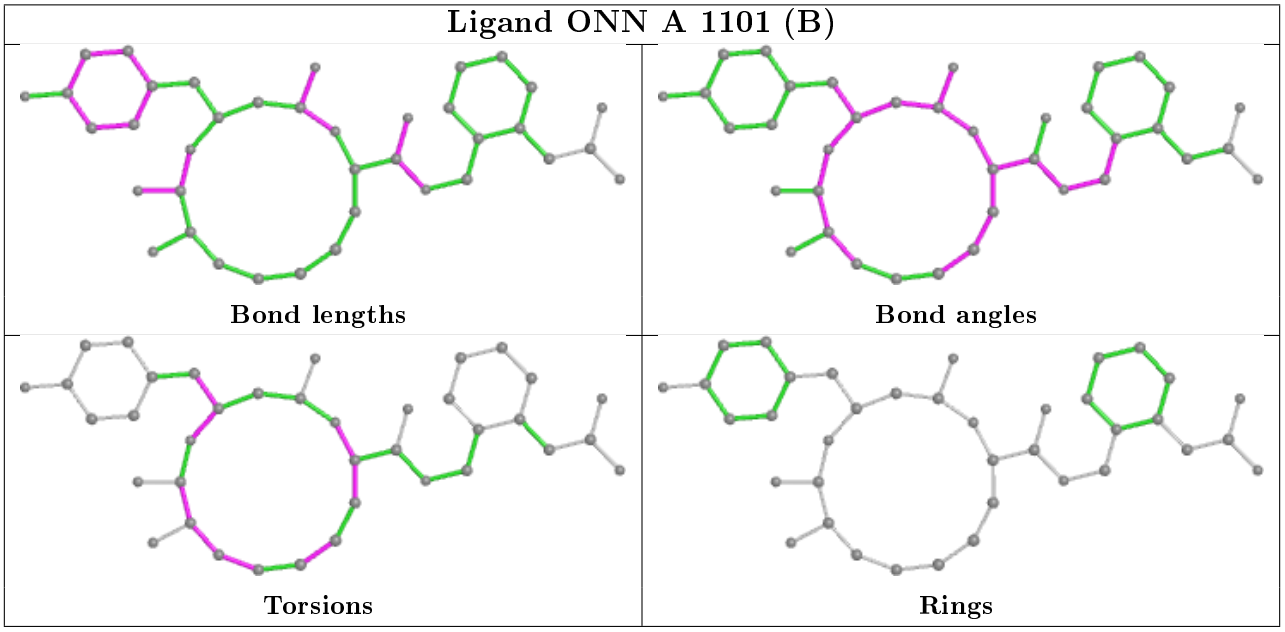
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1118	PEG	1	0
4	A	1101[B]	ONN	3	0
6	A	1112	NAG	2	0
6	A	1106	NAG	2	0
4	B	1101[B]	ONN	2	0
4	B	1101[A]	ONN	1	0
6	A	1116	NAG	1	0
8	A	1118	EDO	1	0
6	A	1115	NAG	1	0

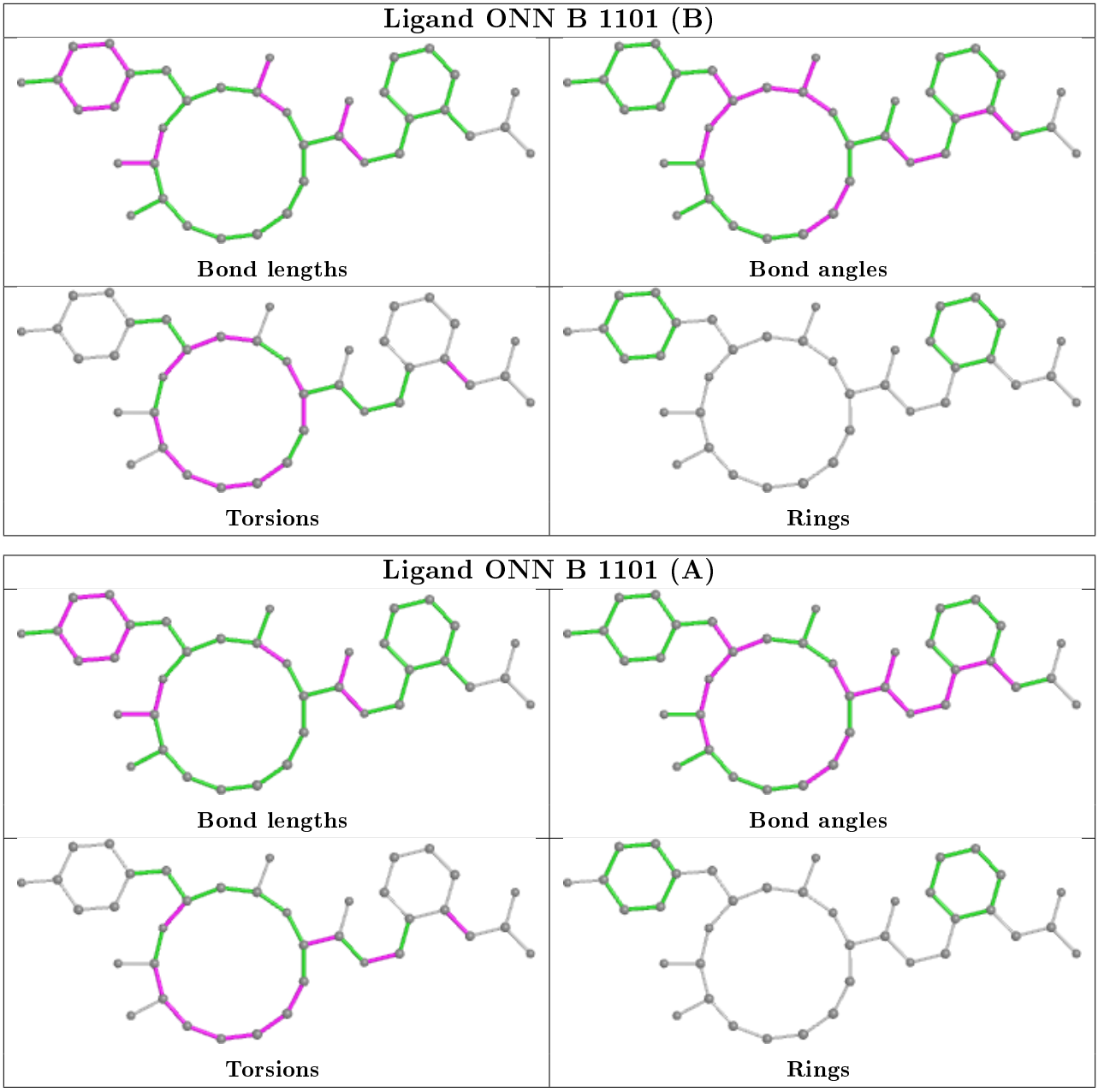
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ONN A 1101 (A)



