Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 05:23 PM JST

PDB ID	:	7VN3
Title	:	Crystal structure of MBP-fused BIL1/BZR1 (21-90) in complex with double-stranded DNA contaning CACACGTGTG
Authors	:	Nosaki, S.; Tanokura, M.; Miyakawa, T.
Deposited on	:	2021-10-10
Resolution	:	1.94 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

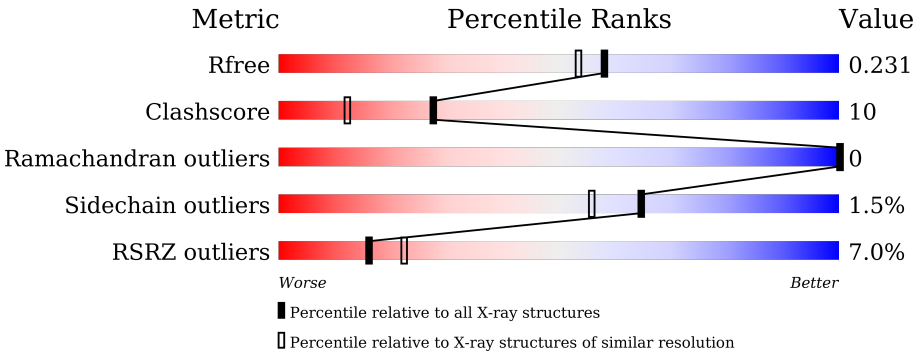
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	9% 80% 18%
1	B	439	10% 82% 16%
1	C	439	3% 88% 12%
1	D	439	8% 75% 24%
2	E	15	80% 20%
2	F	15	47% 53%

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Mol	Chain	Length	Quality of chain
2	G	15	53% 47%
2	H	15	87% 13%
3	K	2	100%
3	L	2	50% 50%
3	M	2	100%
3	N	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15454 atoms, of which 42 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 Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	437	Total	C	N	O	S	0	1	0
			3413	2177	586	641	9			
1	D	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			
1	A	437	Total	C	N	O	S	0	1	0
			3413	2177	586	641	9			
1	B	436	Total	C	N	O	S	0	0	0
			3394	2166	581	639	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
C	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
C	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
C	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
C	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
C	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
D	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
D	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
D	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
D	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
D	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
A	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
A	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
A	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
A	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
A	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-368	MET	-	initiating methionine	UNP A0A4P1LXE0
B	-286	ALA	ASP	engineered mutation	UNP A0A4P1LXE0
B	-285	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-196	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-195	ALA	ASN	engineered mutation	UNP A0A4P1LXE0
B	-129	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-9	ALA	GLU	engineered mutation	UNP A0A4P1LXE0
B	-6	ALA	LYS	engineered mutation	UNP A0A4P1LXE0
B	-5	ALA	ASP	engineered mutation	UNP A0A4P1LXE0

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*CP*AP*CP*AP*CP*GP*TP*GP*TP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	E	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			
2	F	15	Total	C	N	O	P	0	0	0
			305	147	57	87	14			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	K	2	Total	C	O	0	0	0
			23	12	11			
3	L	2	Total	C	O	0	0	0
			23	12	11			

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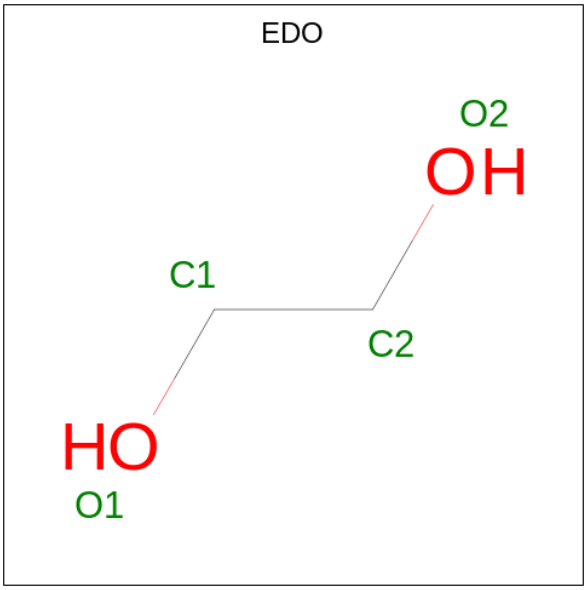
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	M	2	Total C O 23 12 11	0	0	0
3	N	2	Total C O 23 12 11	0	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is water.

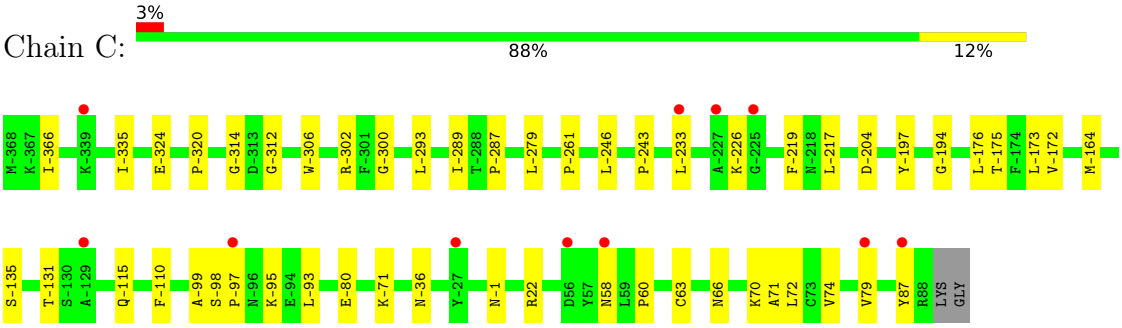
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	105	Total O 105 105	0	0
5	D	50	Total O 50 50	0	0
5	G	22	Total O 22 22	0	0
5	H	25	Total O 25 25	0	0
5	A	97	Total O 97 97	0	0
5	B	143	Total O 143 143	0	0
5	E	5	Total O 5 5	0	0
5	F	11	Total O 11 11	0	0

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.

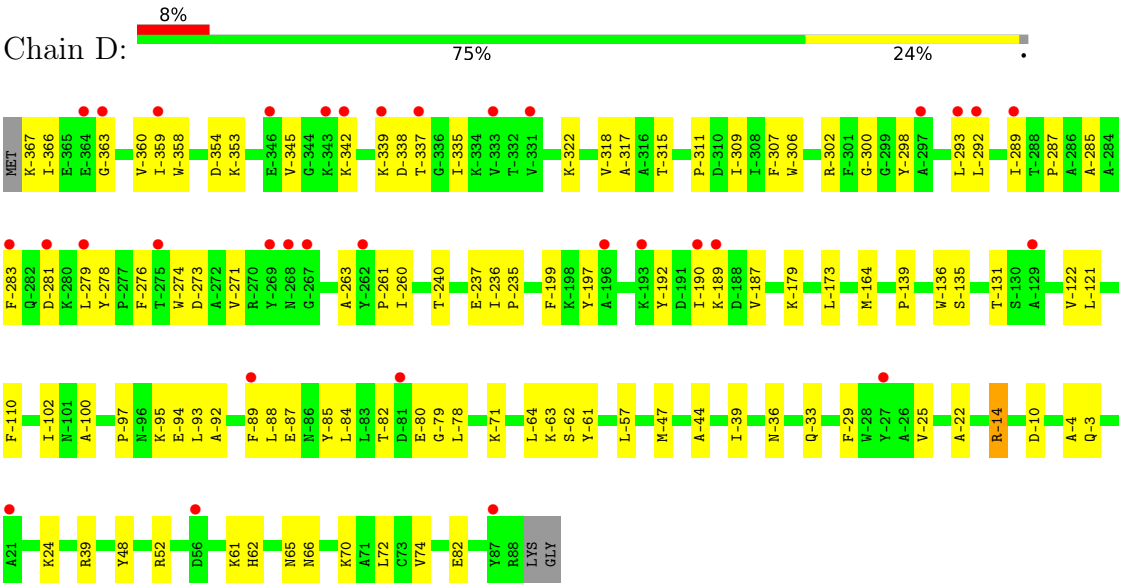
• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

Chain C:



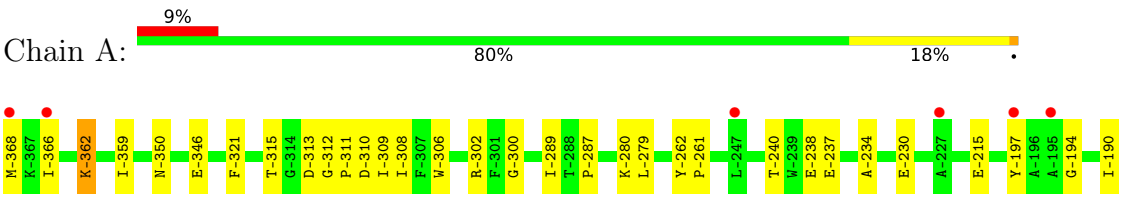
• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

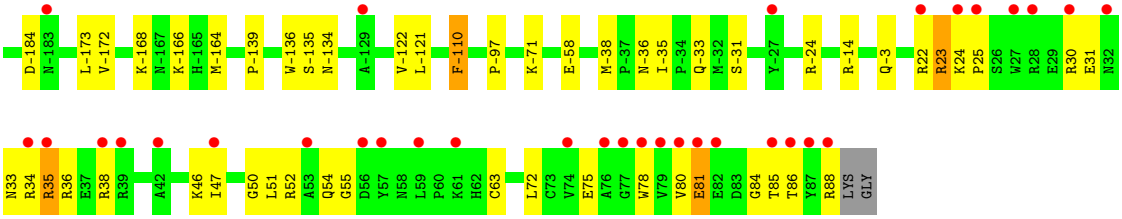
Chain D:



• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

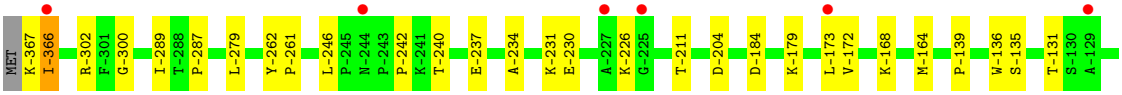
Chain A:

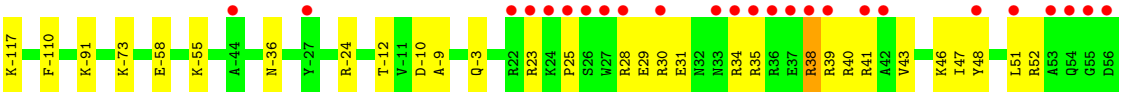


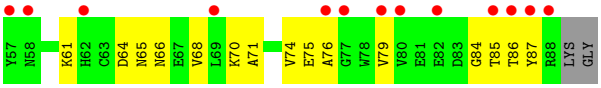


• Molecule 1: Maltodextrin-binding protein,Protein BRASSINAZOLE-RESISTANT 1

Chain B:

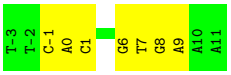






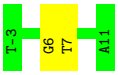
• Molecule 2: DNA (5'-D(*TP*TP*CP*AP*CP*AP*CP*GP*TP*GP*TP*GP*AP*AP*A)-3')

Chain G:



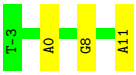
• Molecule 2: DNA (5'-D(*TP*TP*CP*AP*CP*AP*CP*GP*TP*GP*TP*GP*AP*AP*A)-3')

Chain H:



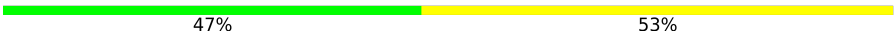
• Molecule 2: DNA (5'-D(*TP*TP*CP*AP*CP*AP*CP*GP*TP*GP*TP*GP*AP*AP*A)-3')

Chain E:



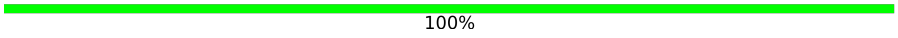
• Molecule 2: DNA (5'-D(*TP*TP*CP*AP*CP*AP*CP*GP*TP*GP*TP*GP*AP*AP*A)-3')

Chain F:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:

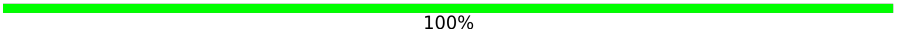


• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:

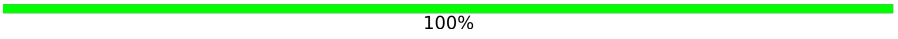
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:



• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.66Å 92.91Å 111.94Å 90.00° 100.33° 90.00°	Depositor
Resolution (Å)	35.50 – 1.94 35.50 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.50-1.94) 99.5 (35.50-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.202 , 0.231 0.202 , 0.231	Depositor DCC
R_{free} test set	7618 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15454	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 56.58 % 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 2.6827e-05. 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: GLC, EDO

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	0.34	0/3492	0.45	0/4737
1	B	0.32	0/3473	0.45	0/4713
1	C	0.37	0/3492	0.44	0/4737
1	D	0.34	0/3473	0.44	0/4713
2	E	0.57	0/342	1.02	2/526 (0.4%)
2	F	0.58	0/342	1.07	2/526 (0.4%)
2	G	0.68	0/342	0.98	0/526
2	H	0.72	0/342	1.01	0/526
All	All	0.38	0/15298	0.53	4/21004 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	11	DA	C1'-O4'-C4'	-6.71	103.39	110.10
2	E	11	DA	C1'-O4'-C4'	-5.72	104.38	110.10
2	F	8	DG	O4'-C1'-N9	5.72	112.00	108.00
2	E	8	DG	O4'-C1'-N9	5.33	111.73	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3413	0	3386	75	0
1	B	3394	0	3365	66	0
1	C	3413	0	3386	46	0
1	D	3394	0	3365	101	0
2	E	305	0	171	1	0
2	F	305	0	171	6	0
2	G	305	0	171	9	0
2	H	305	0	171	1	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0
3	M	23	0	21	0	0
3	N	23	0	21	0	0
4	A	8	12	12	1	0
4	B	4	6	6	0	0
4	C	12	18	18	0	0
4	D	4	6	6	2	0
5	A	97	0	0	3	0
5	B	143	0	0	5	0
5	C	105	0	0	3	0
5	D	50	0	0	3	0
5	E	5	0	0	0	0
5	F	11	0	0	0	0
5	G	22	0	0	0	0
5	H	25	0	0	0	0
All	All	15412	42	14312	292	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 10.

