Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:01 AM BST

PDB ID	:	3O95
Title	:	Crystal Structure of Human DPP4 Bound to TAK-100
Authors	:	Yano, J.K.; Aertgeerts, K.
Deposited on	:	2010-08-03
Resolution	:	2.85 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:

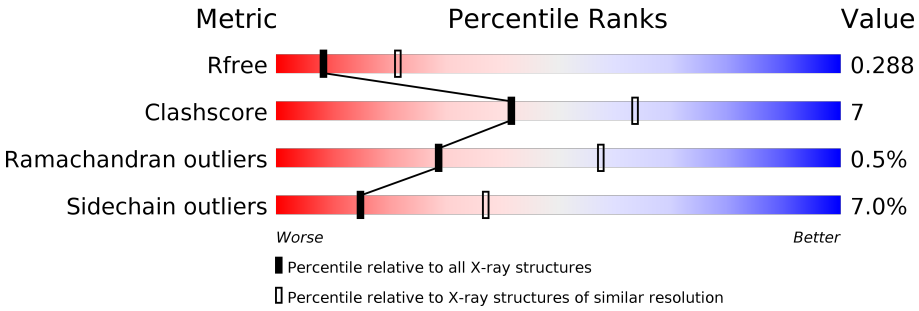
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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%

Mol	Chain	Length	Quality of chain
1	A	740	77% 19%
1	B	740	78% 19%
1	C	740	78% 19%
1	D	740	76% 20%
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	50% 50%
2	I	2	100%
2	J	2	100%
2	L	2	50% 50%
3	K	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	I	1	X	-	-	-
4	NAG	D	5201	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24870 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	726	Total	C	N	O	S	0	0	0
			5946	3818	977	1125	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- 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	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			

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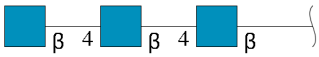
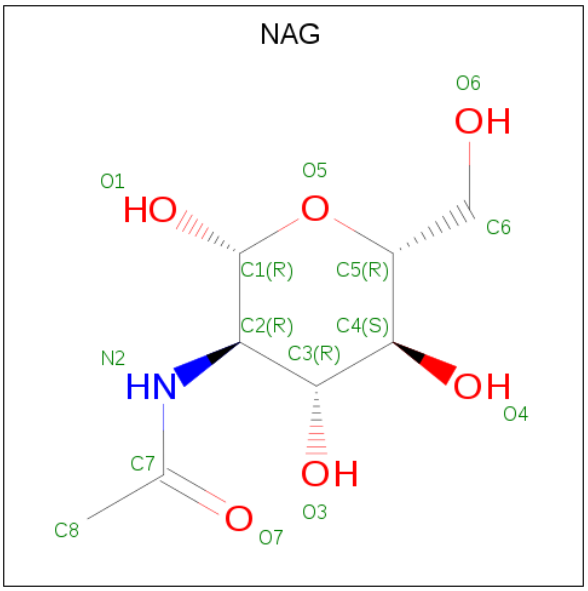
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	2	Total C N O 28 16 2 10	0	0	0
2	I	2	Total C N O 28 16 2 10	0	0	0
2	J	2	Total C N O 28 16 2 10	0	0	0
2	L	2	Total C N O 28 16 2 10	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	3	Total C N O 42 24 3 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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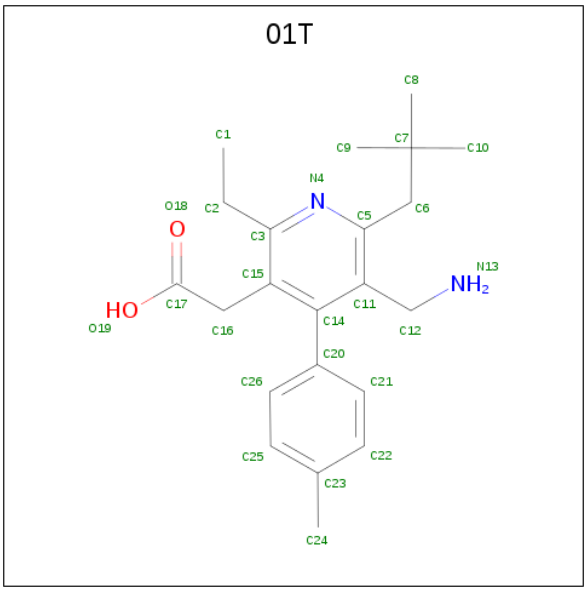
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total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

- Molecule 5 is [5-(aminomethyl)-6-(2,2-dimethylpropyl)-2-ethyl-4-(4-methylphenyl)pyridin-3-yl]acetic acid (three-letter code: 01T) (formula: $C_{22}H_{30}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	22	2	2		
5	B	1	Total	C	N	O	0	0
			26	22	2	2		
5	C	1	Total	C	N	O	0	0
			26	22	2	2		
5	D	1	Total	C	N	O	0	0
			26	22	2	2		

- Molecule 6 is water.

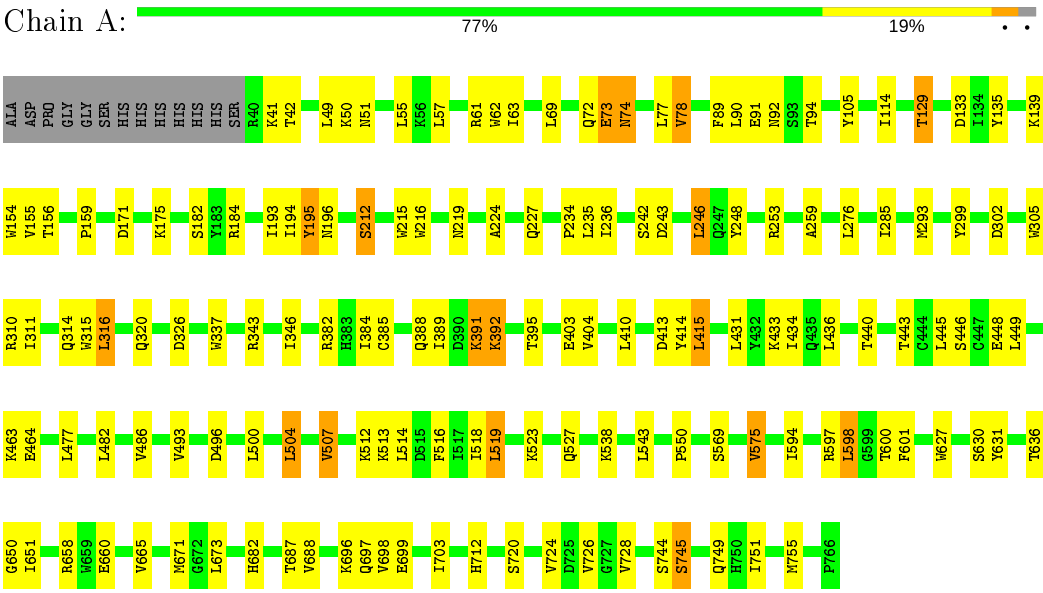
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	B	134	Total	O	0	0
			134	134		
6	C	76	Total	O	0	0
			76	76		
6	D	132	Total	O	0	0
			132	132		

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. 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. 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.

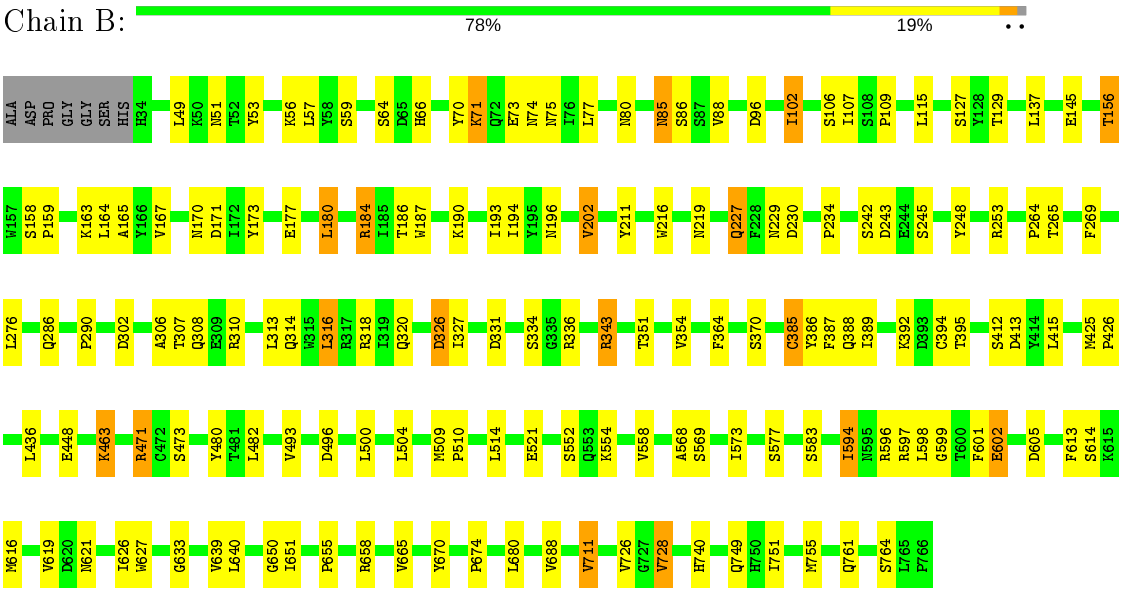
- Molecule 1: Dipeptidyl peptidase 4

Chain A:



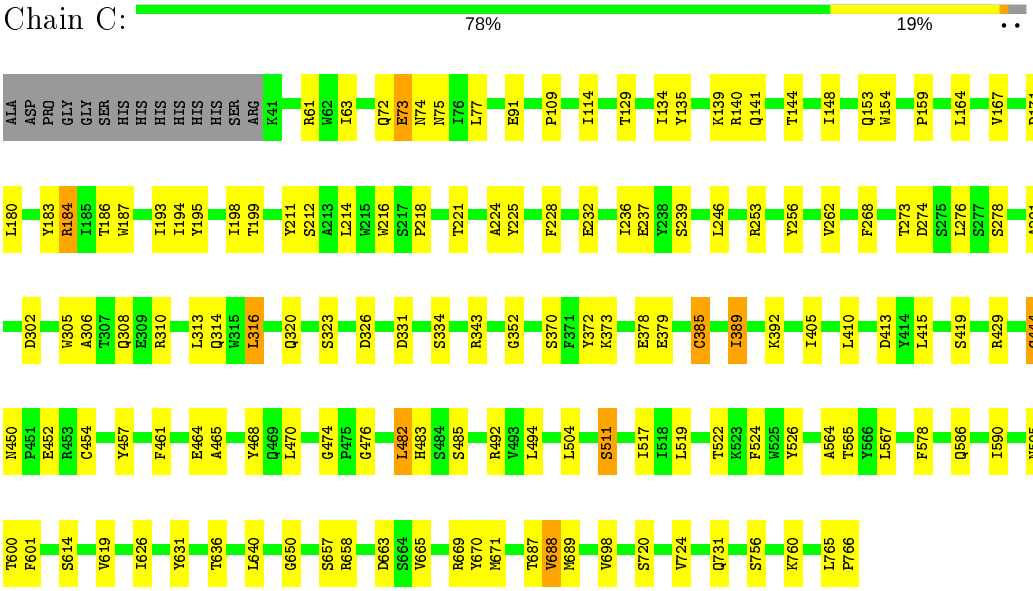
- Molecule 1: Dipeptidyl peptidase 4

Chain B:



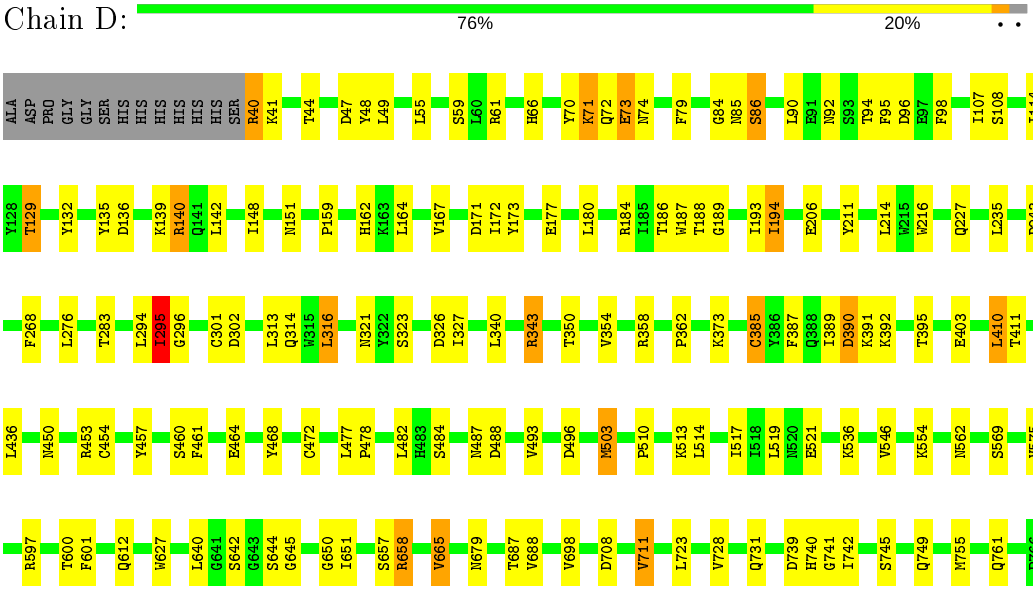
• Molecule 1: Dipeptidyl peptidase 4

Chain C:



• Molecule 1: Dipeptidyl peptidase 4

Chain D:



• 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 H:

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

Chain I:

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

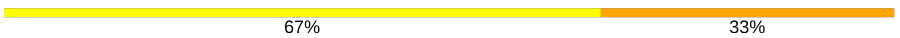
Chain J:

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

Chain L:

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

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.72Å 123.33Å 144.42Å 90.00° 114.78° 90.00°	Depositor
Resolution (Å)	35.00 – 2.85 34.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.00-2.85) 99.2 (34.83-2.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.248 0.242 , 0.288	Depositor DCC
R_{free} test set	4489 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24870	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 01T, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.55	1/6129 (0.0%)	0.62	0/8336
1	B	0.52	0/6190	0.61	0/8419
1	C	0.49	0/6118	0.59	0/8322
1	D	0.54	0/6129	0.61	0/8336
All	All	0.52	1/24566 (0.0%)	0.61	0/33413

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	GLN	CD-OE1	5.07	1.35	1.24

There are no bond angle outliers.