Ligand ONN A 1101 (B)





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	856/912 (93%)	-0.11	22 (2%) 56 40	17, 38, 64, 103	0
1	B	853/912 (93%)	-0.11	9 (1%) 80 69	18, 34, 53, 90	0
All	All	1709/1824 (93%)	-0.11	31 (1%) 68 55	17, 36, 59, 103	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	SER	4.4
1	A	247	ALA	4.4
1	A	248	PRO	4.0
1	B	164	ALA	3.5
1	A	1029	THR	3.5
1	A	249	GLU	3.3
1	B	1025	LEU	3.3
1	A	1028	GLU	3.3
1	B	854	SER	3.2
1	A	258	THR	3.2
1	A	225	VAL	3.0
1	B	598	ASN	2.8
1	A	1027	THR	2.8
1	B	375	GLY	2.8
1	A	222	MET	2.7
1	A	598	ASN	2.7
1	A	326	THR	2.4
1	B	227	SER	2.3
1	A	229	GLU	2.3
1	A	220	THR	2.2
1	A	375	GLY	2.2
1	A	219	VAL	2.2
1	B	491	THR	2.2
1	A	223	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	600	THR	2.1
1	B	853	GLN	2.1
1	A	217	SER	2.0
1	A	180	SER	2.0
1	A	226	SER	2.0
1	A	991	SER	2.0
1	A	636	PHE	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)

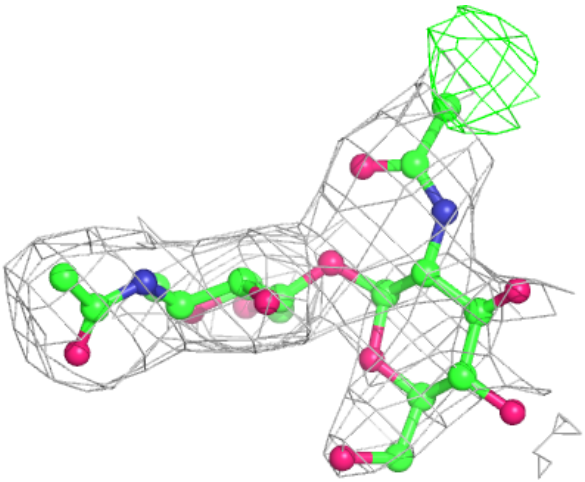
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