All (292) 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:C:-366:ILE:CD1	1:C:-97:PRO:HD2	1.75	1.15
1:C:-289:ILE:HG22	1:C:-287:PRO:HD3	1.32	1.08
1:D:-317:ALA:HB3	1:D:-293:LEU:HD22	1.46	0.97
1:C:-366:ILE:HD11	1:C:-97:PRO:HD2	1.47	0.97
1:D:-359:ILE:HD12	1:D:-309:ILE:HB	1.47	0.94
1:D:-359:ILE:HD11	1:D:-309:ILE:HD12	1.51	0.91
1:A:-240:THR:HG22	1:A:-237:GLU:OE1	1.74	0.88
1:D:-366:ILE:HD13	1:D:-97:PRO:HD3	1.52	0.88
1:A:-366:ILE:HG21	1:A:-97:PRO:HD2	1.56	0.88
1:C:-246:LEU:HD11	1:C:-233:LEU:HD21	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-190:ILE:HD11	1:A:-35:ILE:HD12	1.55	0.86
1:D:-289:ILE:HG22	1:D:-287:PRO:HD3	1.54	0.86
1:B:-12:THR:HG23	1:B:-9:ALA:H	1.41	0.84
1:A:24:LYS:HE2	1:A:24:LYS:HA	1.60	0.82
1:C:-366:ILE:HD11	1:C:-98:SER:HA	1.60	0.82
2:G:9:DA:H5'	2:G:9:DA:H8	1.45	0.81
1:C:-217:LEU:HD21	5:C:274:HOH:O	1.81	0.81
1:C:-366:ILE:CD1	1:C:-98:SER:HA	2.11	0.80
1:A:31:GLU:HA	1:A:34:ARG:HE	1.46	0.80
1:D:-190:ILE:HD11	1:D:-33:GLN:HG2	1.63	0.80
1:D:-14:ARG:HG3	1:D:-14:ARG:HH11	1.45	0.78
1:D:-363:GLY:O	1:D:-335:ILE:HG23	1.83	0.78
1:D:-317:ALA:CB	1:D:-293:LEU:HD22	2.15	0.76
1:B:-289:ILE:HG22	1:B:-287:PRO:HD3	1.69	0.75
1:D:-354:ASP:OD1	1:D:-353:LYS:HE2	1.86	0.75
1:D:-47:MET:HE3	1:D:-47:MET:HA	1.69	0.75
1:D:-240:THR:HG22	1:D:-237:GLU:OE1	1.86	0.74
1:C:-366:ILE:HD12	1:C:-97:PRO:HD2	1.67	0.74
1:D:-300:GLY:HA3	1:D:-36:ASN:O	1.88	0.73
1:A:-197:TYR:OH	1:A:-194:GLY:HA2	1.89	0.72
1:A:-240:THR:HG23	1:A:-237:GLU:H	1.56	0.71
1:D:-271:VAL:HG11	1:D:-261:PRO:HD3	1.72	0.71
1:D:-39:ILE:HD12	1:D:-39:ILE:O	1.91	0.70
1:A:86:THR:OG1	1:B:47:ILE:HA	1.92	0.70
2:G:9:DA:H5'	2:G:9:DA:C8	2.25	0.69
1:A:50:GLY:HA3	1:B:86:THR:HG23	1.73	0.69
1:D:-279:LEU:HD23	1:D:-64:LEU:HA	1.75	0.68
1:D:-14:ARG:HG3	1:D:-14:ARG:NH1	2.05	0.68
1:B:23:ARG:HH22	1:B:25:PRO:HA	1.57	0.68
1:D:-366:ILE:HD13	1:D:-97:PRO:CD	2.23	0.67
1:A:-366:ILE:CG2	1:A:-97:PRO:HD2	2.24	0.67
1:D:-173:LEU:HD12	1:D:-164:MET:HE1	1.75	0.67
1:D:-14:ARG:HH11	1:D:-14:ARG:CG	2.08	0.66
1:A:-368:MET:HG2	1:A:-313:ASP:HB3	1.78	0.66
1:C:-246:LEU:HD22	1:C:-243:PRO:HA	1.77	0.66
1:B:-173:LEU:CD1	1:B:-164:MET:HE1	2.26	0.66
1:B:31:GLU:OE2	1:B:35:ARG:NE	2.28	0.65
1:C:-219:PHE:O	1:C:-217:LEU:HD22	1.97	0.65
1:D:-135:SER:O	1:D:-131:THR:HG23	1.97	0.65
1:C:-80:GLU:CD	1:C:-80:GLU:H	2.00	0.65
1:B:70:LYS:O	1:B:74:VAL:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-366:ILE:HD11	1:C:-97:PRO:CD	2.22	0.65
1:C:-173:LEU:CD1	1:C:-164:MET:HE1	2.27	0.64
1:A:-173:LEU:HD11	1:A:-164:MET:HE1	1.77	0.64
1:A:-58:GLU:OE1	1:A:-58:GLU:HA	1.97	0.64
1:D:-359:ILE:CD1	1:D:-309:ILE:HD12	2.24	0.64
1:A:50:GLY:HA3	1:B:86:THR:CG2	2.26	0.64
1:B:-367:LYS:O	1:B:-367:LYS:HG2	1.98	0.64
1:B:30:ARG:O	1:B:34:ARG:HG3	1.98	0.64
1:C:-300:GLY:HA3	1:C:-36:ASN:O	1.97	0.64
1:B:41:ARG:NH2	2:F:3:DC:H2'	2.12	0.63
1:A:35:ARG:HB2	1:A:38:ARG:HH22	1.63	0.63
1:D:-135:SER:OG	1:D:-71:LYS:HD3	1.99	0.63
1:D:-47:MET:HE3	1:D:-44:ALA:HB3	1.79	0.63
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.63	0.63
1:B:-234:ALA:O	1:B:-230:GLU:HG2	1.99	0.62
1:B:48:TYR:O	1:B:52:ARG:HG3	2.00	0.62
1:D:-240:THR:HG23	1:D:-237:GLU:H	1.64	0.62
1:B:-300:GLY:HA3	1:B:-36:ASN:O	2.00	0.62
1:B:-302:ARG:NH1	5:B:201:HOH:O	2.27	0.61
1:B:-24:ARG:HD2	5:B:325:HOH:O	2.00	0.61
1:A:-289:ILE:HG22	1:A:-287:PRO:HD3	1.83	0.61
1:C:-197:TYR:OH	1:C:-194:GLY:HA2	2.00	0.61
1:A:35:ARG:HB2	1:A:38:ARG:NH2	2.15	0.61
1:D:-342:LYS:O	1:D:-339:LYS:HG2	2.01	0.60
1:A:30:ARG:O	1:A:34:ARG:HG3	2.00	0.60
1:D:-335:ILE:HG12	1:D:-93:LEU:HD11	1.83	0.60
1:A:-173:LEU:CD1	1:A:-164:MET:HE1	2.32	0.60
1:A:51:LEU:HD21	1:A:72:LEU:HD22	1.82	0.60
1:C:-135:SER:OG	1:C:-71:LYS:HD3	2.02	0.59
1:A:-135:SER:OG	1:A:-71:LYS:HD3	2.02	0.59
1:C:-173:LEU:HD11	1:C:-164:MET:HE1	1.82	0.59
1:A:33:ASN:HA	1:A:36:ARG:HH12	1.66	0.59
1:A:-234:ALA:O	1:A:-230:GLU:HG2	2.03	0.59
1:B:-172:VAL:O	1:B:-168:LYS:HG3	2.03	0.59
1:B:71:ALA:O	1:B:74:VAL:HG22	2.02	0.59
1:D:-122:VAL:HG12	1:D:-121:LEU:O	2.04	0.58
1:D:-190:ILE:HD11	1:D:-33:GLN:CG	2.31	0.58
1:A:81:GLU:CD	1:A:85:THR:HB	2.24	0.58
1:B:43:VAL:O	1:B:47:ILE:HD13	2.04	0.58
1:A:81:GLU:CG	1:A:85:THR:HB	2.34	0.57
1:A:24:LYS:HA	1:A:24:LYS:CE	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ALA:O	1:C:74:VAL:HG22	2.05	0.57
1:A:80:VAL:HG22	1:A:86:THR:HG23	1.87	0.57
1:C:-217:LEU:CD2	5:C:274:HOH:O	2.46	0.57
1:B:-24:ARG:HD3	5:B:301:HOH:O	2.05	0.57
1:B:31:GLU:OE2	1:B:35:ARG:CZ	2.52	0.56
1:D:39:ARG:HD3	5:D:250:HOH:O	2.05	0.56
1:B:47:ILE:O	1:B:51:LEU:HG	2.04	0.56
1:A:-215:GLU:OE1	1:A:-24:ARG:NH2	2.37	0.56
1:B:41:ARG:HH22	2:F:3:DC:H2'	1.71	0.56
1:D:-366:ILE:CD1	1:D:-97:PRO:HD3	2.30	0.56
1:C:-324:GLU:HG3	1:C:-302[A]:ARG:HE	1.70	0.56
1:C:-204:ASP:OD1	1:C:-115:GLN:NE2	2.33	0.55
1:D:-366:ILE:HD13	1:D:-97:PRO:HG3	1.88	0.55
1:D:-173:LEU:CD1	1:D:-164:MET:HE1	2.36	0.55
1:D:-307:PHE:HE2	1:D:-260:ILE:HD12	1.70	0.55
1:A:-306:TRP:CD1	1:A:-302[A]:ARG:HG3	2.42	0.55
1:D:-190:ILE:HD11	1:D:-33:GLN:HB2	1.89	0.55
1:D:82:GLU:OE2	1:D:82:GLU:N	2.39	0.55
1:B:-204:ASP:OD2	1:B:-117:LYS:HE2	2.07	0.55
1:A:52:ARG:NH1	1:A:63:CYS:O	2.40	0.55
1:B:-211:THR:HG23	5:B:228:HOH:O	2.07	0.55
1:C:-1:ASN:OD1	1:C:22:ARG:NH2	2.41	0.54
1:D:-271:VAL:O	1:D:-271:VAL:HG22	2.08	0.54
1:B:-289:ILE:HD12	1:B:-262:TYR:CE2	2.42	0.54
2:F:6:DG:H2'	2:F:7:DT:H72	1.88	0.54
1:C:-246:LEU:CD2	1:C:-243:PRO:HA	2.37	0.54
1:A:33:ASN:HA	1:A:36:ARG:NH1	2.21	0.54
1:C:79:VAL:HG11	1:C:87:TYR:CE2	2.43	0.54
1:D:-47:MET:HE3	1:D:-47:MET:CA	2.34	0.54
1:D:-187:VAL:HG23	1:D:-3:GLN:HG3	1.89	0.54
1:D:-102:ILE:HD13	1:D:-92:ALA:HB3	1.90	0.54
1:A:-300:GLY:HA3	1:A:-36:ASN:O	2.07	0.54
1:D:-190:ILE:CD1	1:D:-33:GLN:HG2	2.37	0.53
1:A:22:ARG:NH2	1:A:22:ARG:HB3	2.23	0.53
1:D:-187:VAL:CG2	1:D:-3:GLN:HG3	2.38	0.53
1:D:-82:THR:HG23	1:D:-79:GLY:H	1.73	0.53
1:A:24:LYS:HD3	1:A:25:PRO:HD2	1.90	0.53
1:C:-279:LEU:HD23	1:C:-261:PRO:HG2	1.88	0.53
1:D:-260:ILE:HD13	1:D:-84:LEU:HD21	1.91	0.53
1:A:-280:LYS:NZ	5:A:202:HOH:O	2.42	0.53
1:A:46:LYS:HD3	1:B:85:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-85:TYR:O	1:D:-82:THR:HG22	2.08	0.53
1:B:23:ARG:HG3	1:B:23:ARG:O	2.09	0.53
1:A:-366:ILE:HD13	1:A:-310:ASP:OD1	2.09	0.52
1:C:72:LEU:HD23	1:D:72:LEU:HD23	1.89	0.52
1:C:-175:THR:O	1:C:-172:VAL:HG22	2.09	0.52
1:A:-197:TYR:OH	1:A:-194:GLY:CA	2.58	0.52
1:D:-197:TYR:HB2	1:D:-192:TYR:CE1	2.45	0.52
1:C:-366:ILE:HD13	1:C:-98:SER:HA	1.92	0.52
1:C:-306:TRP:CD1	1:C:-302[B]:ARG:HG3	2.45	0.52
1:D:61:LYS:HE2	1:D:62:HIS:NE2	2.25	0.51
1:B:-91:LYS:HE2	5:B:203:HOH:O	2.10	0.51
1:C:-226:LYS:O	1:C:-226:LYS:HG2	2.10	0.51
1:C:-175:THR:HA	1:C:-172:VAL:HG22	1.93	0.51
1:A:-321:PHE:CG	1:A:-308:ILE:HD12	2.46	0.51
1:B:-179:LYS:HE3	1:B:-10:ASP:OD1	2.10	0.51
1:D:39:ARG:CD	5:D:250:HOH:O	2.58	0.51
1:A:-134:ASN:HB3	4:A:102:EDO:H22	1.92	0.51
1:D:-358:TRP:CG	1:D:-311:PRO:HG3	2.46	0.50