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	5957	0	5673	87	0
1	B	6013	0	5714	81	0
1	C	5946	0	5663	81	0
1	D	5957	0	5674	87	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
2	L	28	0	25	1	0
3	K	42	0	37	1	0
4	A	28	0	26	0	0
4	B	42	0	39	0	0
4	C	42	0	39	0	0
4	D	56	0	52	1	0
5	A	26	0	29	2	0
5	B	26	0	29	1	0
5	C	26	0	29	0	0
5	D	26	0	29	1	0
6	A	145	0	0	1	0
6	B	134	0	0	3	0
6	C	76	0	0	2	0
6	D	132	0	0	6	0
All	All	24870	0	23208	332	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 7.

All (332) 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:D:193:ILE:HG22	1:D:194:ILE:HD13	1.49	0.94
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.94	0.91
4:D:2811:NAG:H2	6:D:845:HOH:O	1.70	0.89
1:C:511:SER:HB3	6:C:812:HOH:O	1.74	0.88
1:B:73:GLU:HA	6:B:866:HOH:O	1.79	0.82
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.64	0.81
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.63	0.80
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.66	0.78
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.78	0.77
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.20	0.76
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.78	0.76
1:A:91:GLU:O	1:A:94:THR:HG22	1.86	0.75
1:C:72:GLN:O	1:C:73:GLU:HB2	1.86	0.75
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.33	0.73
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD23	1:B:86:SER:HB2	1.72	0.71
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.71	0.71
1:B:614:SER:HA	1:B:619:VAL:HB	1.73	0.70
1:A:343:ARG:HD3	1:A:389:ILE:CG2	2.21	0.69
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.74	0.69
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.74	0.69
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.76	0.68
1:A:343:ARG:HD3	1:A:389:ILE:HG23	1.75	0.67
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.77	0.66
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.78	0.66
1:C:184:ARG:HD3	1:C:186:THR:O	1.96	0.66
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.78	0.65
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.77	0.65
1:B:290:PRO:HG3	1:B:326:ASP:OD1	1.97	0.64
1:A:74:ASN:HB2	1:A:92:ASN:CB	2.28	0.64
2:I:1:NAG:H61	2:I:2:NAG:C7	2.29	0.63
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.62	0.63
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.34	0.62
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.80	0.62
1:B:471:ARG:HG2	1:B:480:TYR:CE1	2.34	0.62
1:A:74:ASN:HB2	1:A:92:ASN:HB3	1.80	0.62
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.35	0.62
1:D:84:GLY:C	1:D:86:SER:H	2.03	0.62
1:A:751:ILE:O	1:A:755:MET:HG3	2.00	0.61
1:D:723:LEU:HD22	1:D:728:VAL:HG11	1.82	0.61
1:B:316:LEU:HD13	1:B:320:GLN:HG2	1.83	0.60
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.37	0.60
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.82	0.60
1:B:184:ARG:HD3	1:B:186:THR:O	2.01	0.59
1:C:614:SER:HA	1:C:619:VAL:HB	1.83	0.59
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.36	0.59
1:C:177:GLU:HB2	1:C:180:LEU:HG	1.83	0.59
1:D:723:LEU:HB3	1:D:728:VAL:HG13	1.84	0.59
1:B:242:SER:OG	1:B:243:ASP:N	2.36	0.59
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.38	0.58
1:B:613:PHE:O	1:B:616:MET:HB2	2.03	0.58
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.85	0.58
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.03	0.58
1:C:167:VAL:HA	1:C:171:ASP:O	2.03	0.58
1:B:73:GLU:O	1:B:74:ASN:HB2	2.04	0.57
1:D:70:TYR:CE2	1:D:71:LYS:HE3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.39	0.57
1:C:72:GLN:O	1:C:73:GLU:CB	2.53	0.57
1:A:72:GLN:O	1:A:73:GLU:HB2	2.05	0.57
1:D:72:GLN:C	1:D:74:ASN:H	2.08	0.56
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.88	0.56
1:C:657:SER:HA	1:C:688:VAL:CG1	2.36	0.56
1:D:206:GLU:HB3	1:D:665:VAL:CG2	2.35	0.56
1:C:172:ILE:HD13	1:C:214:LEU:HD21	1.88	0.56
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.88	0.56
1:B:202:VAL:HG22	6:B:799:HOH:O	2.05	0.55
1:B:127:SER:HB3	1:B:211:TYR:CG	2.41	0.55
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.36	0.55
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.88	0.55
1:B:554:LYS:HE3	6:B:797:HOH:O	2.06	0.55
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.37	0.55
1:A:253:ARG:NH2	1:B:253:ARG:HH21	2.04	0.55
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.41	0.55
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.90	0.54
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.08	0.53
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.90	0.53
1:A:518:ILE:O	1:A:519:LEU:HD13	2.08	0.53
1:B:751:ILE:O	1:B:755:MET:HG3	2.07	0.53
1:A:433:LYS:HD2	1:A:445:LEU:HD21	1.90	0.53
1:C:598:LEU:HG	1:C:631:TYR:OH	2.07	0.53
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.90	0.53
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.90	0.53
1:B:64:SER:O	1:B:463:LYS:HB2	2.09	0.53
1:B:493:VAL:HG11	1:B:496:ASP:HB3	1.91	0.53
1:D:73:GLU:O	1:D:74:ASN:HB2	2.09	0.53
1:A:63:ILE:HD11	1:A:69:LEU:HG	1.92	0.52
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.90	0.52
1:A:242:SER:OG	1:A:243:ASP:N	2.41	0.52
1:C:465:ALA:O	1:C:485:SER:OG	2.24	0.52
1:B:626:ILE:HD13	1:B:639:VAL:HG11	1.91	0.52
1:D:761:GLN:HB3	6:D:880:HOH:O	2.10	0.52
1:A:129:THR:HG23	1:A:151:ASN:HA	1.91	0.52
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.74	0.52
1:B:102:ILE:HD12	1:B:102:ILE:H	1.75	0.51
1:A:598:LEU:HG	1:A:631:TYR:OH	2.11	0.51
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.92	0.51
1:D:184:ARG:HD3	1:D:186:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.45	0.51
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.44	0.51
1:D:79:PHE:HA	1:D:86:SER:HB3	1.93	0.51
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.93	0.51
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.93	0.51
1:A:550:PRO:HB3	1:A:594:ILE:HD11	1.92	0.51
1:C:731:GLN:NE2	1:D:731:GLN:OE1	2.44	0.51
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.46	0.50
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.40	0.50
1:A:346:ILE:H	1:A:392:LYS:NZ	2.09	0.50
1:C:75:ASN:HD22	1:C:91:GLU:HG2	1.76	0.50
1:D:410:LEU:HD22	1:D:411:THR:O	2.11	0.50
1:B:471:ARG:CG	1:B:480:TYR:CE1	2.94	0.50
1:C:522:THR:HB	1:C:524:PHE:CE2	2.46	0.50
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.46	0.50
1:D:107:ILE:HG22	1:D:108:SER:O	2.11	0.50
1:D:389:ILE:HG22	1:D:390:ASP:OD1	2.12	0.50
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.92	0.50
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.47	0.50
1:D:189:GLY:HA2	1:D:194:ILE:HG22	1.94	0.50
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.42	0.49
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.42	0.49
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.45	0.49
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.94	0.49
1:C:756:SER:O	1:C:760:LYS:HG3	2.12	0.49
1:A:42:THR:HB	1:A:569:SER:OG	2.12	0.49
1:A:63:ILE:CD1	1:A:69:LEU:HG	2.42	0.49
1:C:586:GLN:HB3	1:C:590:ILE:HD12	1.95	0.49
1:A:154:TRP:CD1	1:A:212:SER:HB2	2.47	0.49
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.95	0.49
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.95	0.49
1:B:554:LYS:HB3	1:B:577:SER:HB3	1.93	0.49
1:B:651:ILE:HD13	1:B:755:MET:HB3	1.94	0.49
1:C:343:ARG:HD3	1:C:389:ILE:HG23	1.94	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.48
1:C:195:TYR:CD1	1:C:195:TYR:N	2.81	0.48
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.94	0.48
1:C:482:LEU:HB2	1:C:494:LEU:HD21	1.94	0.48
1:C:91:GLU:HB3	6:C:818:HOH:O	2.12	0.48
1:D:127:SER:HB3	1:D:211:TYR:CG	2.48	0.48
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ASP:HB3	1:B:334:SER:HB2	1.95	0.48
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.29	0.48
1:B:243:ASP:OD2	1:B:245:SER:HB2	2.13	0.48
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.95	0.48
1:C:221:THR:HG23	1:C:274:ASP:OD2	2.12	0.48
1:D:268:PHE:CD2	1:D:313:LEU:HD11	2.48	0.48
1:B:334:SER:HB3	1:B:336:ARG:H	1.78	0.47
1:C:291:ALA:O	1:C:295:ILE:HG23	2.14	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.47
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.50	0.47
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.95	0.47
1:B:674:PRO:O	1:B:680:LEU:HD13	2.15	0.47
1:C:139:LYS:HB2	1:C:141:GLN:HG2	1.96	0.47
1:C:268:PHE:CE2	1:C:313:LEU:HD11	2.48	0.47
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.95	0.47
1:C:372:TYR:HA	1:C:385:CYS:O	2.15	0.47
1:A:308:GLN:HA	1:A:308:GLN:OE1	2.15	0.47
1:B:308:GLN:OE1	1:B:308:GLN:HA	2.14	0.47
1:A:195:TYR:N	1:A:195:TYR:CD1	2.82	0.47
1:A:744:SER:O	1:A:745:SER:C	2.54	0.47
1:D:642:SER:OG	1:D:644:SER:HB3	2.15	0.47
1:A:299:TYR:CE1	1:A:665:VAL:HG22	2.50	0.46
1:B:568:ALA:HA	1:B:573:ILE:O	2.15	0.46
1:B:170:ASN:O	1:B:196:ASN:HB2	2.15	0.46
1:C:195:TYR:HB3	1:C:198:ILE:HG13	1.97	0.46
1:D:294:LEU:C	1:D:296:GLY:H	2.19	0.46
1:D:600:THR:OG1	1:D:601:PHE:N	2.47	0.46
1:C:331:ASP:HB3	1:C:334:SER:HB2	1.97	0.46
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.98	0.46
1:B:415:LEU:HD23	1:B:415:LEU:C	2.35	0.46
1:B:599:GLY:N	1:B:602:GLU:OE2	2.37	0.46
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.98	0.46
1:B:343:ARG:HD2	1:B:389:ILE:HG23	1.97	0.46
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.97	0.46
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.97	0.46
1:D:708:ASP:OD1	1:D:740:HIS:HA	2.15	0.46
1:D:194:ILE:HG13	2:L:1:NAG:H82	1.98	0.46
1:C:429:ARG:HB2	1:C:457:TYR:H	1.81	0.46
1:C:444:CYS:SG	1:C:445:LEU:N	2.88	0.46
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.15	0.46
1:D:44:THR:O	1:D:47:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:CE2	1:B:286:GLN:HB2	2.51	0.45
1:B:109:PRO:HG2	1:B:158:SER:O	2.16	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.47	0.45
1:C:218:PRO:HD3	1:C:305:TRP:HB3	1.98	0.45
1:C:405:ILE:HG12	1:C:419:SER:HA	1.97	0.45
1:D:450:ASN:O	1:D:454:CYS:HB2	2.16	0.45
1:D:472:CYS:O	1:D:478:PRO:HA	2.17	0.45
1:A:253:ARG:HH21	1:B:253:ARG:NH2	2.08	0.45
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.99	0.45
1:D:139:LYS:O	1:D:139:LYS:HG2	2.15	0.45
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.97	0.45
1:D:301:CYS:SG	1:D:316:LEU:HB2	2.57	0.45
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.98	0.45
1:D:132:TYR:HB2	1:D:148:ILE:HG21	1.98	0.45
1:D:162:HIS:NE2	1:D:177:GLU:OE2	2.45	0.45
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.99	0.45
1:C:464:GLU:O	1:C:464:GLU:HG3	2.16	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.17	0.45
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.30	0.45
1:A:171:ASP:OD1	1:A:184:ARG:NH2	2.50	0.45
1:A:139:LYS:O	1:A:140:ARG:HB2	2.17	0.45
1:B:71:LYS:HA	1:B:75:ASN:O	2.17	0.45
1:B:156:THR:HG23	1:B:165:ALA:HB3	1.99	0.45
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.47	0.45
1:A:433:LYS:HB3	1:A:445:LEU:HD11	1.99	0.44
1:B:425:MET:HA	1:B:426:PRO:HD3	1.80	0.44
1:B:473:SER:HB3	1:B:558:VAL:HG13	1.99	0.44
1:D:136:ASP:CG	1:D:139:LYS:HB3	2.37	0.44
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.52	0.44
1:D:484:SER:O	1:D:488:ASP:HA	2.17	0.44
1:D:640:LEU:HB3	1:D:698:VAL:HG21	1.99	0.44
1:A:453:ARG:NH2	1:A:477:LEU:O	2.41	0.44
1:A:293:MET:HG3	1:A:315:TRP:HB2	1.98	0.44
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.98	0.44
1:C:316:LEU:HD13	1:C:320:GLN:HG2	1.99	0.44
1:C:352:GLY:HA2	1:C:595:ASN:OD1	2.17	0.44
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.52	0.44
6:A:859:HOH:O	1:D:40:ARG:HG2	2.17	0.44
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.98	0.44
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.48	0.44
1:D:321:ASN:ND2	6:D:843:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:THR:HA	1:C:228:PHE:CE2	2.53	0.44
1:C:474:GLY:HA2	1:C:476:GLY:O	2.18	0.44
1:D:167:VAL:HA	1:D:171:ASP:O	2.18	0.44
1:D:173:TYR:CE1	1:D:184:ARG:HG3	2.53	0.43
1:C:232:GLU:HB2	1:C:262:VAL:HG11	2.00	0.43
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.43
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.99	0.43
1:A:703:ILE:HG21	1:A:751:ILE:HD12	2.00	0.43
1:C:657:SER:HA	1:C:688:VAL:HG12	1.99	0.43
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.99	0.43
1:C:218:PRO:HD3	1:C:305:TRP:CB	2.49	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HB3	2.01	0.43
1:C:236:ILE:HD12	1:D:249:PRO:HD2	2.00	0.43
1:D:487:ASN:O	1:D:488:ASP:HB2	2.17	0.43
1:D:645:GLY:HA2	6:D:841:HOH:O	2.18	0.43
1:A:215:TRP:HB2	1:A:224:ALA:HB3	1.99	0.43
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.01	0.43
1:B:53:TYR:HB3	1:B:500:LEU:CD1	2.48	0.43
1:B:219:ASN:HB3	1:B:308:GLN:NE2	2.33	0.43
1:B:307:THR:OG1	1:B:310:ARG:HB3	2.18	0.43
1:D:385:CYS:HB3	1:D:387:PHE:CE2	2.53	0.43
1:A:636:THR:HG21	1:A:651:ILE:O	2.18	0.43
1:C:720:SER:O	1:C:724:VAL:HG23	2.19	0.43
1:D:657:SER:HA	1:D:688:VAL:HG13	1.99	0.43
1:D:453:ARG:HD2	1:D:477:LEU:O	2.19	0.43
1:A:446:SER:HA	1:A:449:LEU:HG	2.01	0.43
1:B:167:VAL:HA	1:B:171:ASP:O	2.19	0.43
1:B:318:ARG:O	1:B:320:GLN:HG3	2.19	0.43
1:B:59:SER:O	1:B:70:TYR:CD1	2.72	0.43
1:C:153:GLN:HB3	1:C:211:TYR:CE1	2.54	0.43
1:A:431:LEU:HD13	1:A:459:VAL:HG11	2.01	0.42
1:A:62:TRP:C	1:A:63:ILE:HD12	2.40	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.52	0.42
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.49	0.42
1:D:554:LYS:HB3	1:D:577:SER:HB3	2.02	0.42
1:A:391:LYS:HE2	1:A:391:LYS:HB3	1.85	0.42
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.84	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.55	0.42
1:C:183:TYR:CD2	1:C:276:LEU:HD23	2.55	0.42
1:A:219:ASN:HB3	1:A:308:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:HD22	1:A:671:MET:HG2	2.01	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.42
1:C:598:LEU:HD22	1:C:671:MET:HG2	2.01	0.42
1:A:316:LEU:HD13	1:A:320:GLN:HG2	2.02	0.42
1:C:564:ALA:HA	1:C:567:LEU:HD12	2.02	0.42
1:D:142:LEU:H	1:D:142:LEU:HD23	1.84	0.42
1:D:562:ASN:HB2	6:D:869:HOH:O	2.20	0.42
1:A:543:LEU:O	1:A:575:VAL:HA	2.19	0.42
1:B:177:GLU:HB2	1:B:180:LEU:HD22	2.02	0.42
1:A:219:ASN:HB3	1:A:308:GLN:NE2	2.35	0.42
1:C:657:SER:HB2	1:C:689:MET:SD	2.60	0.42
5:D:1:01T:C26	5:D:1:01T:H12	2.49	0.42
1:C:194:ILE:HD13	3:K:1:NAG:H82	2.01	0.42
1:A:382:ARG:H	1:A:403:GLU:HG2	1.85	0.41
1:A:597:ARG:HH11	1:A:682:HIS:CB	2.32	0.41
1:A:49:LEU:HD22	1:A:749:GLN:HA	2.01	0.41
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.41
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.55	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.86	0.41
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.02	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:A:90:LEU:CD2	1:A:114:ILE:HD13	2.50	0.41
1:B:552:SER:O	1:B:583:SER:HB2	2.20	0.41
1:C:114:ILE:HG22	1:C:135:TYR:HB2	2.02	0.41
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.41
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.55	0.41
1:D:739:ASP:HB2	6:D:828:HOH:O	2.21	0.41
1:D:651:ILE:HD13	1:D:755:MET:HG2	2.02	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.41
1:A:600:THR:OG1	1:A:601:PHE:N	2.51	0.41
1:A:720:SER:O	1:A:724:VAL:HG23	2.20	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.41
1:C:73:GLU:HB3	1:C:74:ASN:H	1.65	0.41
1:D:314:GLN:OE1	1:D:362:PRO:HD3	2.19	0.41
1:D:503:MET:HG2	1:D:503:MET:H	1.46	0.41
1:A:285:ILE:HG21	1:A:337:TRP:HD1	1.86	0.41
1:A:493:VAL:HG11	1:A:496:ASP:HB3	2.03	0.41
1:B:633:GLY:HA3	1:B:655:PRO:HB3	2.03	0.41
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.56	0.41
1:D:295:ILE:O	1:D:295:ILE:HG23	2.21	0.41
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.02	0.41
5:B:1:01T:H12A	5:B:1:01T:H6A	1.90	0.41
1:A:630:SER:OG	5:A:1:01T:C22	2.69	0.41
1:B:386:TYR:O	1:B:394:CYS:HB2	2.21	0.41
1:B:601:PHE:O	1:B:605:ASP:N	2.47	0.41
1:B:80:ASN:HB2	1:B:85:ASN:HB2	2.03	0.41
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.56	0.41
1:D:139:LYS:O	1:D:140:ARG:HB2	2.20	0.41
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.02	0.41
5:A:1:01T:H6A	5:A:1:01T:H12A	1.84	0.41
1:A:414:TYR:CD2	1:A:433:LYS:HE2	2.56	0.41
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.02	0.41
1:B:102:ILE:H	1:B:102:ILE:CD1	2.34	0.41
1:C:154:TRP:CD2	1:C:212:SER:HB3	2.56	0.41
1:D:429:ARG:HB2	1:D:457:TYR:H	1.86	0.40
1:D:493:VAL:HG11	1:D:496:ASP:HB3	2.02	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.02	0.40
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.21	0.40
1:B:49:LEU:HB3	1:B:749:GLN:HG2	2.03	0.40
1:C:517:ILE:HD11	1:C:578:PHE:CE1	2.56	0.40
1:C:626:ILE:HG12	1:C:636:THR:HG23	2.03	0.40
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.56	0.40
1:B:594:ILE:HG12	1:B:598:LEU:HD23	2.03	0.40
1:D:129:THR:HG23	1:D:151:ASN:HA	2.04	0.40
1:C:299:TYR:CE1	1:C:665:VAL:HG22	2.56	0.40
1:C:658:ARG:CB	1:C:687:THR:HG22	2.50	0.40
1:D:741:GLY:O	1:D:742:ILE:C	2.59	0.40
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.03	0.40
1:C:450:ASN:O	1:C:454:CYS:HB2	2.22	0.40
2:J:1:NAG:H62	2:J:2:NAG:N2	2.36	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	725/740 (98%)	674 (93%)	47 (6%)	4 (1%)	25	53
1	B	731/740 (99%)	682 (93%)	47 (6%)	2 (0%)	41	68
1	C	724/740 (98%)	667 (92%)	54 (8%)	3 (0%)	34	62
1	D	725/740 (98%)	675 (93%)	44 (6%)	6 (1%)	19	46
All	All	2905/2960 (98%)	2698 (93%)	192 (7%)	15 (0%)	29	57