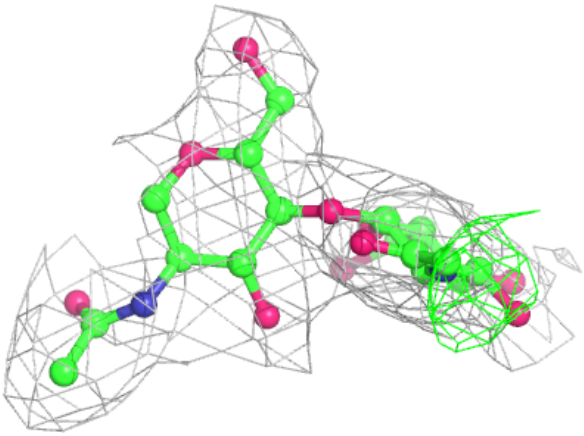
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.67	0.30	58,60,61,61	0
2	NAG	G	2	14/15	0.67	0.29	63,70,79,80	0
2	NAG	I	1	14/15	0.79	0.24	54,54,55,55	0
3	BMA	D	3	11/12	0.80	0.21	74,75,75,75	0
2	NAG	F	2	14/15	0.81	0.17	66,66,67,67	0
2	NAG	E	2	14/15	0.83	0.16	70,71,73,73	0
2	NAG	G	1	14/15	0.84	0.26	54,61,72,73	0
3	NAG	D	2	14/15	0.85	0.29	67,72,74,75	0
2	NAG	E	1	14/15	0.85	0.16	69,73,80,81	0
3	NAG	D	1	14/15	0.85	0.34	71,78,82,83	0
2	NAG	I	2	14/15	0.86	0.14	54,55,55,55	0
2	NAG	C	1	14/15	0.88	0.14	46,54,59,62	0
3	NAG	H	2	14/15	0.89	0.19	50,50,51,51	0
2	NAG	F	1	14/15	0.89	0.20	56,56,57,57	0
3	NAG	H	1	14/15	0.91	0.17	41,42,43,43	0
3	BMA	H	3	11/12	0.91	0.16	53,54,54,54	0

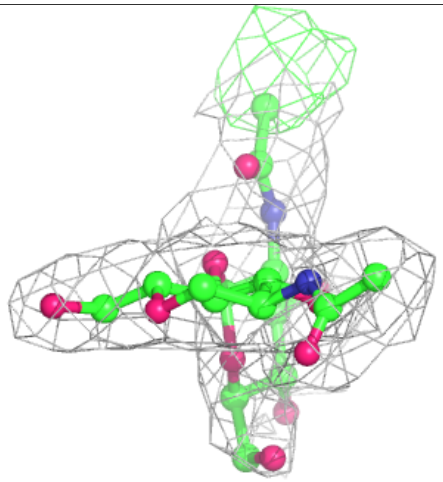
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

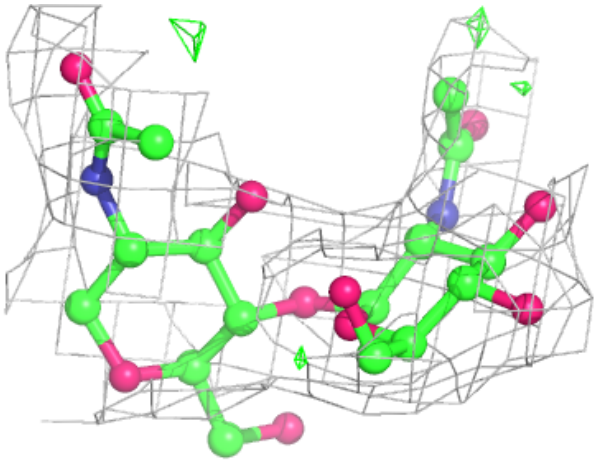


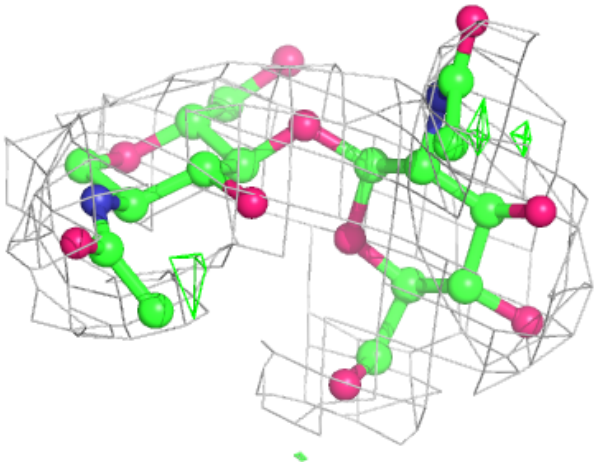


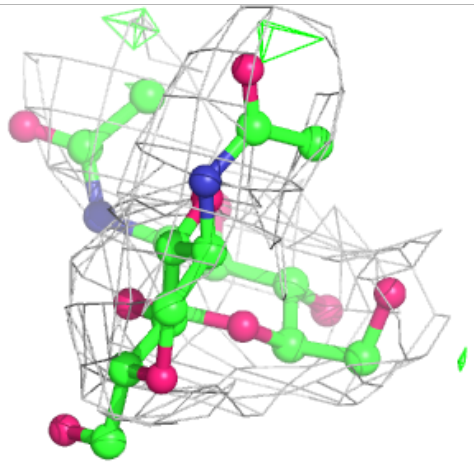


Electron density around Chain E:

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

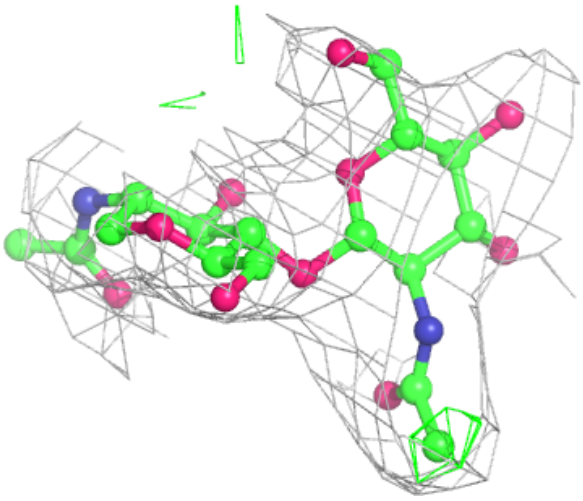


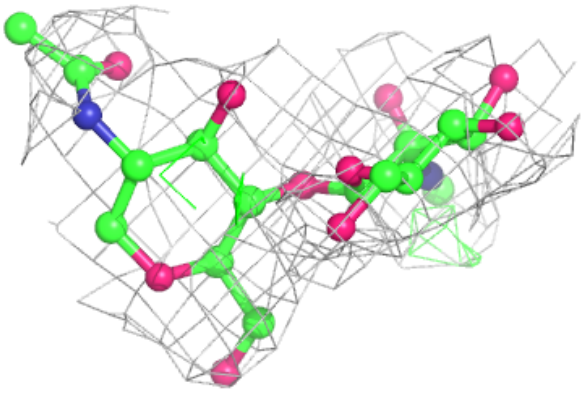


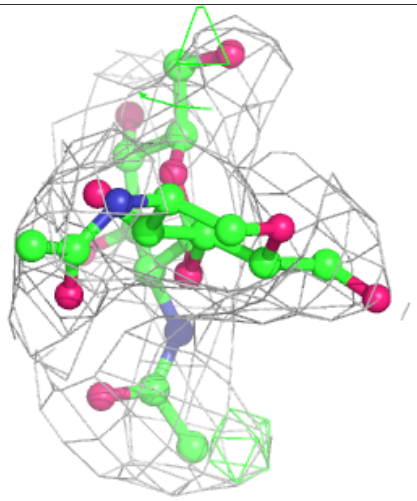


Electron density around Chain F:

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

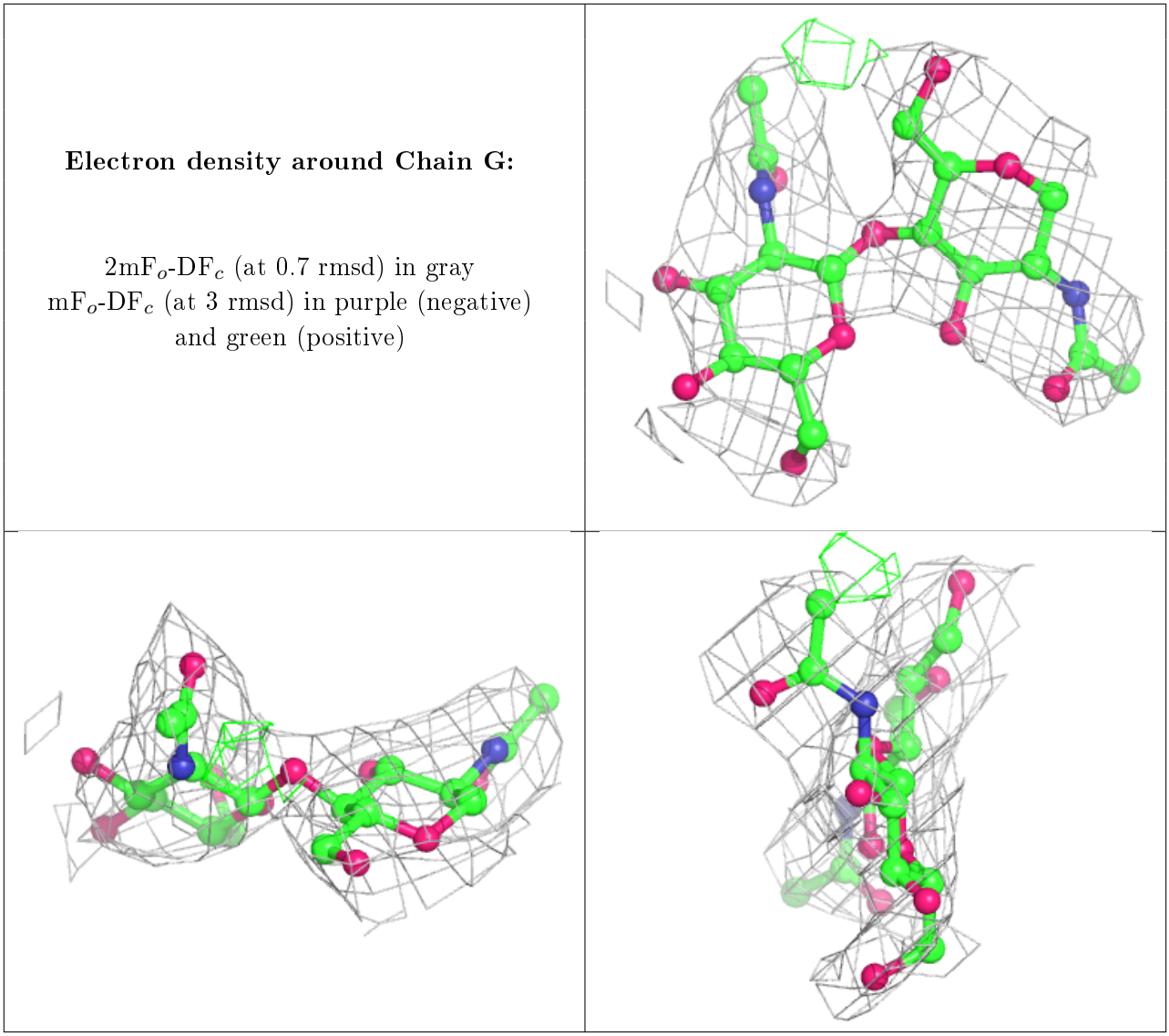






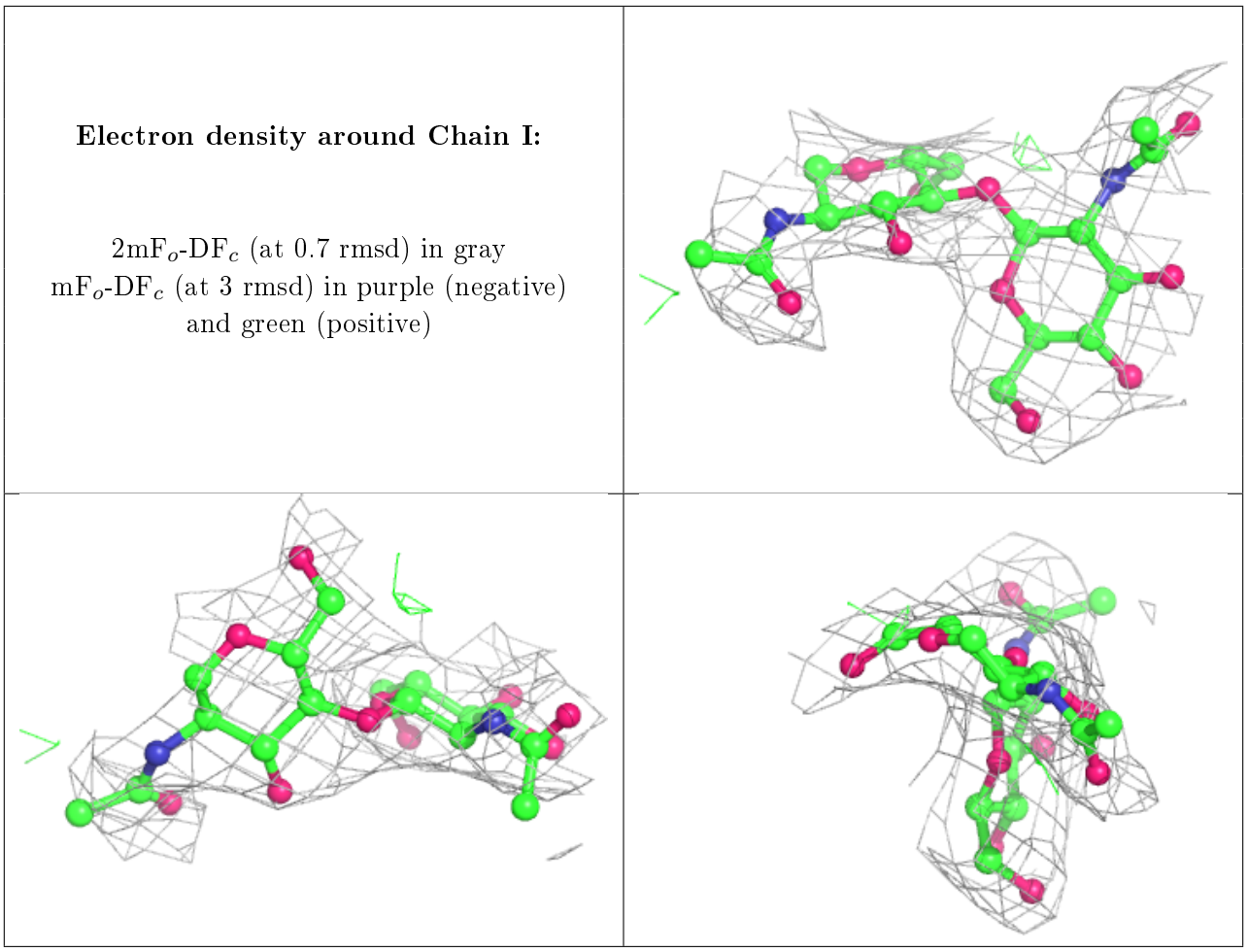
Electron density around Chain G:

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



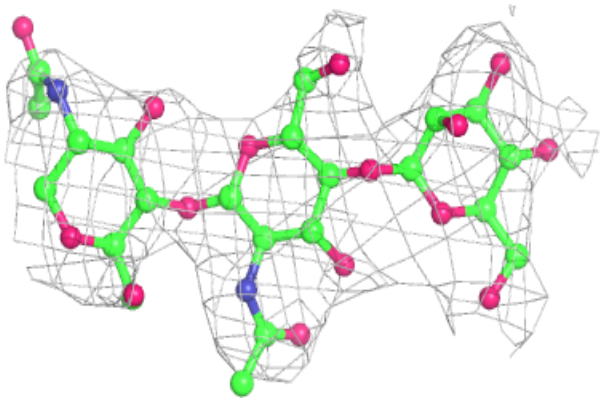
Electron density around Chain I:

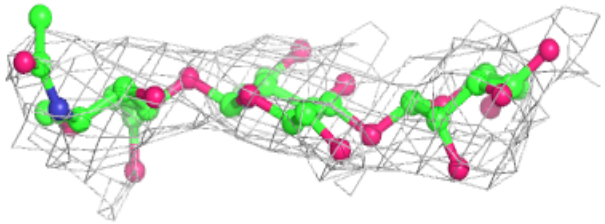
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

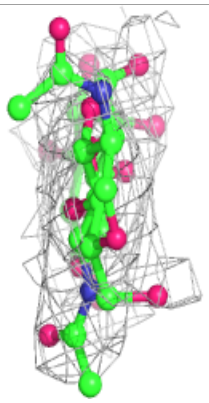


Electron density around Chain D:

$2mF_o$-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 H:

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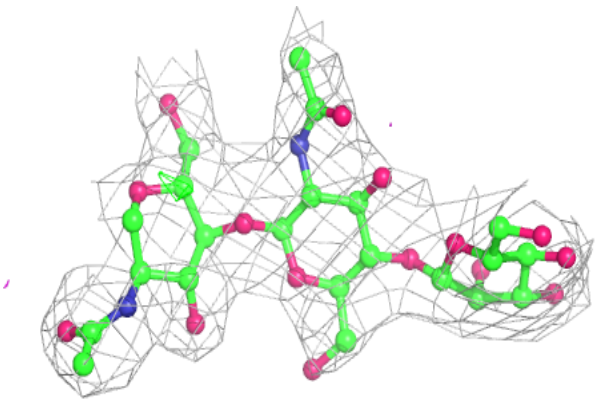
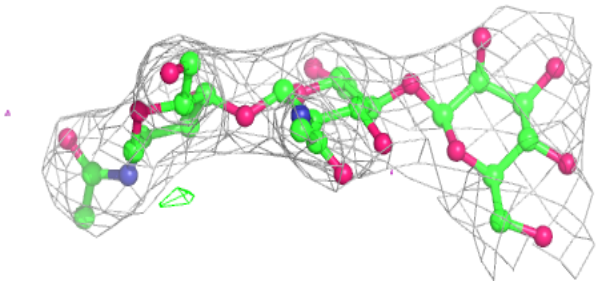
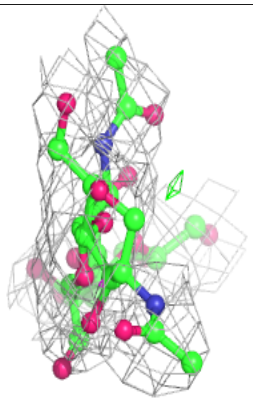
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.4 Ligands (i)

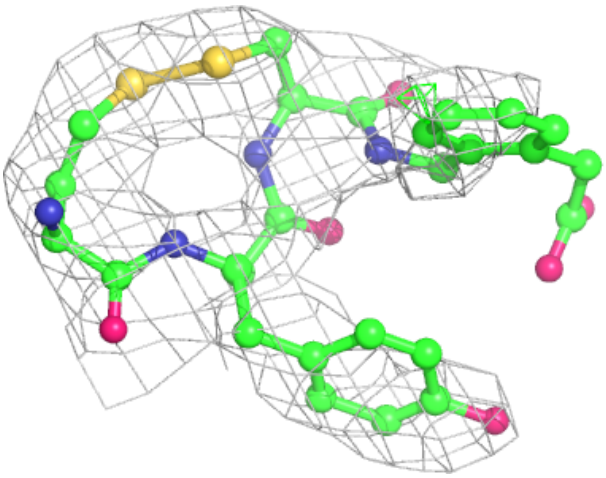
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