1:D:-307:PHE:HE2	1:D:-260:ILE:CD1	2.24	0.50
1:A:88:ARG:NH2	1:B:75:GLU:OE2	2.35	0.50
1:D:-276:PHE:HA	1:D:-273:ASP:OD2	2.11	0.50
1:B:31:GLU:OE2	1:B:35:ARG:NH2	2.45	0.50
1:D:-80:GLU:H	1:D:-80:GLU:CD	2.15	0.50
1:A:-190:ILE:CD1	1:A:-35:ILE:HD12	2.36	0.50
1:A:84:GLY:HA2	1:B:47:ILE:HD11	1.94	0.50
1:C:-335:ILE:HG13	1:C:-93:LEU:HD13	1.94	0.50
1:D:39:ARG:CG	5:D:250:HOH:O	2.59	0.50
1:A:-240:THR:OG1	1:A:-238:GLU:OE1	2.30	0.50
1:C:-135:SER:O	1:C:-131:THR:HG23	2.12	0.50
1:A:-172:VAL:HG12	1:A:-168:LYS:HE3	1.93	0.50
1:D:-338:ASP:OD2	1:D:-85:TYR:OH	2.20	0.49
1:A:-359:ILE:HG12	1:A:-309:ILE:HB	1.93	0.49
1:D:-61:TYR:CE2	1:D:-57:LEU:HD11	2.47	0.49
1:B:34:ARG:O	1:B:38:ARG:HG3	2.12	0.49
1:B:-279:LEU:HD23	1:B:-261:PRO:HG2	1.94	0.49
1:D:-366:ILE:HD13	1:D:-97:PRO:CG	2.41	0.49
1:A:81:GLU:HG3	1:A:85:THR:HB	1.93	0.49
1:D:-84:LEU:O	1:D:-78:LEU:HD13	2.12	0.49
1:D:-322:LYS:O	1:D:-318:VAL:HG13	2.12	0.48
2:G:-1:DC:H2"	2:G:0:DA:C8	2.48	0.48
1:D:-139:PRO:HA	1:D:-136:TRP:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:HA	1:B:34:ARG:HG3	1.96	0.48
1:D:-359:ILE:CD1	1:D:-309:ILE:HB	2.32	0.48
1:B:40:ARG:NH2	2:E:0:DA:H2'	2.28	0.48
1:A:-306:TRP:CD1	1:A:-302[B]:ARG:HG3	2.49	0.48
1:D:-271:VAL:CG2	1:D:-263:ALA:HB3	2.43	0.47
1:C:-173:LEU:HD12	1:C:-164:MET:HE1	1.96	0.47
1:D:-100:ALA:O	1:D:-95:LYS:NZ	2.32	0.47
2:G:8:DG:H2"	2:G:9:DA:H5"	1.96	0.47
1:A:-190:ILE:HD11	1:A:-35:ILE:CD1	2.37	0.47
1:D:-307:PHE:CE2	1:D:-260:ILE:HD12	2.50	0.47
1:D:24:LYS:HA	1:D:24:LYS:HD3	1.63	0.47
4:D:101:EDO:H11	2:G:1:DC:H5"	1.97	0.47
1:B:-240:THR:OG1	1:B:-237:GLU:HG3	2.15	0.47
1:D:70:LYS:O	1:D:74:VAL:HG13	2.15	0.47
1:B:65:ASN:HA	1:B:68:VAL:HG12	1.96	0.47
1:A:-240:THR:HG23	1:A:-237:GLU:N	2.28	0.46
1:B:39:ARG:O	1:B:43:VAL:HG23	2.14	0.46
1:C:58:ASN:OD1	1:C:58:ASN:O	2.32	0.46
1:A:-122:VAL:HG12	1:A:-121:LEU:O	2.15	0.46
2:G:6:DG:H2'	2:G:7:DT:H72	1.97	0.46
1:A:-14:ARG:CZ	1:A:-14:ARG:HB2	2.45	0.46
1:B:31:GLU:HB2	1:B:34:ARG:NH2	2.30	0.46
1:D:-342:LYS:HA	1:D:-339:LYS:HG2	1.98	0.46
1:C:-314:GLY:HA2	1:C:-99:ALA:CB	2.46	0.46
1:D:-345:VAL:HG12	1:D:-89:PHE:CE2	2.51	0.46
4:D:101:EDO:H11	2:G:1:DC:H3'	1.97	0.46
1:A:-184:ASP:HB2	1:A:-3:GLN:HB2	1.98	0.46
1:D:-298:TYR:HB2	1:D:-292:LEU:HD11	1.98	0.46
1:A:-14:ARG:HB2	1:A:-14:ARG:NH1	2.31	0.46
2:F:-3:DT:H2"	2:F:-2:DT:H5'	1.97	0.46
1:A:-366:ILE:HD11	1:A:-311:PRO:C	2.37	0.45
1:B:23:ARG:HG3	1:B:23:ARG:NH1	2.30	0.45
1:D:-366:ILE:HD12	1:D:-366:ILE:O	2.17	0.45
1:D:-279:LEU:HD12	1:D:-274:TRP:CZ2	2.50	0.45
1:D:-64:LEU:HG	1:D:-62:SER:HB3	1.98	0.45
1:B:-184:ASP:HB2	1:B:-3:GLN:HB2	1.99	0.45
1:B:-73:LYS:HA	1:B:-73:LYS:HD3	1.55	0.45
1:D:66:ASN:O	1:D:70:LYS:HG3	2.15	0.45
2:G:8:DG:H2"	2:G:9:DA:C5'	2.46	0.45
1:D:-285:ALA:O	1:D:-281:ASP:OD1	2.35	0.45
1:A:-279:LEU:HD23	1:A:-261:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:HD12	1:B:47:ILE:N	2.32	0.45
1:D:52:ARG:HH21	1:D:65:ASN:ND2	2.15	0.45
1:B:64:ASP:OD1	1:B:65:ASN:N	2.50	0.45
1:B:66:ASN:O	1:B:70:LYS:HG3	2.16	0.45
1:C:-366:ILE:HG23	1:C:-312:GLY:O	2.16	0.45
1:B:-139:PRO:HA	1:B:-136:TRP:CE2	2.52	0.45
1:B:51:LEU:HD13	1:B:68:VAL:CG2	2.46	0.44
1:D:-89:PHE:HD1	1:D:-88:LEU:HD23	1.82	0.44
1:B:-58:GLU:O	1:B:-55:LYS:HG3	2.18	0.44
1:D:-179:LYS:HE2	1:D:-10:ASP:OD1	2.17	0.44
1:D:-89:PHE:CD1	1:D:-88:LEU:HD23	2.53	0.44
1:A:-350:ASN:O	1:A:-346:GLU:HG3	2.17	0.44
1:C:66:ASN:O	1:C:70:LYS:HG3	2.17	0.44
1:B:51:LEU:CD1	1:B:68:VAL:HG21	2.47	0.44
1:D:-287:PRO:HB3	1:D:-87:GLU:OE2	2.18	0.44
1:C:60:PRO:HG2	1:C:63:CYS:HB3	2.00	0.44
1:D:-190:ILE:HD11	1:D:-33:GLN:CB	2.47	0.43
1:D:-47:MET:CE	1:D:-44:ALA:HB3	2.46	0.43
1:A:-366:ILE:HG23	5:A:240:HOH:O	2.17	0.43
1:A:23:ARG:HB2	1:A:23:ARG:CZ	2.48	0.43
1:B:29:GLU:O	1:B:29:GLU:HG3	2.17	0.43
1:D:-283:PHE:CE2	1:D:-87:GLU:HA	2.53	0.43
2:G:8:DG:C2'	2:G:9:DA:H5"	2.48	0.43
1:A:-302[B]:ARG:HE	1:A:-302[B]:ARG:HB3	1.50	0.43
1:D:-271:VAL:HG21	1:D:-263:ALA:HB3	1.99	0.43
1:B:-366:ILE:H	1:B:-366:ILE:HG12	1.56	0.43
1:A:54:GLN:HG2	1:A:54:GLN:O	2.19	0.43
1:C:-366:ILE:HD12	1:C:-366:ILE:O	2.17	0.43
1:D:-367:LYS:HG2	1:D:-366:ILE:N	2.34	0.43
1:A:-289:ILE:HD12	1:A:-262:TYR:CE2	2.53	0.43
1:A:-139:PRO:HA	1:A:-136:TRP:CE2	2.53	0.43
1:C:-176:LEU:O	1:C:-172:VAL:HG13	2.18	0.43
1:A:-368:MET:HE2	1:A:-313:ASP:OD2	2.18	0.43
1:B:43:VAL:O	1:B:47:ILE:CD1	2.67	0.43
1:D:-306:TRP:NE1	1:D:-302:ARG:HG3	2.33	0.43
1:B:-246:LEU:HD21	1:B:-242:PRO:HD3	2.00	0.43
1:D:61:LYS:HE2	1:D:62:HIS:HE2	1.83	0.43
1:D:-199:PHE:CE1	1:D:-187:VAL:HG12	2.53	0.43
1:D:-190:ILE:HG23	1:D:-189:LYS:HG2	2.01	0.43
1:A:-366:ILE:HG13	1:A:-312:GLY:O	2.19	0.42
1:B:-173:LEU:HD11	1:B:-164:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-22:ALA:HB2	1:D:-4:ALA:HB2	2.00	0.42
1:A:-190:ILE:HD12	1:A:-33:GLN:HB2	2.02	0.42
1:A:78:TRP:CH2	1:B:51:LEU:HA	2.55	0.42
1:D:-366:ILE:HD12	1:D:-366:ILE:C	2.39	0.42
1:C:-324:GLU:CG	1:C:-302[A]:ARG:HE	2.32	0.42
1:A:-197:TYR:OH	1:A:-194:GLY:C	2.59	0.42
1:A:51:LEU:O	1:A:55:GLY:HA3	2.20	0.42
1:C:-320:PRO:HA	1:C:-293:LEU:CD1	2.51	0.41
1:C:-98:SER:O	1:C:-95:LYS:HG3	2.21	0.41
1:D:-236:ILE:N	1:D:-235:PRO:CD	2.82	0.41
1:A:75:GLU:HG2	1:B:76:ALA:HB1	2.02	0.41
2:F:6:DG:H2"	2:F:7:DT:C6	2.55	0.41
1:D:-278:TYR:CE1	1:D:-63:LYS:HG2	2.56	0.41
1:D:-190:ILE:CG2	1:D:-189:LYS:HG2	2.50	0.41
1:D:-29:PHE:O	1:D:-25:VAL:HG23	2.19	0.41
1:A:52:ARG:NH2	1:A:63:CYS:O	2.51	0.41
2:F:3:DC:H2"	2:F:4:DG:C8	2.56	0.41
1:B:-226:LYS:HG2	1:B:-226:LYS:O	2.20	0.41
1:B:-135:SER:O	1:B:-131:THR:HG23	2.19	0.41
1:B:46:LYS:HB2	1:B:46:LYS:HE3	1.66	0.41
1:D:48:TYR:O	1:D:52:ARG:HG3	2.20	0.41
1:D:-358:TRP:CD2	1:D:-311:PRO:HG3	2.56	0.41
1:D:-278:TYR:CZ	1:D:-63:LYS:HG2	2.55	0.41
1:D:-271:VAL:HG21	1:D:-263:ALA:O	2.21	0.41
2:H:6:DG:H2'	2:H:7:DT:H72	2.03	0.41
1:B:79:VAL:O	1:B:86:THR:HA	2.21	0.41
1:B:79:VAL:HG12	1:B:87:TYR:O	2.21	0.41
1:D:-271:VAL:HG21	1:D:-263:ALA:C	2.42	0.41
1:C:79:VAL:CG1	1:C:87:TYR:CE2	3.04	0.40
1:D:-260:ILE:CD1	1:D:-84:LEU:HD21	2.50	0.40
1:A:-190:ILE:HD12	1:A:-33:GLN:CB	2.51	0.40
1:A:-110:PHE:CG	1:A:-38:MET:HG2	2.56	0.40
1:D:-360:VAL:O	1:D:-359:ILE:HD13	2.21	0.40
1:A:-362:LYS:HG3	5:A:240:HOH:O	2.21	0.40
1:A:47:ILE:HD11	1:B:84:GLY:HA2	2.04	0.40
1:C:-302[A]:ARG:NH2	5:C:202:HOH:O	2.26	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	436/439 (99%)	431 (99%)	5 (1%)	0	100	100
1	B	434/439 (99%)	430 (99%)	4 (1%)	0	100	100
1	C	436/439 (99%)	429 (98%)	7 (2%)	0	100	100
1	D	434/439 (99%)	426 (98%)	8 (2%)	0	100	100
All	All	1740/1756 (99%)	1716 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	345/345 (100%)	337 (98%)	8 (2%)	50	38
1	B	343/345 (99%)	337 (98%)	6 (2%)	60	49
1	C	345/345 (100%)	344 (100%)	1 (0%)	92	93
1	D	343/345 (99%)	338 (98%)	5 (2%)	65	56
All	All	1376/1380 (100%)	1356 (98%)	20 (2%)	65	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-110	PHE
1	D	-337	THR