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	85	ASN
1	C	73	GLU
1	D	85	ASN
1	D	140	ARG
1	A	140	ARG
1	D	73	GLU
1	D	86	SER
1	D	521	GLU
1	A	745	SER
1	B	88	VAL
1	C	389	ILE
1	C	109	PRO
1	A	486	VAL
1	D	295	ILE

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	652/662 (98%)	607 (93%)	45 (7%)	15	38
1	B	658/662 (99%)	608 (92%)	50 (8%)	13	33
1	C	651/662 (98%)	617 (95%)	34 (5%)	23	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	652/662 (98%)	598 (92%)	54 (8%)	11 29
All	All	2613/2648 (99%)	2430 (93%)	183 (7%)	15 37

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	50	LYS
1	A	51	ASN
1	A	57	LEU
1	A	61	ARG
1	A	74	ASN
1	A	77	LEU
1	A	78	VAL
1	A	129	THR
1	A	133	ASP
1	A	155	VAL
1	A	156	THR
1	A	195	TYR
1	A	212	SER
1	A	235	LEU
1	A	246	LEU
1	A	276	LEU
1	A	316	LEU
1	A	326	ASP
1	A	385	CYS
1	A	388	GLN
1	A	391	LYS
1	A	392	LYS
1	A	395	THR
1	A	410	LEU
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	443	THR
1	A	448	GLU
1	A	453	ARG
1	A	463	LYS
1	A	464	GLU
1	A	482	LEU
1	A	504	LEU

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Mol	Chain	Res	Type
1	A	507	VAL
1	A	512	LYS
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	575	VAL
1	A	598	LEU
1	A	673	LEU
1	A	688	VAL
1	B	51	ASN
1	B	56	LYS
1	B	57	LEU
1	B	66	HIS
1	B	71	LYS
1	B	96	ASP
1	B	102	ILE
1	B	107	ILE
1	B	129	THR
1	B	137	LEU
1	B	145	GLU
1	B	156	THR
1	B	164	LEU
1	B	180	LEU
1	B	184	ARG
1	B	190	LYS
1	B	202	VAL
1	B	227	GLN
1	B	276	LEU
1	B	313	LEU
1	B	316	LEU
1	B	326	ASP
1	B	343	ARG
1	B	351	THR
1	B	354	VAL
1	B	370	SER
1	B	385	CYS
1	B	388	GLN
1	B	392	LYS
1	B	395	THR
1	B	412	SER
1	B	413	ASP
1	B	448	GLU

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Mol	Chain	Res	Type
1	B	463	LYS
1	B	471	ARG
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	521	GLU
1	B	594	ILE
1	B	597	ARG
1	B	602	GLU
1	B	627	TRP
1	B	658	ARG
1	B	665	VAL
1	B	688	VAL
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	B	764	SER
1	C	61	ARG
1	C	63	ILE
1	C	77	LEU
1	C	129	THR
1	C	140	ARG
1	C	144	THR
1	C	164	LEU
1	C	184	ARG
1	C	239	SER
1	C	246	LEU
1	C	278	SER
1	C	308	GLN
1	C	316	LEU
1	C	323	SER
1	C	326	ASP
1	C	370	SER
1	C	373	LYS
1	C	378	GLU
1	C	379	GLU
1	C	385	CYS
1	C	392	LYS
1	C	413	ASP
1	C	444	CYS
1	C	447	CYS
1	C	452	GLU

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Mol	Chain	Res	Type
1	C	482	LEU
1	C	492	ARG
1	C	504	LEU
1	C	511	SER
1	C	519	LEU
1	C	565	THR
1	C	597	ARG
1	C	598	LEU
1	C	688	VAL
1	D	40	ARG
1	D	41	LYS
1	D	55	LEU
1	D	59	SER
1	D	61	ARG
1	D	66	HIS
1	D	71	LYS
1	D	92	ASN
1	D	94	THR
1	D	96	ASP
1	D	98	PHE
1	D	123	GLN
1	D	129	THR
1	D	164	LEU
1	D	180	LEU
1	D	188	THR
1	D	194	ILE
1	D	227	GLN
1	D	235	LEU
1	D	243	ASP
1	D	276	LEU
1	D	283	THR
1	D	295	ILE
1	D	316	LEU
1	D	323	SER
1	D	326	ASP
1	D	327	ILE
1	D	343	ARG
1	D	350	THR
1	D	354	VAL
1	D	358	ARG
1	D	373	LYS
1	D	385	CYS