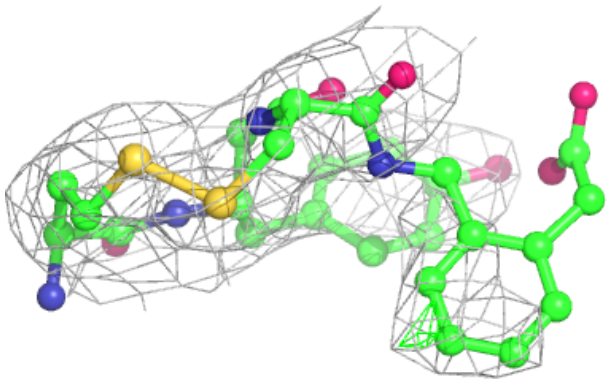
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	B	1110	14/15	0.68	0.30	58,59,59,59	0
6	NAG	A	1116	14/15	0.73	0.28	75,76,77,77	0
6	NAG	A	1112	14/15	0.74	0.32	50,54,58,64	0
6	NAG	B	1113	14/15	0.75	0.23	60,60,61,61	0
6	NAG	A	1115	14/15	0.78	0.35	57,57,57,57	0
6	NAG	B	1114	14/15	0.79	0.21	49,50,50,50	0
12	PEG	B	1118	7/7	0.81	0.15	56,56,56,56	0
6	NAG	A	1105	14/15	0.82	0.35	77,81,84,85	0
4	ONN	B	1101[B]	38/38	0.86	0.40	40,48,53,59	38
4	ONN	B	1101[A]	38/38	0.86	0.40	33,38,40,46	38
6	NAG	B	1105	14/15	0.87	0.19	52,57,65,66	0
6	NAG	A	1106	14/15	0.88	0.26	55,66,69,69	0
9	PGE	A	1120	10/10	0.88	0.12	41,51,55,60	0
4	ONN	A	1101[B]	38/38	0.90	0.34	33,38,42,48	38
10	PG4	A	1121	13/13	0.90	0.16	41,49,55,56	0
8	EDO	B	1115	4/4	0.90	0.13	36,39,39,41	0
6	NAG	B	1106	14/15	0.90	0.18	55,60,63,64	0
4	ONN	A	1101[A]	38/38	0.90	0.34	33,39,43,48	38
7	SIN	A	1117	8/8	0.90	0.17	38,42,45,48	0
8	EDO	B	1117	4/4	0.90	0.30	24,28,31,33	0
8	EDO	A	1118	4/4	0.92	0.17	35,38,38,40	0
11	PO4	A	1122	5/5	0.95	0.30	59,59,59,59	0
8	EDO	A	1119	4/4	0.95	0.09	26,26,26,26	0
8	EDO	B	1116	4/4	0.95	0.13	37,39,40,41	0
5	ZN	A	1102	1/1	0.98	0.15	49,49,49,49	0
5	ZN	B	1102	1/1	0.99	0.17	35,35,35,35	0

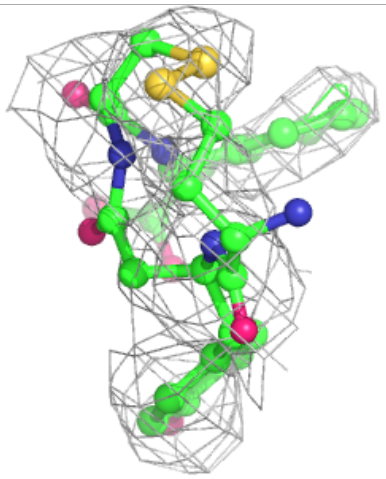
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ONN B 1101 (B):

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

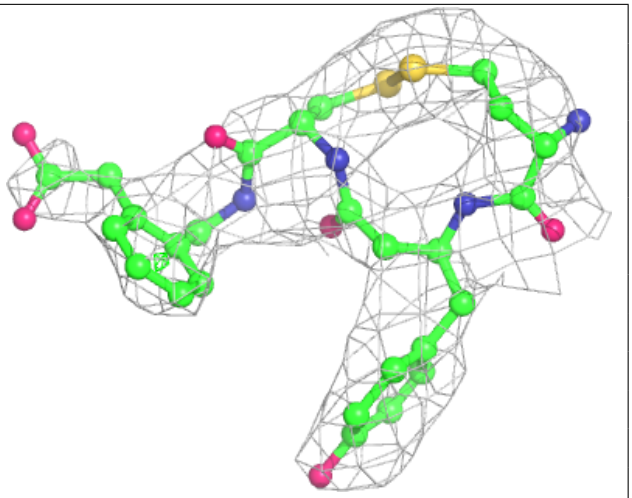


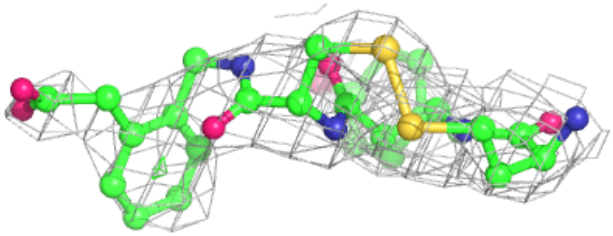


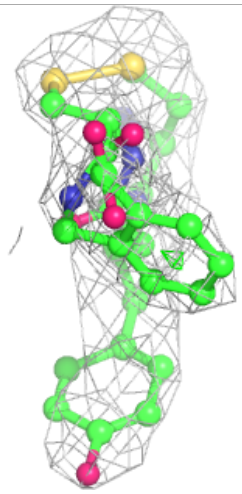


Electron density around ONN B 1101 (A):