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Mol	Chain	Res	Type
1	D	-315	THR
1	D	-110	PHE
1	D	-94	GLU
1	D	-14	ARG
1	A	-362	LYS
1	A	-315	THR
1	A	-166	LYS
1	A	-110	PHE
1	A	-31	SER
1	A	23	ARG
1	A	35	ARG
1	A	81	GLU
1	B	-366	ILE
1	B	-231	LYS
1	B	-110	PHE
1	B	28	ARG
1	B	38	ARG
1	B	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
1	A	-319	GLN
1	A	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 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	$\#\|Z\| > 2$
3	GLC	K	1	3	12,12,12	0.51	0	17,17,17	0.62	0
3	GLC	K	2	3	11,11,12	0.62	0	15,15,17	0.74	0
3	GLC	L	1	3	12,12,12	0.49	0	17,17,17	0.86	0
3	GLC	L	2	3	11,11,12	0.61	0	15,15,17	0.98	1 (6%)
3	GLC	M	1	3	12,12,12	0.52	0	17,17,17	0.58	0
3	GLC	M	2	3	11,11,12	0.63	0	15,15,17	0.78	0
3	GLC	N	1	3	12,12,12	0.56	0	17,17,17	0.62	0
3	GLC	N	2	3	11,11,12	0.61	0	15,15,17	0.72	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
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	1	3	-	0/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	N	1	3	-	0/2/22/22	0/1/1/1
3	GLC	N	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	2	GLC	C1-O5-C5	2.59	115.70	112.19