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Mol	Chain	Res	Type
1	D	390	ASP
1	D	391	LYS
1	D	392	LYS
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	460	SER
1	D	464	GLU
1	D	482	LEU
1	D	503	MET
1	D	513	LYS
1	D	514	LEU
1	D	519	LEU
1	D	536	LYS
1	D	546	VAL
1	D	575	VAL
1	D	658	ARG
1	D	665	VAL
1	D	711	VAL
1	D	745	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	508	GLN

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)

17 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	E	1	1,2	14,14,15	0.64	0	17,19,21	2.04	4 (23%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	0.88	0
2	NAG	F	1	1,2	14,14,15	0.65	0	17,19,21	1.45	1 (5%)
2	NAG	F	2	2	14,14,15	0.70	0	17,19,21	1.45	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.62	0	17,19,21	1.13	2 (11%)
2	NAG	G	2	2	14,14,15	0.61	0	17,19,21	1.34	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.74	0	17,19,21	1.65	3 (17%)
2	NAG	H	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	NAG	I	1	1,2	14,14,15	0.59	0	17,19,21	1.34	1 (5%)
2	NAG	I	2	2	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.61	0	17,19,21	1.30	1 (5%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	1.63	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.43	0	17,19,21	1.29	2 (11%)
3	NAG	K	2	3	14,14,15	0.54	0	17,19,21	2.87	5 (29%)
3	NAG	K	3	3	14,14,15	0.38	0	17,19,21	1.23	3 (17%)
2	NAG	L	1	1,2	14,14,15	0.58	0	17,19,21	1.43	3 (17%)
2	NAG	L	2	2	14,14,15	0.51	0	17,19,21	0.89	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
2	NAG	E	1	1,2	-	1/6/23/26	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	-	5/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	3	3	-	1/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	2	NAG	C1-O5-C5	7.20	121.95	112.19
3	K	2	NAG	O4-C4-C5	5.65	123.32	109.30
3	K	2	NAG	C4-C3-C2	-5.49	102.97	111.02
2	E	1	NAG	C1-O5-C5	5.27	119.33	112.19
2	H	1	NAG	C4-C3-C2	4.52	117.64	111.02
2	F	1	NAG	C2-N2-C7	4.32	129.06	122.90
2	F	2	NAG	C4-C3-C2	4.02	116.91	111.02
2	J	2	NAG	C3-C4-C5	4.00	117.37	110.24
2	E	1	NAG	C4-C3-C2	-3.59	105.75	111.02
2	J	2	NAG	C4-C3-C2	3.59	116.28	111.02
2	J	1	NAG	C1-O5-C5	3.51	116.94	112.19
2	H	1	NAG	C1-O5-C5	3.28	116.63	112.19
2	E	1	NAG	C2-N2-C7	3.25	127.53	122.90
3	K	2	NAG	C8-C7-N2	3.11	121.37	116.10
3	K	1	NAG	C1-O5-C5	2.95	116.19	112.19
2	L	1	NAG	C1-O5-C5	2.92	116.16	112.19
3	K	3	NAG	C1-O5-C5	2.86	116.07	112.19
2	E	1	NAG	C1-C2-N2	2.85	115.36	110.49
2	G	2	NAG	C1-O5-C5	2.85	116.05	112.19
3	K	3	NAG	O5-C5-C6	2.80	111.60	107.20
2	H	1	NAG	C3-C4-C5	2.75	115.14	110.24
2	G	1	NAG	O5-C1-C2	-2.73	106.97	111.29
2	L	1	NAG	C4-C3-C2	2.70	114.97	111.02
2	L	1	NAG	C3-C4-C5	2.47	114.65	110.24
2	F	2	NAG	C3-C4-C5	2.47	114.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	NAG	O5-C5-C6	2.40	110.97	107.20
2	I	2	NAG	O5-C5-C6	2.35	110.89	107.20
3	K	3	NAG	O5-C1-C2	-2.31	107.64	111.29
3	K	2	NAG	C3-C4-C5	-2.26	106.20	110.24
2	G	1	NAG	C4-C3-C2	2.07	114.05	111.02
3	K	1	NAG	O5-C1-C2	-2.06	108.04	111.29
2	J	2	NAG	O5-C1-C2	-2.01	108.12	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	I	1	NAG	C1

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	L	2	NAG	O5-C5-C6-O6
2	L	2	NAG	C8-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
3	K	2	NAG	C8-C7-N2-C2
2	L	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	G	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
3	K	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C8-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O7-C7-N2-C2
3	K	3	NAG	O5-C5-C6-O6
2	F	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C1-C2-N2-C7
2	F	1	NAG	C3-C2-N2-C7

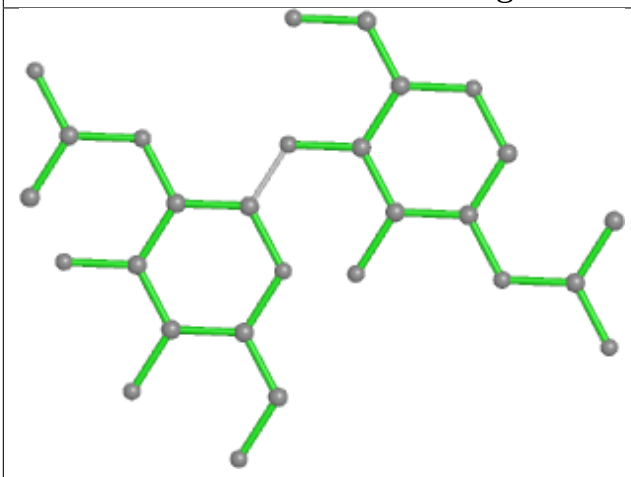
There are no ring outliers.

6 monomers are involved in 4 short contacts:

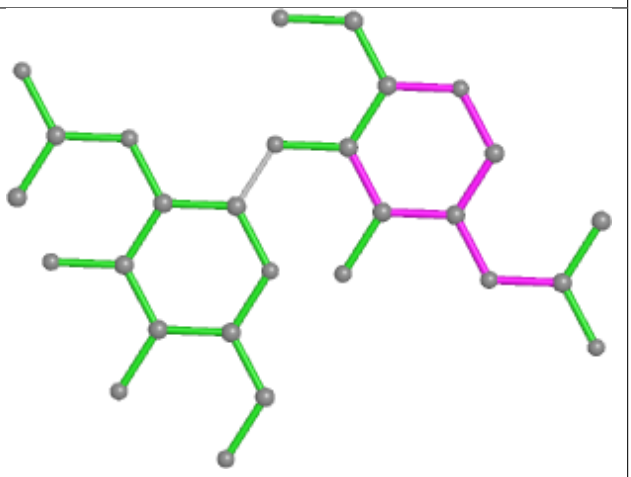
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	1	0
2	L	1	NAG	1	0
3	K	1	NAG	1	0
2	J	1	NAG	1	0
2	I	1	NAG	1	0
2	I	2	NAG	1	0