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

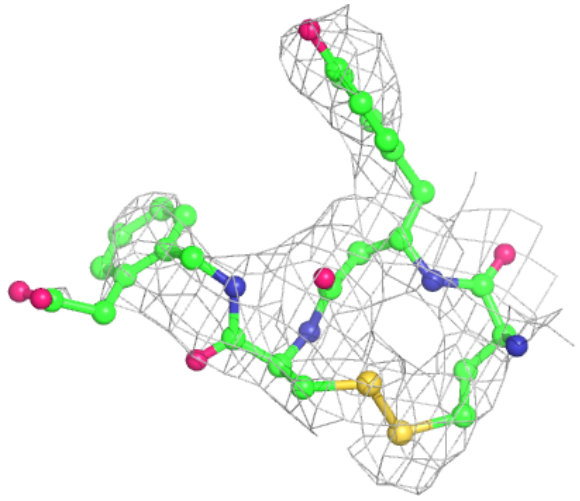


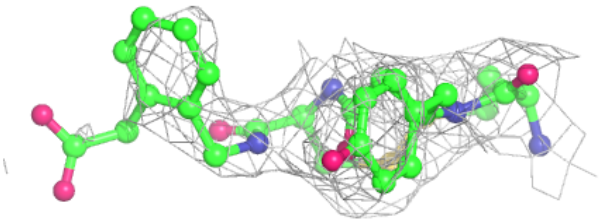


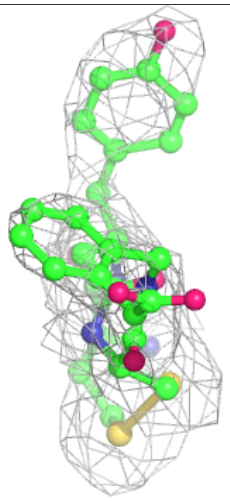


Electron density around ONN A 1101 (B):

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

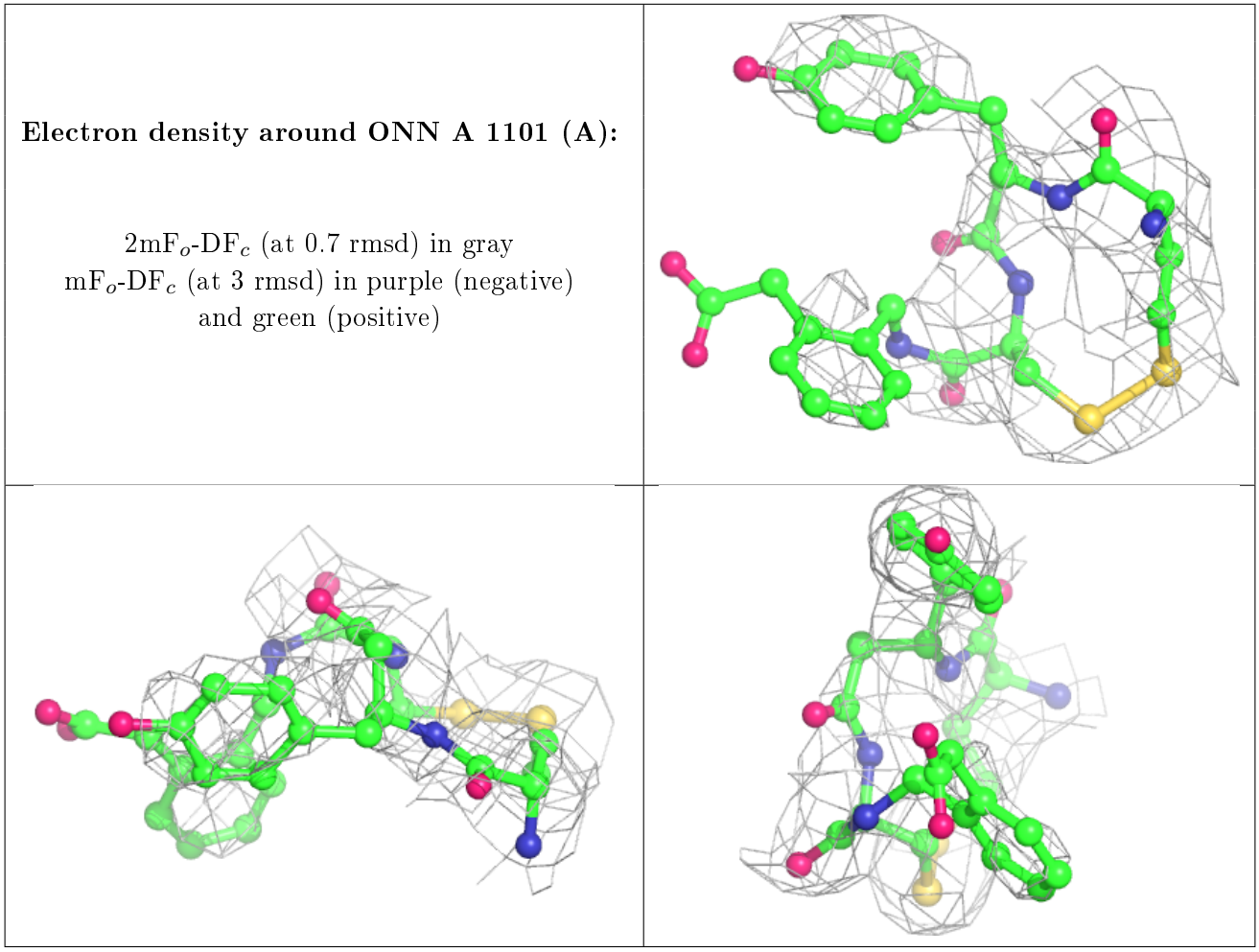






Electron density around ONN A 1101 (A):

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



6.5 Other polymers

There are no such residues in this entry.