There are no chirality outliers.

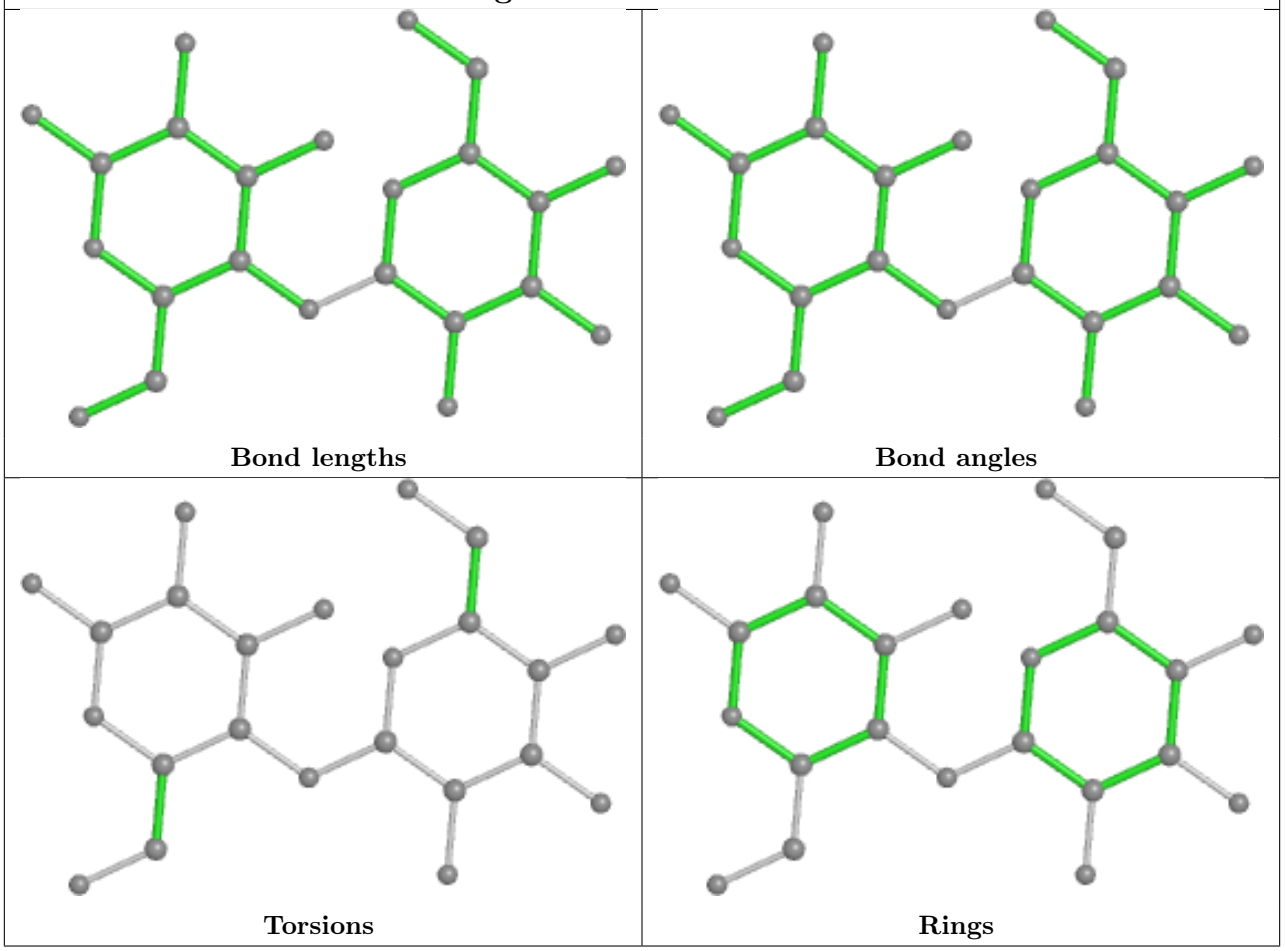
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