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

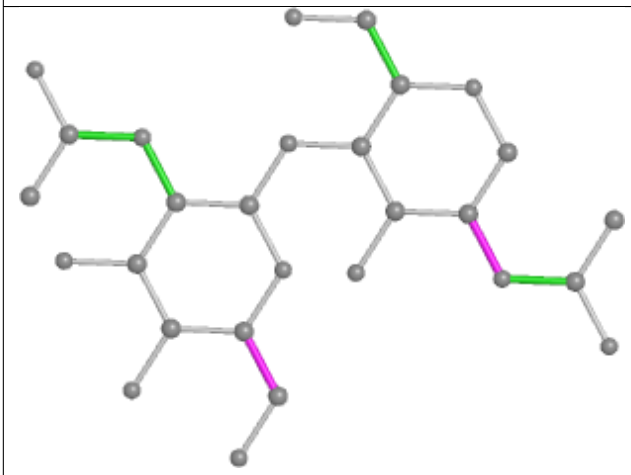
Oligosaccharide Chain E



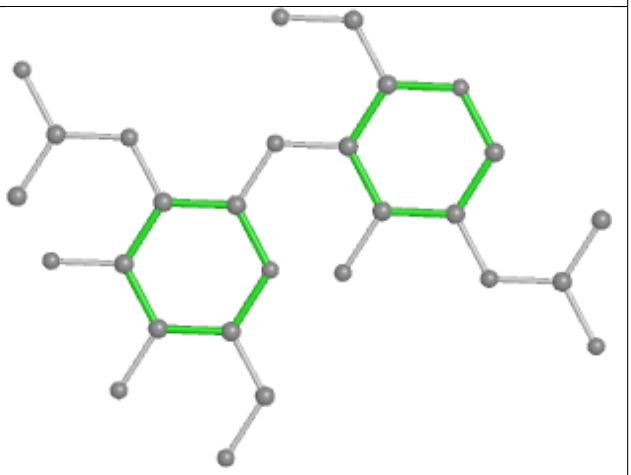
Bond lengths



Bond angles

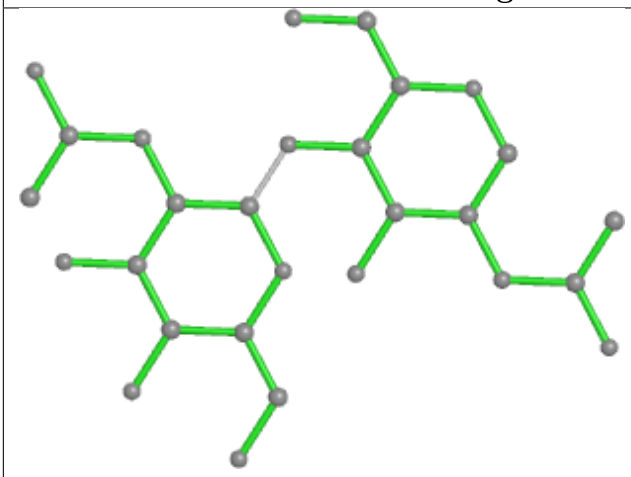


Torsions

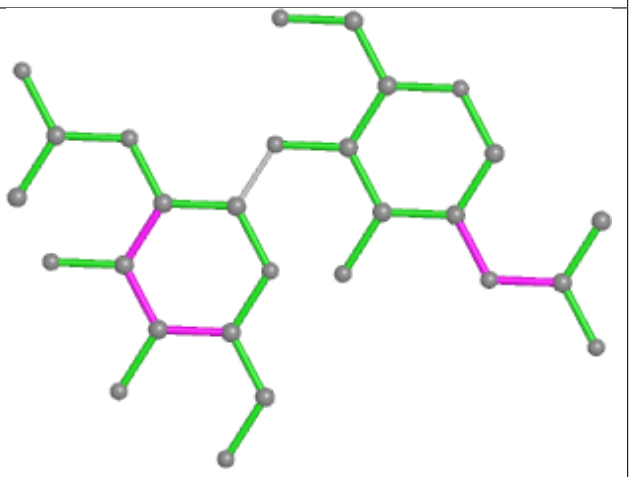


Rings

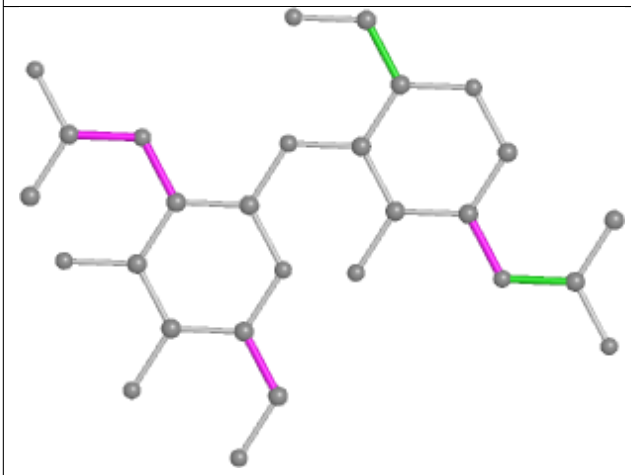
Oligosaccharide Chain F



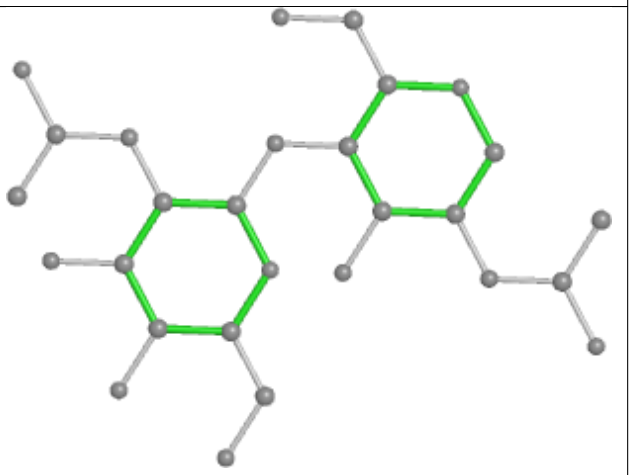
Bond lengths



Bond angles

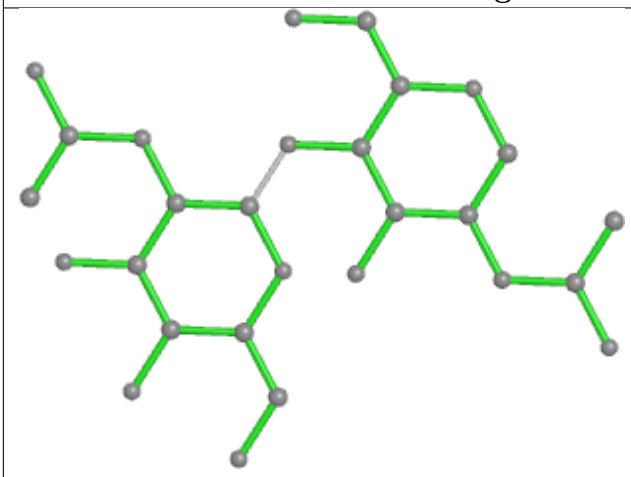


Torsions

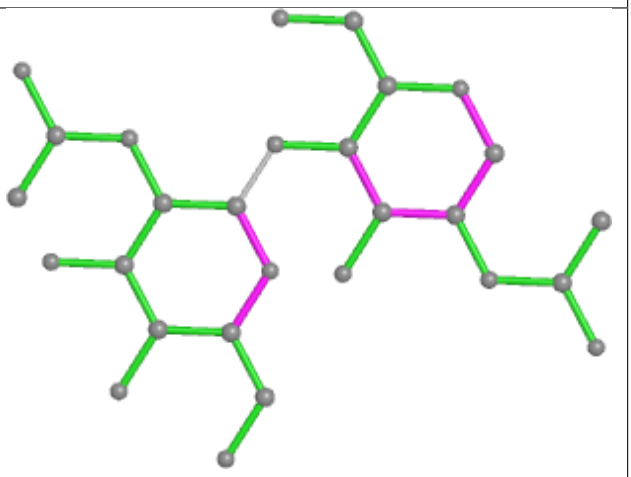


Rings

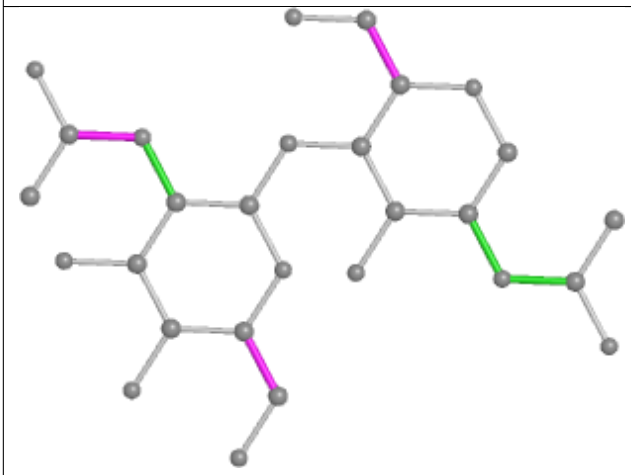
Oligosaccharide Chain G



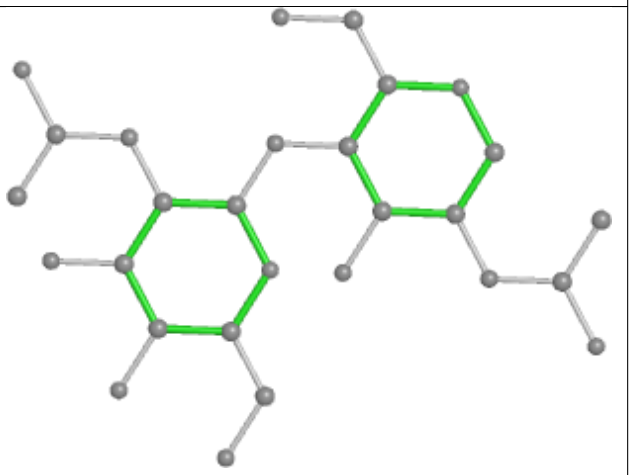
Bond lengths



Bond angles

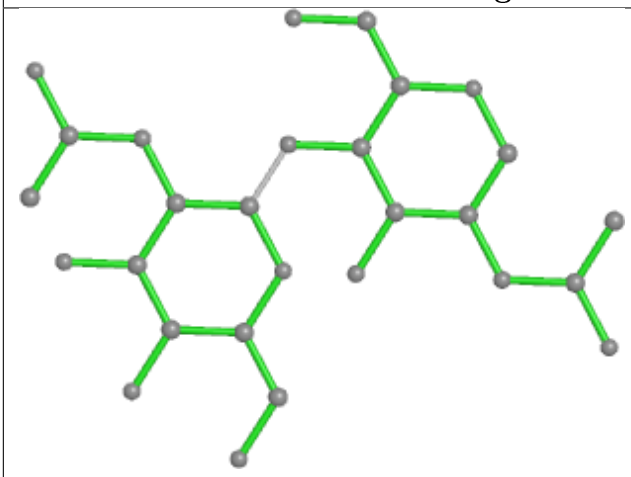


Torsions

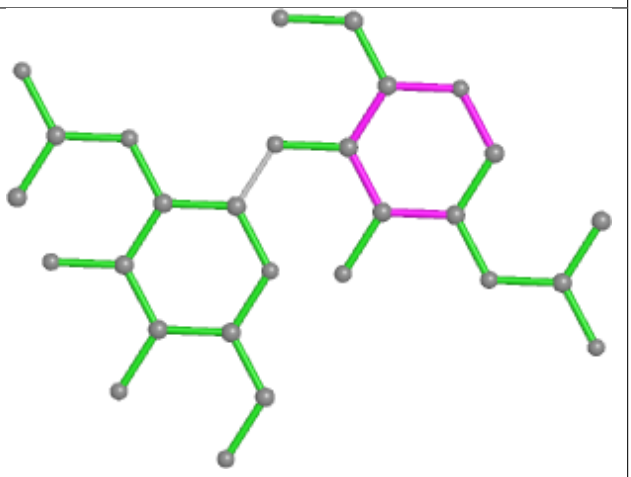


Rings

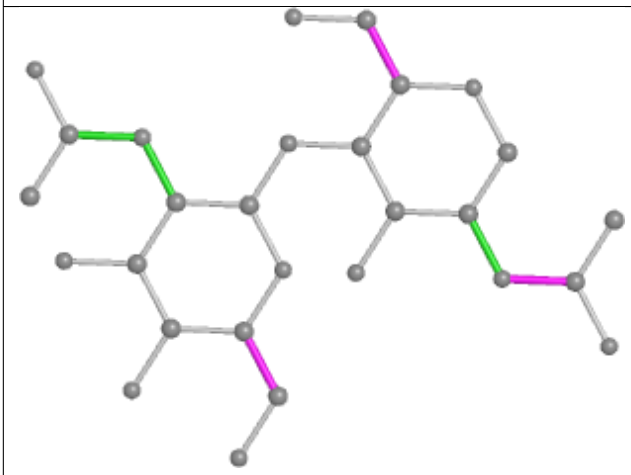
Oligosaccharide Chain H



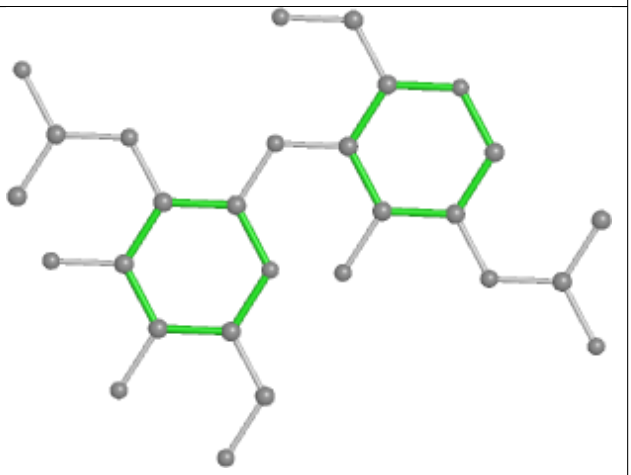
Bond lengths



Bond angles

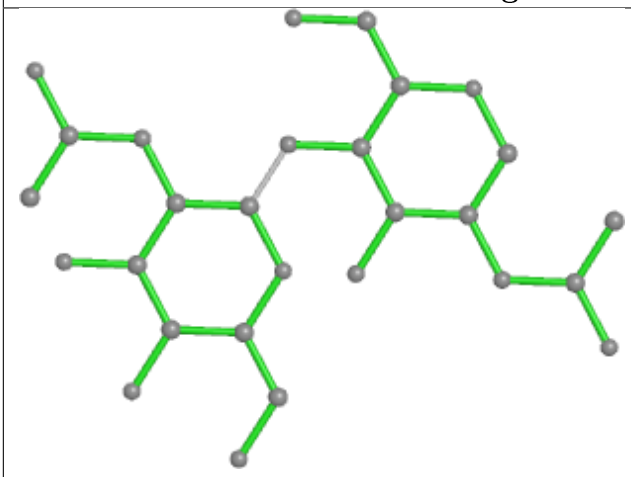


Torsions

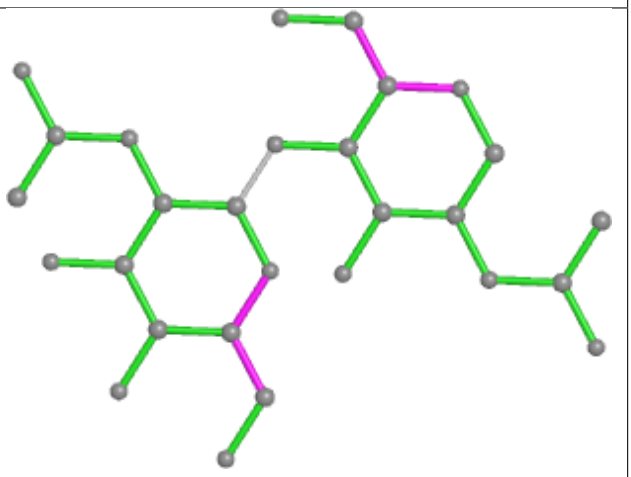


Rings

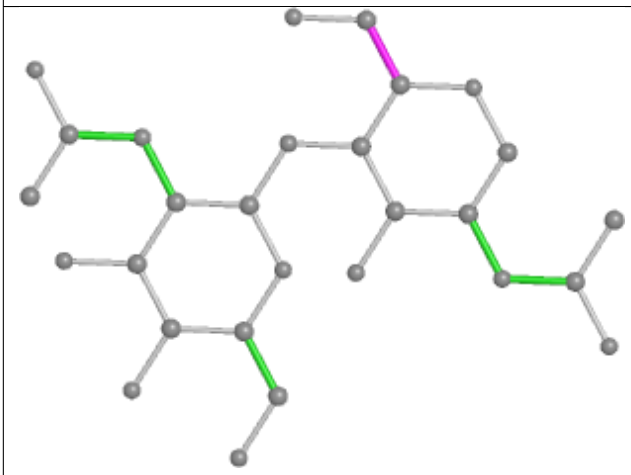
Oligosaccharide Chain I



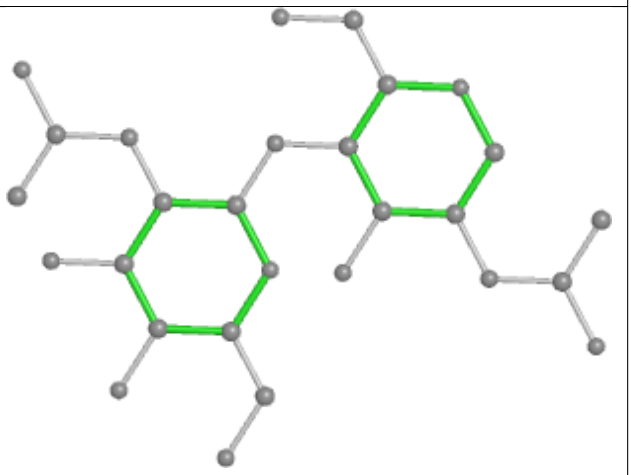
Bond lengths



Bond angles

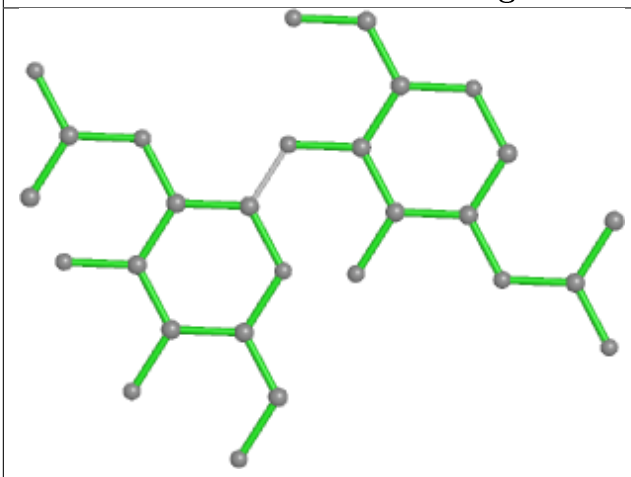


Torsions

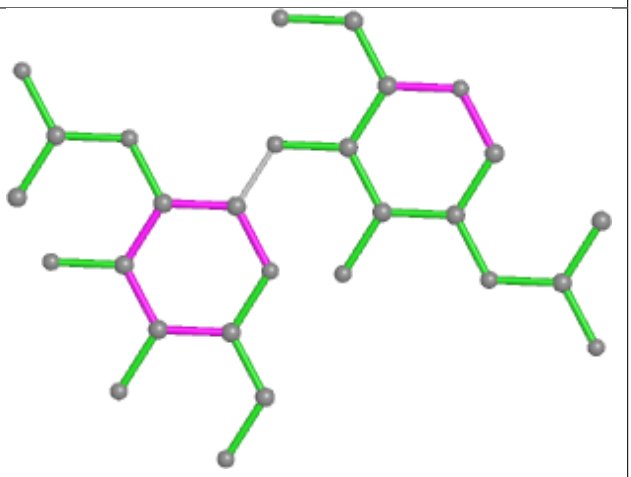


Rings

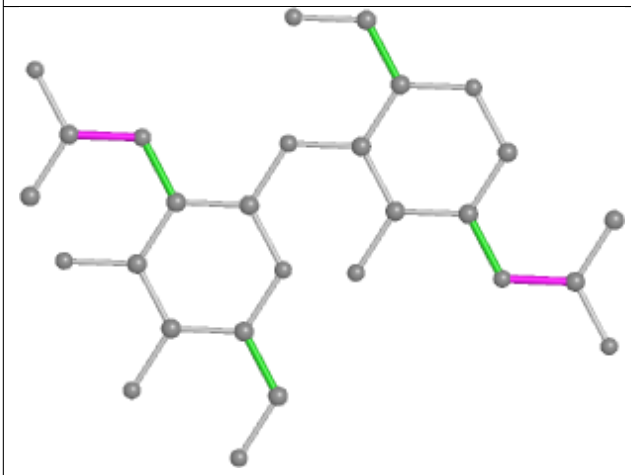
Oligosaccharide Chain J



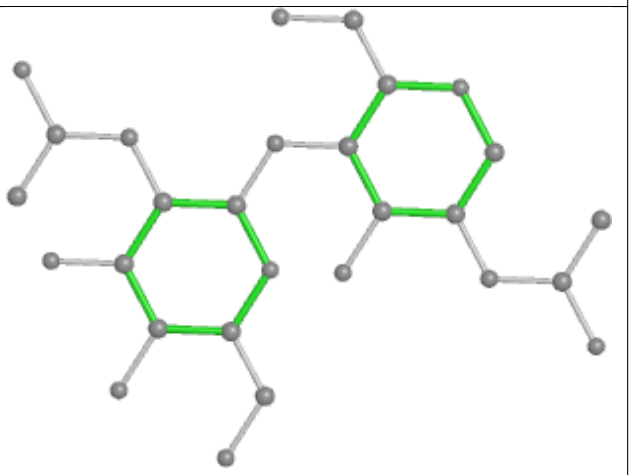
Bond lengths



Bond angles

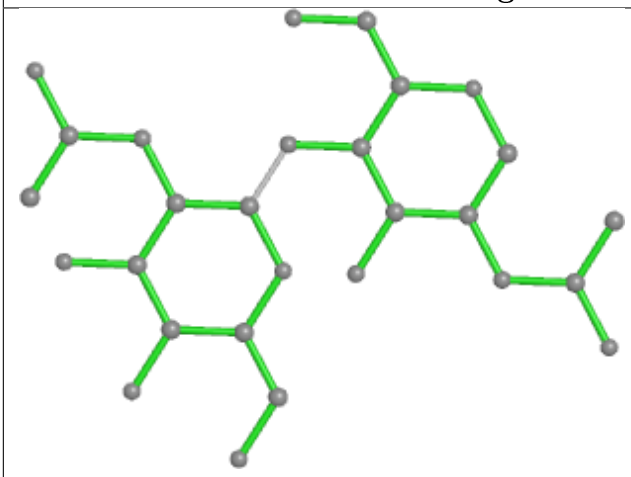


Torsions

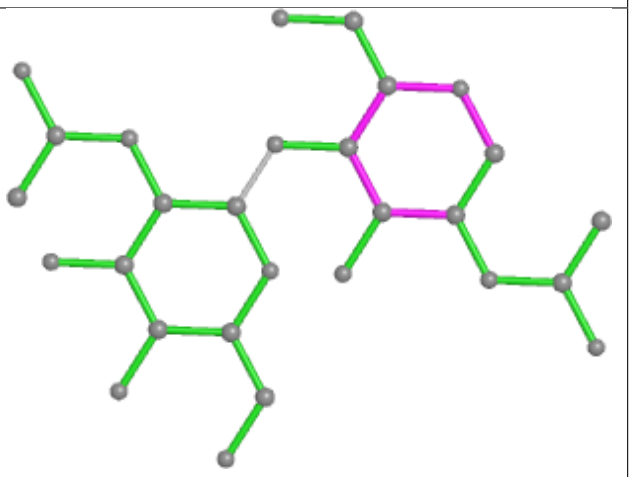


Rings

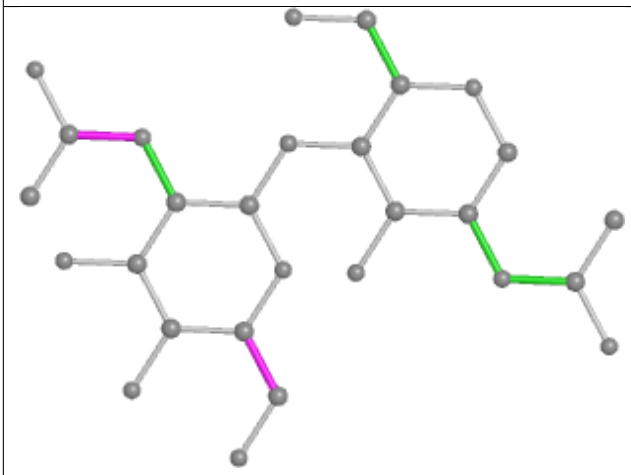
Oligosaccharide Chain L



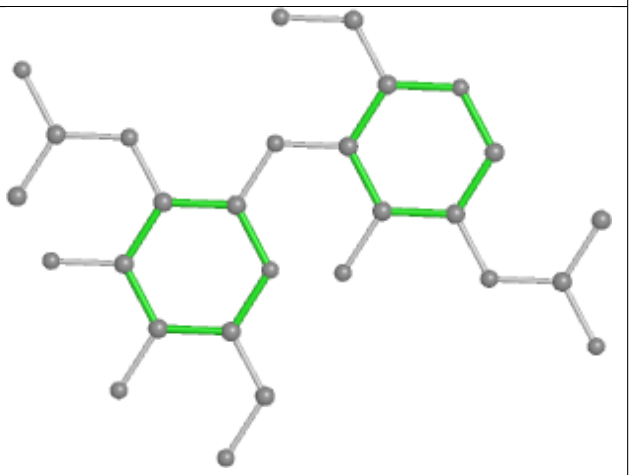
Bond lengths



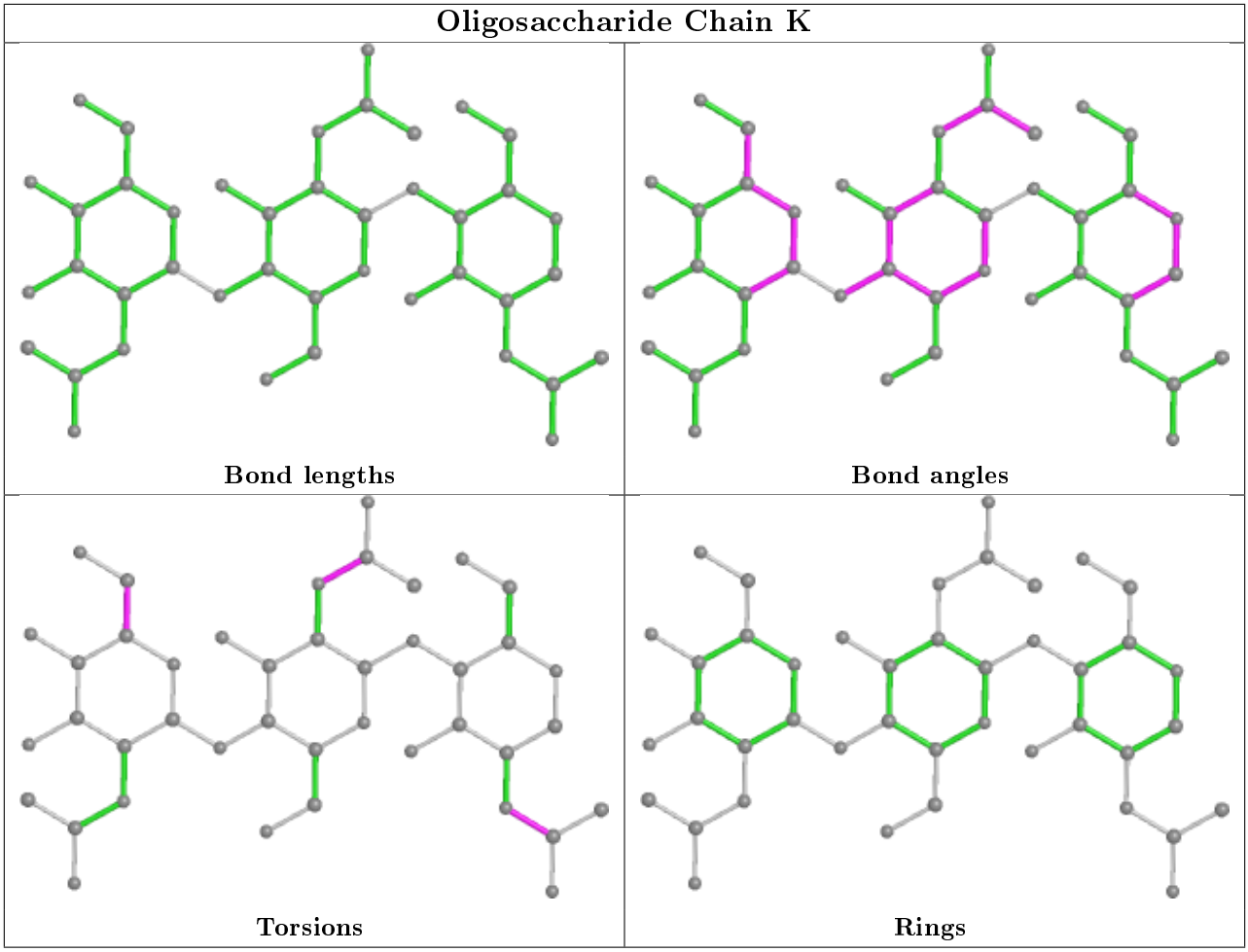
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

16 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	NAG	B	2811	1	14,14,15	0.55	0	17,19,21	1.73	2 (11%)
4	NAG	D	2811	1	14,14,15	0.81	1 (7%)	17,19,21	1.29	2 (11%)
5	01T	C	1	-	23,27,27	0.60	0	29,39,39	1.83	6 (20%)
5	01T	D	1	-	23,27,27	0.63	0	29,39,39	1.80	4 (13%)
4	NAG	A	2191	1	14,14,15	0.58	0	17,19,21	1.37	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	2811	1	14,14,15	0.65	0	17,19,21	1.49	2 (11%)
4	NAG	B	1501	1	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
4	NAG	D	5201	1	14,14,15	0.54	0	17,19,21	1.06	1 (5%)
5	01T	B	1	-	23,27,27	0.53	0	29,39,39	1.65	4 (13%)
4	NAG	D	1501	1	14,14,15	0.69	0	17,19,21	1.92	3 (17%)
4	NAG	B	3211	1	14,14,15	0.69	0	17,19,21	1.56	3 (17%)
4	NAG	A	3211	1	14,14,15	0.58	0	17,19,21	1.46	1 (5%)
4	NAG	C	3211	1	14,14,15	0.73	0	17,19,21	1.35	3 (17%)
4	NAG	D	2191	1	14,14,15	0.64	0	17,19,21	1.55	3 (17%)
4	NAG	C	1501	1	14,14,15	0.60	0	17,19,21	1.99	4 (23%)
5	01T	A	1	-	23,27,27	0.44	0	29,39,39	1.79	6 (20%)