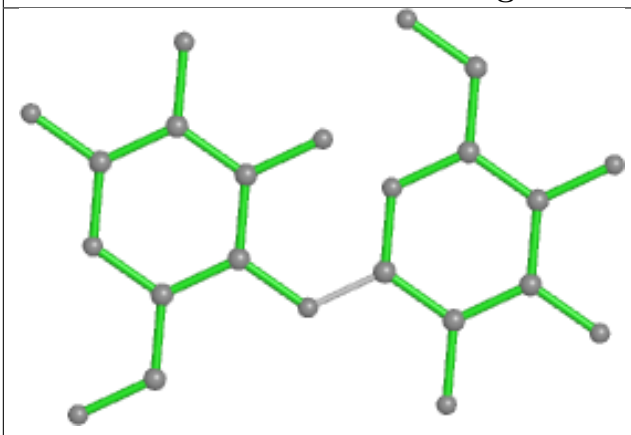
Oligosaccharide Chain K



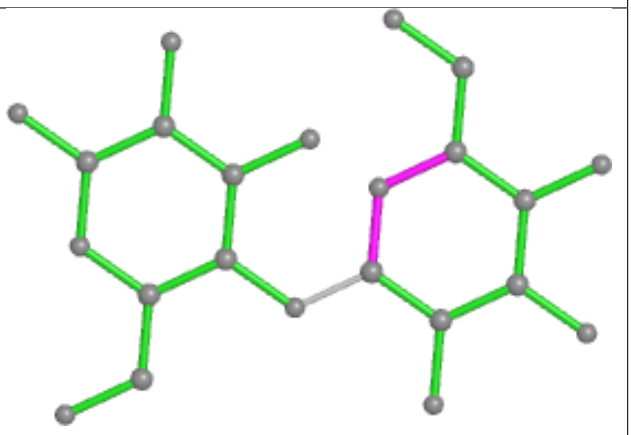
Bond lengths **Bond angles**

Torsions **Rings**

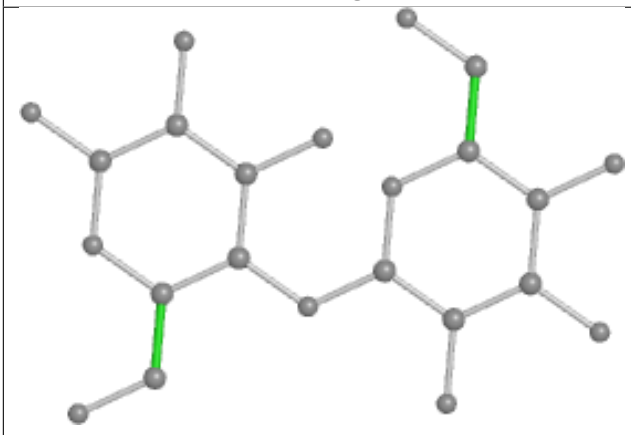
Oligosaccharide Chain L



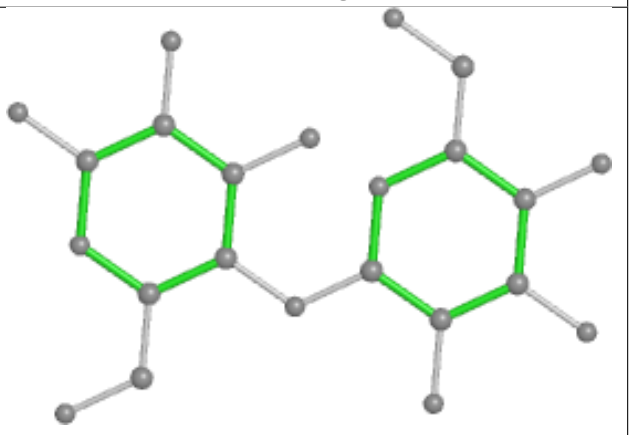
Bond lengths



Bond angles

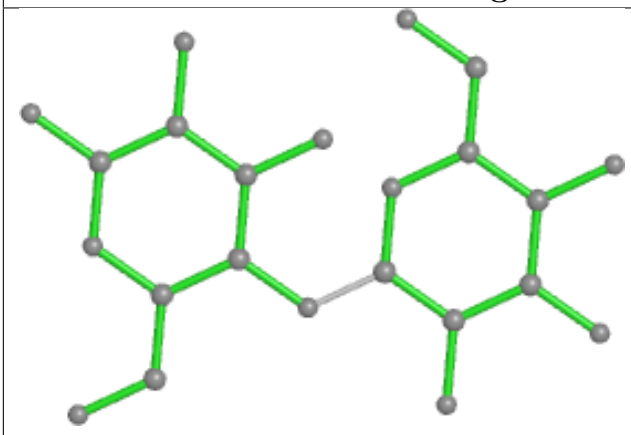


Torsions

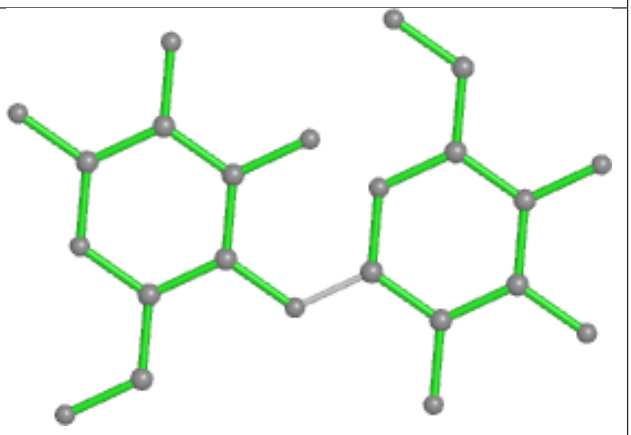


Rings

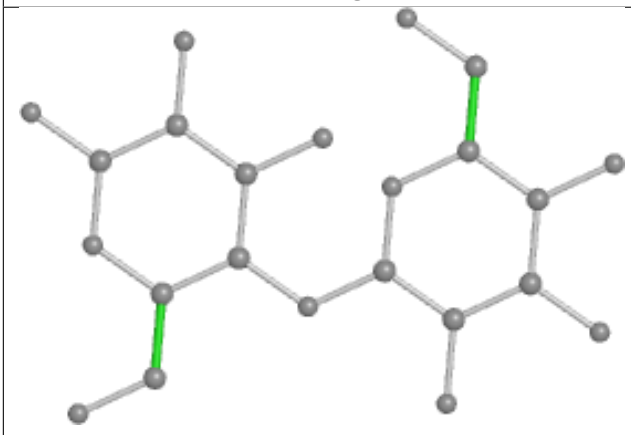
Oligosaccharide Chain M



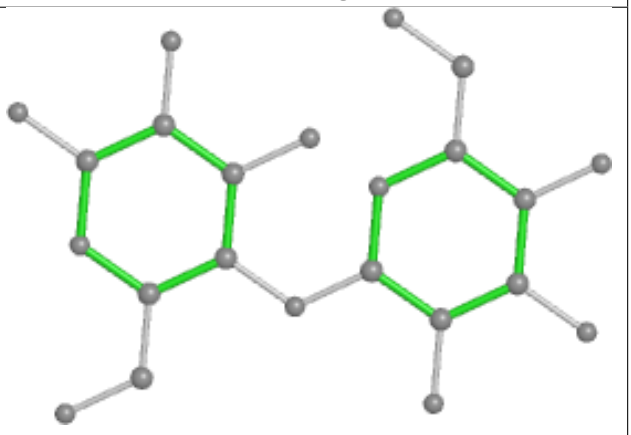
Bond lengths



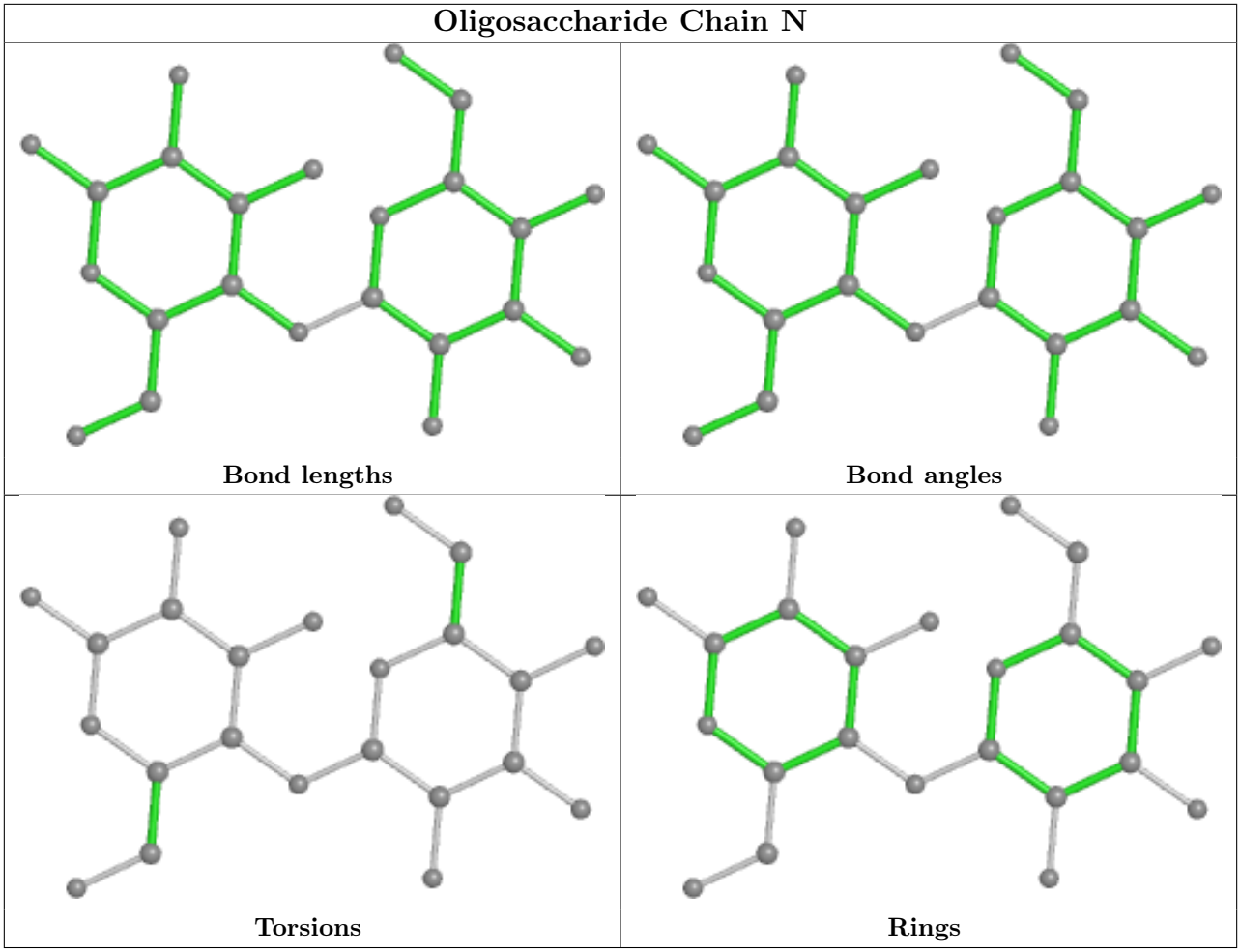
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	101	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	C	101	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	D	101	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	C	103	-	3,3,3	0.47	0	2,2,2	0.58	0
4	EDO	A	101	-	3,3,3	0.48	0	2,2,2	0.28	0
4	EDO	C	102	-	3,3,3	0.47	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	102	-	3,3,3	0.48	0	2,2,2	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	101	-	-	0/1/1/1	-
4	EDO	C	101	-	-	0/1/1/1	-
4	EDO	D	101	-	-	1/1/1/1	-
4	EDO	C	103	-	-	0/1/1/1	-
4	EDO	A	101	-	-	0/1/1/1	-
4	EDO	C	102	-	-	1/1/1/1	-
4	EDO	A	102	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	102	EDO	O1-C1-C2-O2
4	D	101	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	101	EDO	2	0
4	A	102	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	437/439 (99%)	0.41	39 (8%) 9 14	24, 45, 93, 107	0
1	B	436/439 (99%)	0.53	44 (10%) 7 10	22, 42, 97, 121	0
1	C	437/439 (99%)	0.14	11 (2%) 57 64	26, 47, 73, 104	0
1	D	436/439 (99%)	0.56	33 (7%) 13 19	30, 59, 101, 119	0
2	E	15/15 (100%)	-0.05	0 100 100	56, 62, 88, 94	0
2	F	15/15 (100%)	0.10	0 100 100	47, 68, 87, 93	0
2	G	15/15 (100%)	-0.25	0 100 100	32, 37, 63, 65	0
2	H	15/15 (100%)	-0.43	0 100 100	30, 38, 51, 56	0
All	All	1806/1816 (99%)	0.39	127 (7%) 16 22	22, 49, 94, 121	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	TRP	9.5
1	A	27	TRP	6.6
1	C	-129	ALA	6.5
1	B	42	ALA	5.6
1	B	87	TYR	5.5
1	A	87	TYR	5.4
1	D	-297	ALA	5.3
1	B	34	ARG	5.2
1	A	76	ALA	5.1
1	B	76	ALA	5.1
1	B	24	LYS	5.0
1	D	-363	GLY	4.9
1	A	85	THR	4.8
1	B	56	ASP	4.8
1	B	85	THR	4.7
1	B	38	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	-289	ILE	4.6
1	A	56	ASP	4.6
1	A	86	THR	4.3
1	A	59	LEU	4.3
1	B	80	VAL	4.2
1	D	-343	LYS	4.2
1	A	34	ARG	3.9
1	D	-269	TYR	3.9
1	B	57	TYR	3.9
1	B	77	GLY	3.8
1	D	-27	TYR	3.8
1	B	35	ARG	3.8
1	B	-225	GLY	3.8
1	A	-366	ILE	3.8
1	A	79	VAL	3.8
1	D	-292	LEU	3.7
1	C	-225	GLY	3.7
1	A	53	ALA	3.6
1	D	-129	ALA	3.6
1	A	57	TYR	3.6
1	B	28	ARG	3.6
1	B	79	VAL	3.6
1	D	-262	TYR	3.6
1	B	25	PRO	3.6
1	D	-337	THR	3.5
1	A	39	ARG	3.5
1	D	-190	ILE	3.5
1	C	58	ASN	3.5
1	A	-368	MET	3.4
1	D	-267	GLY	3.4
1	B	53	ALA	3.4
1	A	80	VAL	3.4
1	A	-27	TYR	3.4
1	A	74	VAL	3.4
1	D	-339	LYS	3.3
1	B	33	ASN	3.3
1	D	-81	ASP	3.3
1	A	38	ARG	3.2
1	A	-197	TYR	3.2
1	B	-27	TYR	3.2
1	A	22	ARG	3.2
1	D	-346	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLU	3.2
1	A	-195	ALA	3.0
1	B	86	THR	3.0
1	A	-227	ALA	3.0
1	D	-293	LEU	3.0
1	B	88	ARG	2.9
1	B	26	SER	2.9
1	D	-364	GLU	2.9
1	B	36	ARG	2.9
1	C	-27	TYR	2.9
1	D	-333	VAL	2.9
1	A	61	LYS	2.8
1	B	30	ARG	2.8
1	B	39	ARG	2.8
1	C	87	TYR	2.8
1	A	-247	LEU	2.7
1	C	-97	PRO	2.7
1	D	-283	PHE	2.7
1	B	69	LEU	2.7
1	A	35	ARG	2.6
1	B	-129	ALA	2.6
1	B	-44	ALA	2.6
1	D	-331	VAL	2.6
1	A	32	ASN	2.5
1	C	-227	ALA	2.5
1	B	51	LEU	2.5
1	A	30	ARG	2.5
1	B	-244	ASN	2.5
1	B	48	TYR	2.5
1	B	41	ARG	2.4
1	B	54	GLN	2.4
1	D	-342	LYS	2.4
1	A	77	GLY	2.4
1	A	42	ALA	2.4
1	C	79	VAL	2.4
1	B	-227	ALA	2.3
1	D	-89	PHE	2.3
1	D	21	ALA	2.3
1	B	-366	ILE	2.3
1	A	-129	ALA	2.3
1	C	-339	LYS	2.3
1	B	62	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	47	ILE	2.3
1	D	-281	ASP	2.3
1	A	88	ARG	2.3
1	D	-196	ALA	2.2
1	D	-279	LEU	2.2
1	B	82	GLU	2.2
1	A	28	ARG	2.2
1	B	23	ARG	2.2
1	D	-359	ILE	2.2
1	A	78	TRP	2.2
1	D	-275	THR	2.2
1	D	-189	LYS	2.2
1	C	-233	LEU	2.2
1	B	58	ASN	2.2
1	C	56	ASP	2.2
1	A	-183	ASN	2.1
1	D	-268	ASN	2.1
1	A	82	GLU	2.1
1	D	-193	LYS	2.1
1	A	24	LYS	2.1
1	B	-173	LEU	2.1
1	B	55	GLY	2.1
1	B	22	ARG	2.0
1	D	87	TYR	2.0
1	B	37	GLU	2.0
1	A	25	PRO	2.0
1	D	56	ASP	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
3	GLC	N	1	12/12	0.93	0.14	35,44,50,52	0

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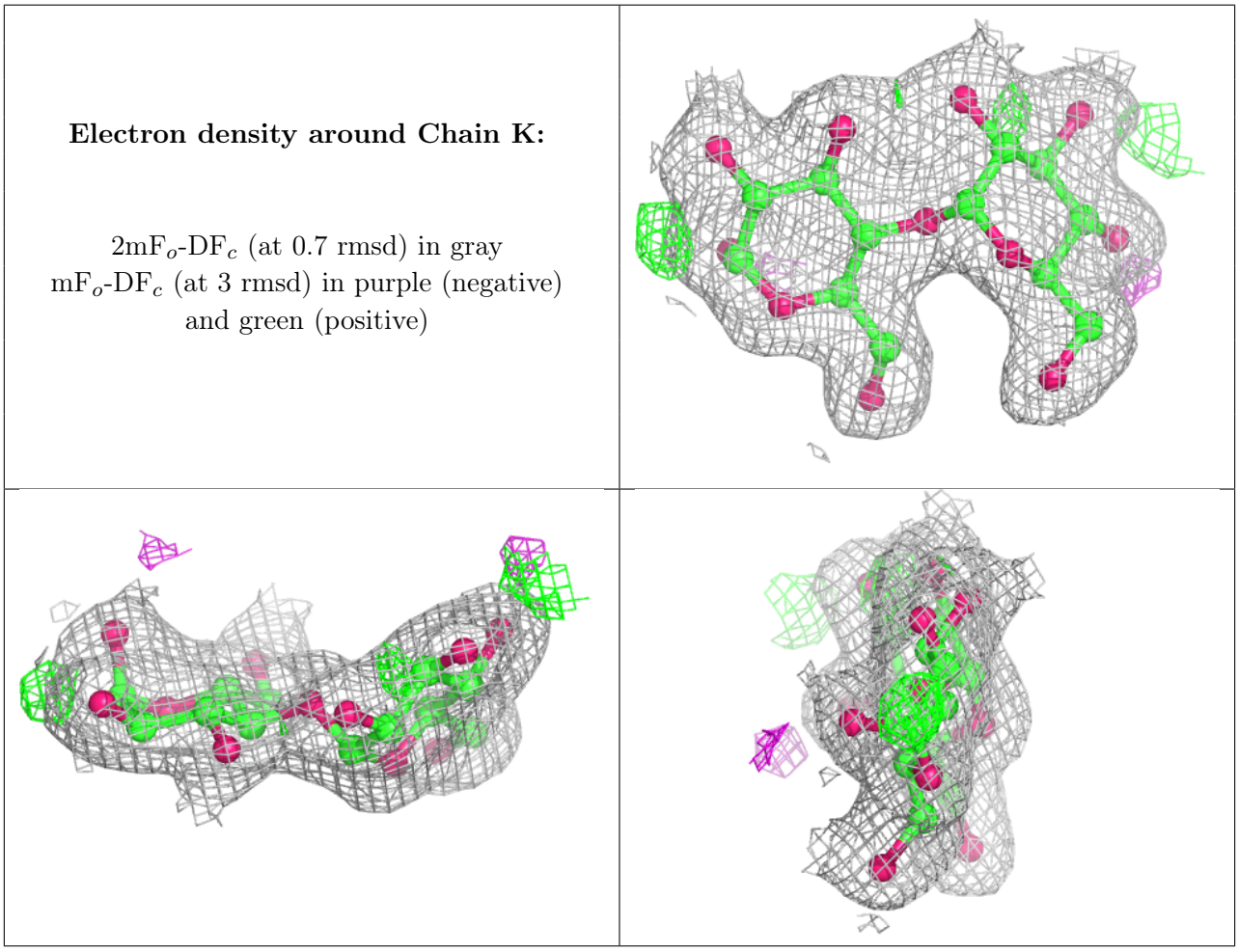
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	N	2	11/12	0.94	0.10	33,41,46,46	0
3	GLC	K	2	11/12	0.95	0.12	25,31,33,33	0
3	GLC	K	1	12/12	0.96	0.17	28,30,36,36	0
3	GLC	M	1	12/12	0.97	0.16	28,31,37,37	0
3	GLC	M	2	11/12	0.97	0.14	27,27,31,33	0
3	GLC	L	1	12/12	0.98	0.16	24,29,32,33	0
3	GLC	L	2	11/12	0.98	0.17	24,27,28,28	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.

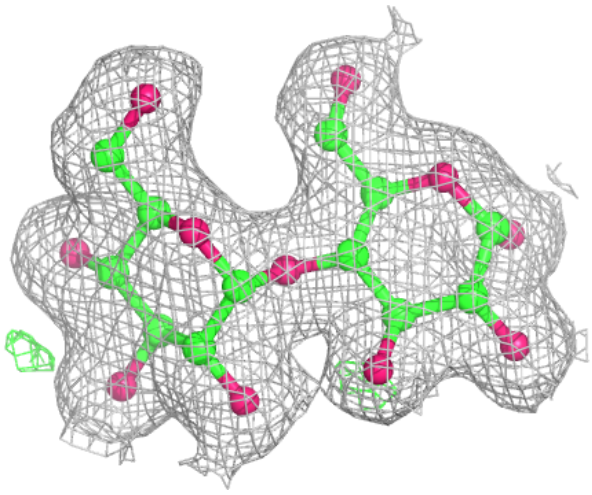
Electron density around Chain K:

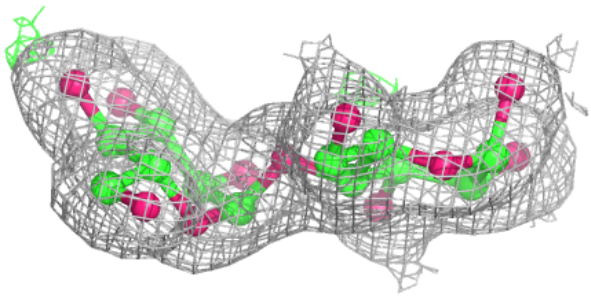
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

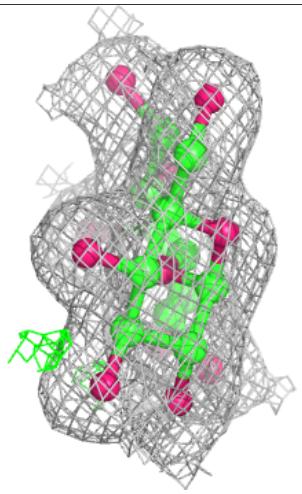


Electron density around Chain L:

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

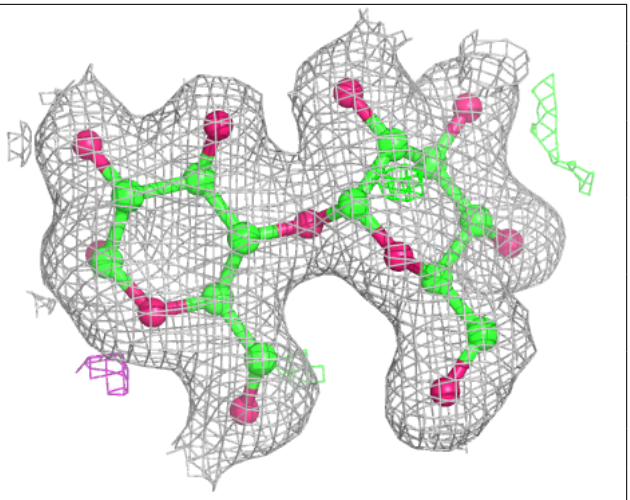


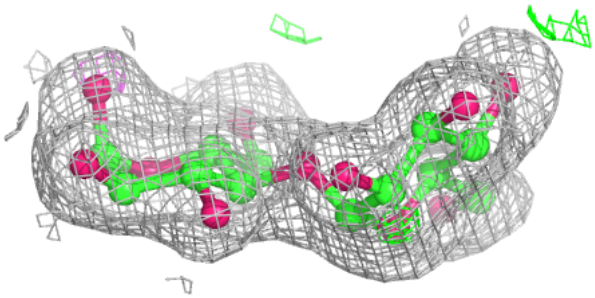


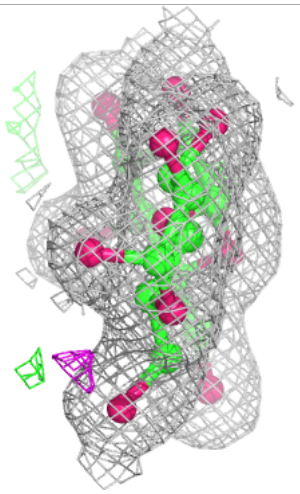


Electron density around Chain M:

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

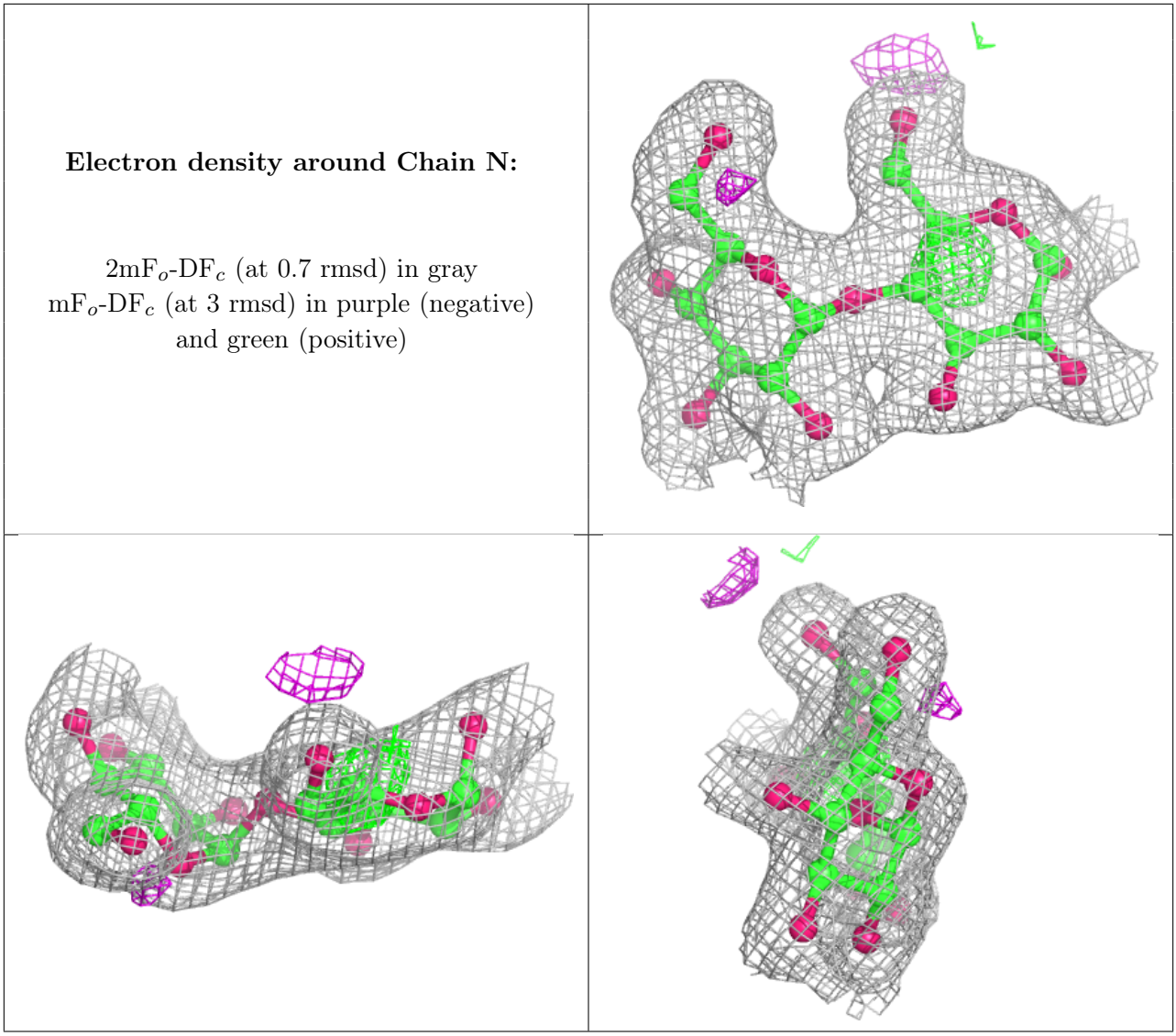






Electron density around Chain N:

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



6.4 Ligands

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	EDO	D	101	4/4	0.73	0.28	40,54,55,65	0
4	EDO	A	102	4/4	0.81	0.25	47,57,59,62	0
4	EDO	C	103	4/4	0.91	0.16	39,49,59,59	0
4	EDO	C	102	4/4	0.94	0.11	47,57,59,67	0
4	EDO	C	101	4/4	0.94	0.11	36,43,53,53	0
4	EDO	A	101	4/4	0.96	0.08	37,46,52,55	0
4	EDO	B	101	4/4	0.97	0.10	32,38,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.