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	NAG	B	2811	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2811	1	-	4/6/23/26	0/1/1/1
5	01T	C	1	-	-	2/14/17/17	0/2/2/2
5	01T	D	1	-	-	2/14/17/17	0/2/2/2
4	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	5201	1	1/1/5/7	4/6/23/26	0/1/1/1
5	01T	B	1	-	-	3/14/17/17	0/2/2/2
4	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	B	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	C	3211	1	-	0/6/23/26	0/1/1/1
4	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
5	01T	A	1	-	-	1/14/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2811	NAG	C1-C2	2.07	1.55	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1501	NAG	C1-O5-C5	6.08	120.42	112.19
5	C	1	01T	C15-C3-N4	-5.81	118.58	123.49
4	D	1501	NAG	C1-O5-C5	5.58	119.75	112.19
4	B	2811	NAG	C1-O5-C5	5.54	119.70	112.19
5	D	1	01T	C11-C5-N4	-5.26	119.05	123.49
4	A	3211	NAG	C1-O5-C5	4.98	118.94	112.19
5	A	1	01T	C11-C5-N4	-4.96	119.30	123.49
5	A	1	01T	C15-C3-N4	-4.77	119.46	123.49
5	D	1	01T	C15-C3-N4	-4.68	119.54	123.49
5	B	1	01T	C11-C5-N4	-4.66	119.56	123.49
4	C	2811	NAG	C1-O5-C5	4.36	118.11	112.19
4	B	3211	NAG	C4-C3-C2	4.19	117.15	111.02
5	B	1	01T	C15-C3-N4	-4.04	120.08	123.49
4	A	2191	NAG	C1-O5-C5	3.99	117.60	112.19
5	C	1	01T	C11-C5-N4	-3.70	120.37	123.49
4	C	2811	NAG	O5-C5-C6	3.57	112.79	107.20
4	D	2191	NAG	C4-C3-C2	3.55	116.22	111.02
4	B	1501	NAG	C1-O5-C5	3.54	116.99	112.19
4	D	2811	NAG	C4-C3-C2	3.40	116.00	111.02
5	D	1	01T	C14-C11-C5	3.38	119.85	117.70
4	C	1501	NAG	O5-C5-C6	3.38	112.50	107.20
4	D	1501	NAG	C2-N2-C7	3.26	127.54	122.90
4	D	2811	NAG	C1-O5-C5	3.12	116.41	112.19
4	D	2191	NAG	C1-O5-C5	3.09	116.38	112.19
4	D	5201	NAG	C1-O5-C5	3.04	116.31	112.19
5	A	1	01T	C14-C11-C5	2.91	119.55	117.70
5	B	1	01T	C14-C11-C5	2.81	119.48	117.70
4	C	3211	NAG	C1-O5-C5	2.79	115.97	112.19
4	B	3211	NAG	C1-O5-C5	2.72	115.88	112.19
4	C	1501	NAG	C3-C4-C5	2.67	115.00	110.24
5	C	1	01T	C14-C15-C3	2.59	119.34	117.70
4	C	3211	NAG	C4-C3-C2	2.58	114.80	111.02
5	C	1	01T	C7-C6-C5	-2.53	111.63	117.97
4	B	2811	NAG	O5-C5-C6	2.49	111.11	107.20
5	A	1	01T	C3-N4-C5	2.47	123.01	118.06
5	C	1	01T	C17-C16-C15	-2.41	111.27	115.96
4	A	2191	NAG	C2-N2-C7	-2.39	119.50	122.90
5	C	1	01T	C3-N4-C5	2.37	122.81	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1501	NAG	C4-C3-C2	2.29	114.38	111.02
4	D	2191	NAG	C3-C4-C5	2.27	114.28	110.24
5	A	1	01T	C1-C2-C3	-2.25	109.33	114.88
5	B	1	01T	C3-N4-C5	2.16	122.39	118.06
5	D	1	01T	C3-N4-C5	2.16	122.38	118.06
4	D	1501	NAG	O3-C3-C2	2.16	113.93	109.47
4	B	3211	NAG	C3-C4-C5	2.14	114.06	110.24
4	C	3211	NAG	C2-N2-C7	2.04	125.80	122.90
5	A	1	01T	C7-C6-C5	-2.02	112.90	117.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	5201	NAG	C1

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	01T	C14-C11-C12-N13
4	C	2811	NAG	O5-C5-C6-O6
4	B	2811	NAG	O5-C5-C6-O6
4	C	2811	NAG	C4-C5-C6-O6
4	D	2811	NAG	C8-C7-N2-C2
4	D	2811	NAG	O7-C7-N2-C2
4	C	1501	NAG	C4-C5-C6-O6
4	B	2811	NAG	C4-C5-C6-O6
4	C	1501	NAG	O5-C5-C6-O6
4	D	5201	NAG	O5-C5-C6-O6
4	B	2811	NAG	C8-C7-N2-C2
4	D	5201	NAG	C4-C5-C6-O6
4	D	2811	NAG	O5-C5-C6-O6
4	B	2811	NAG	O7-C7-N2-C2
4	D	2811	NAG	C4-C5-C6-O6
4	D	5201	NAG	C8-C7-N2-C2
4	D	1501	NAG	C8-C7-N2-C2
4	D	1501	NAG	C3-C2-N2-C7
4	D	5201	NAG	O7-C7-N2-C2
4	D	1501	NAG	O7-C7-N2-C2
4	D	1501	NAG	C4-C5-C6-O6
4	A	3211	NAG	C8-C7-N2-C2
5	B	1	01T	C1-C2-C3-C15
5	C	1	01T	C1-C2-C3-N4

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Mol	Chain	Res	Type	Atoms
4	A	3211	NAG	O7-C7-N2-C2
5	C	1	01T	C1-C2-C3-C15
5	B	1	01T	C1-C2-C3-N4
5	D	1	01T	C1-C2-C3-C15
4	B	3211	NAG	C4-C5-C6-O6
4	B	3211	NAG	O5-C5-C6-O6
5	B	1	01T	C14-C11-C12-N13
5	D	1	01T	C1-C2-C3-N4

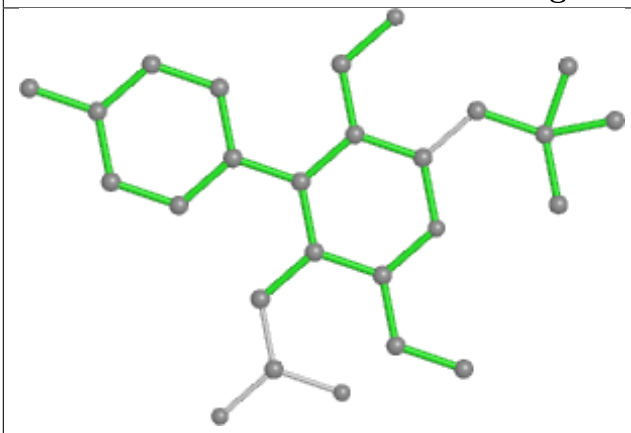
There are no ring outliers.

4 monomers are involved in 5 short contacts:

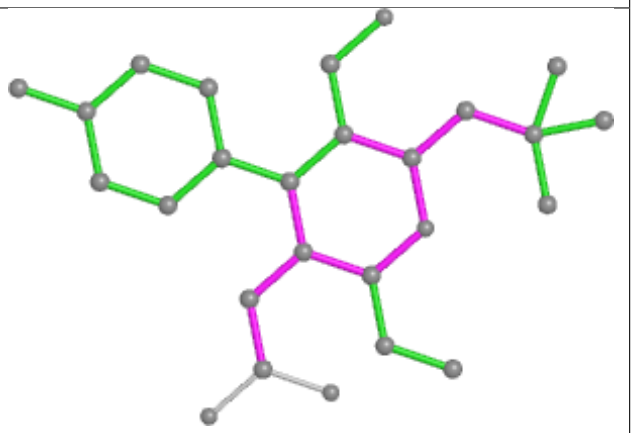
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2811	NAG	1	0
5	D	1	01T	1	0
5	B	1	01T	1	0
5	A	1	01T	2	0

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

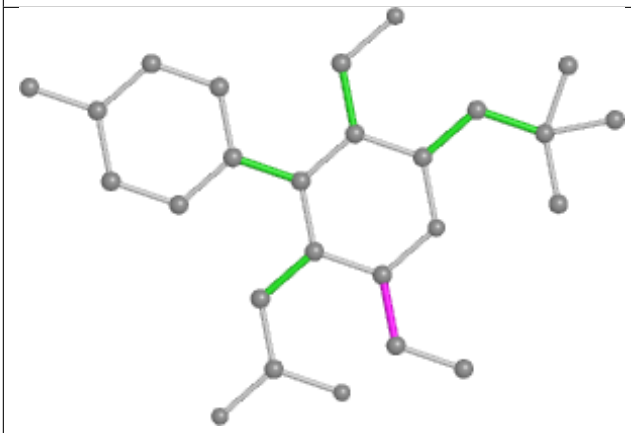
Ligand 01T C 1



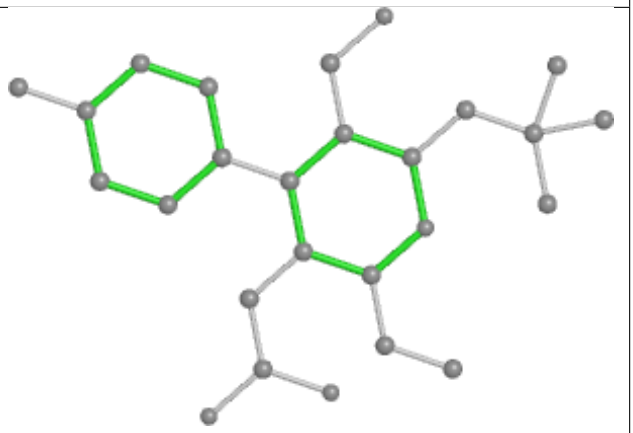
Bond lengths



Bond angles

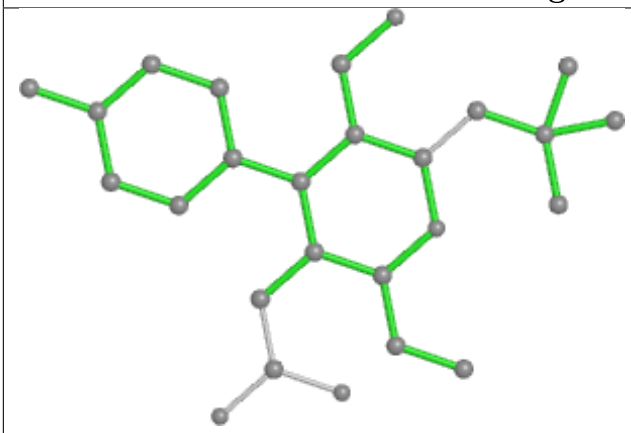


Torsions

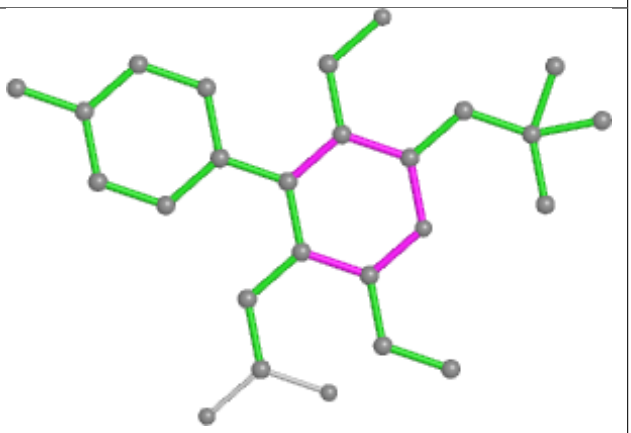


Rings

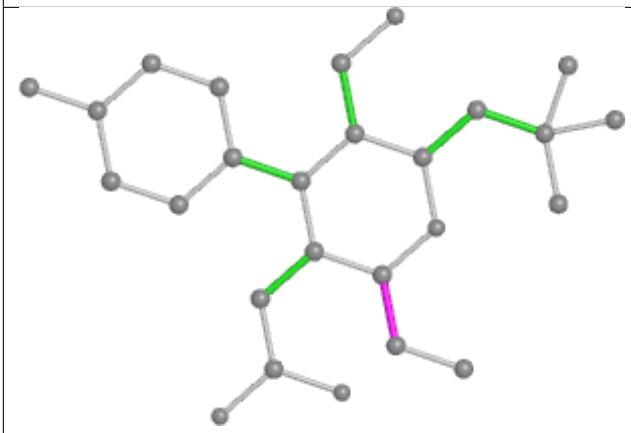
Ligand 01T D 1



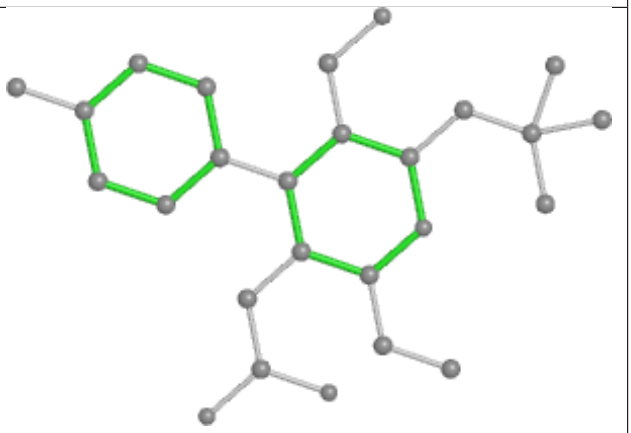
Bond lengths



Bond angles

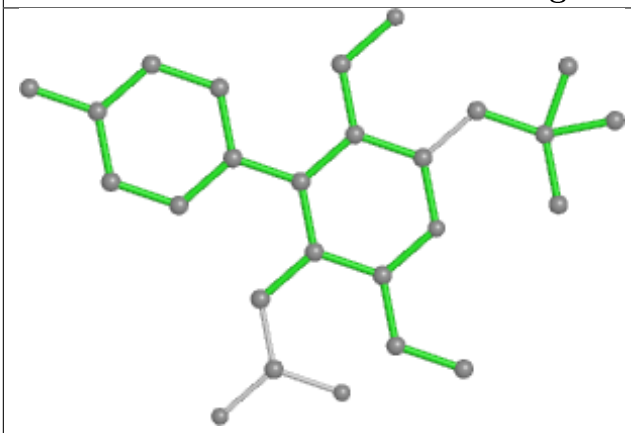


Torsions

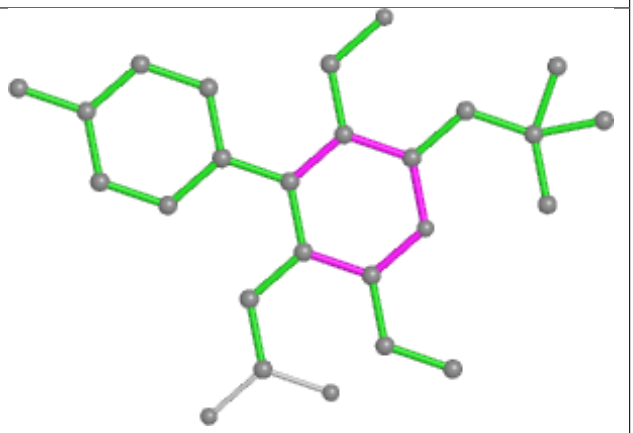


Rings

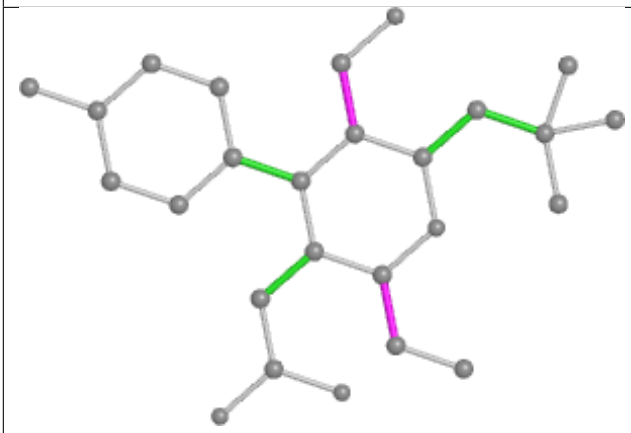
Ligand 01T B 1



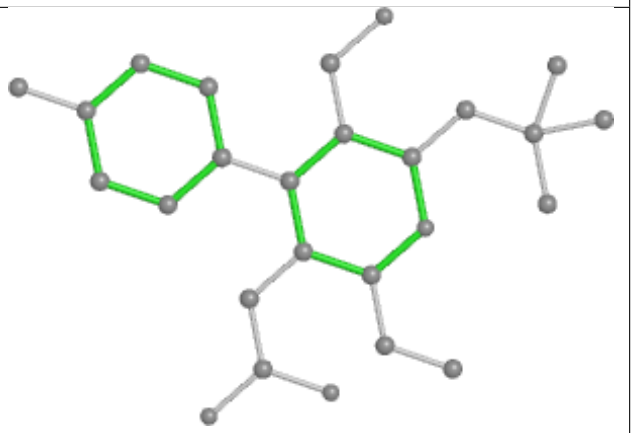
Bond lengths



Bond angles

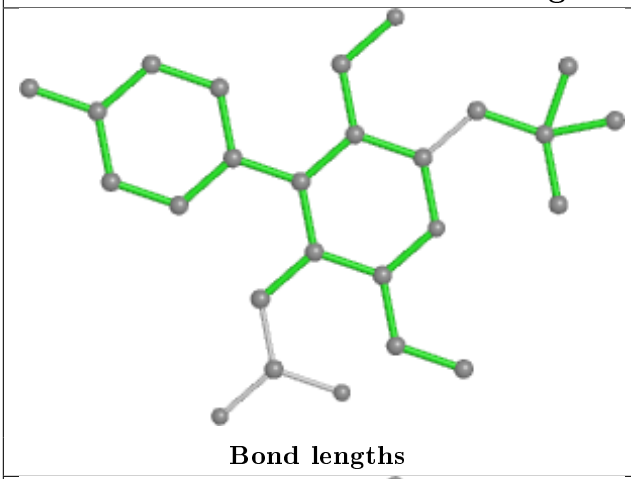


Torsions

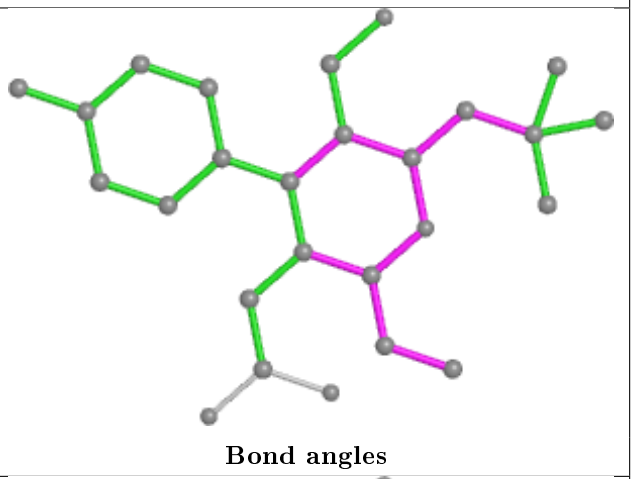


Rings

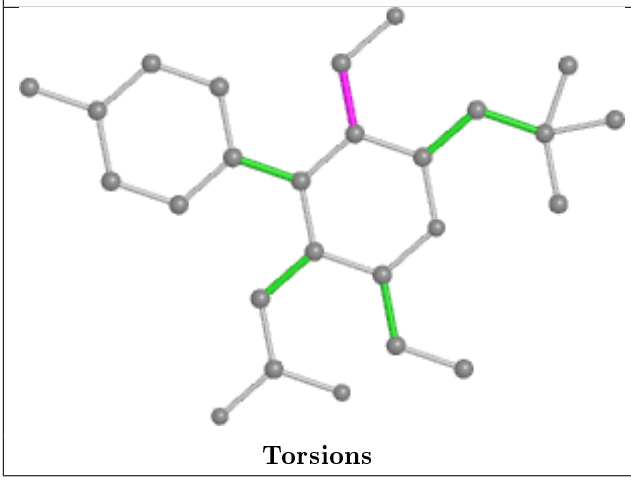
Ligand 01T A 1



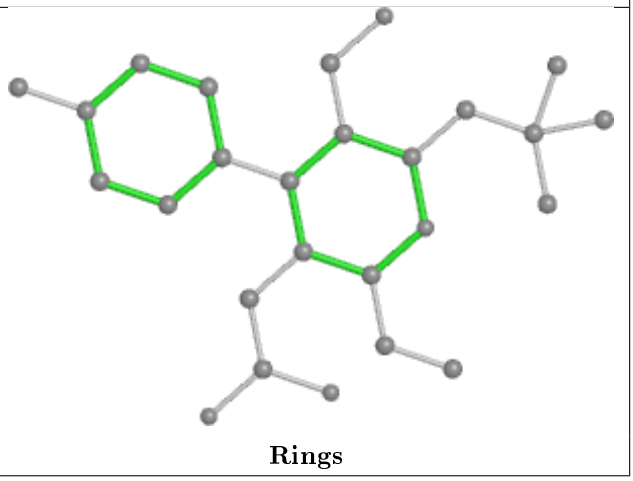
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

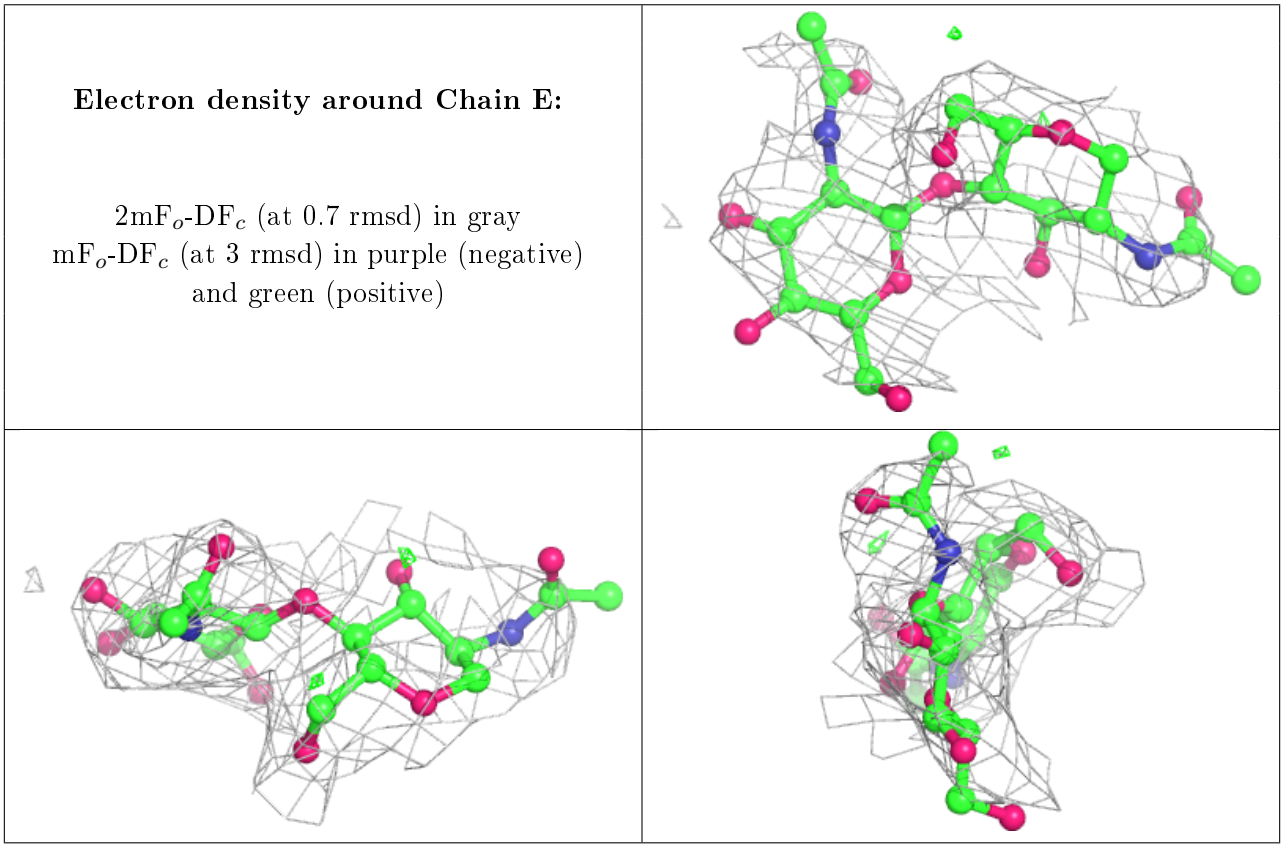
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

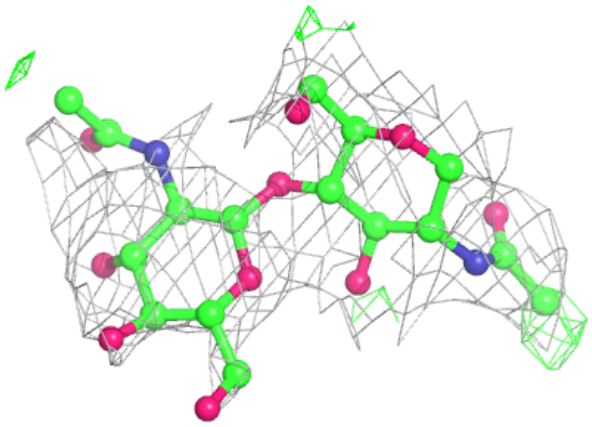
Unable to reproduce the depositors R factor - this section is therefore empty.

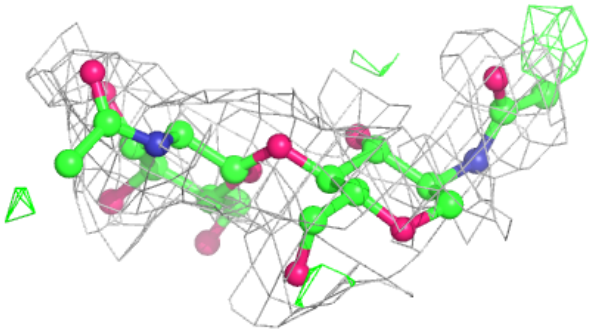
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

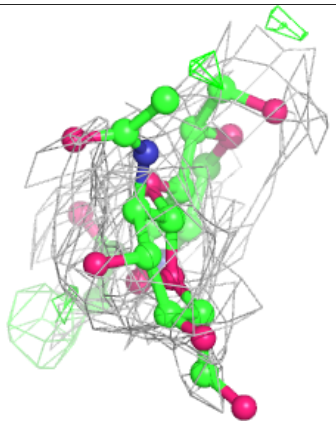


Electron density around Chain F:

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

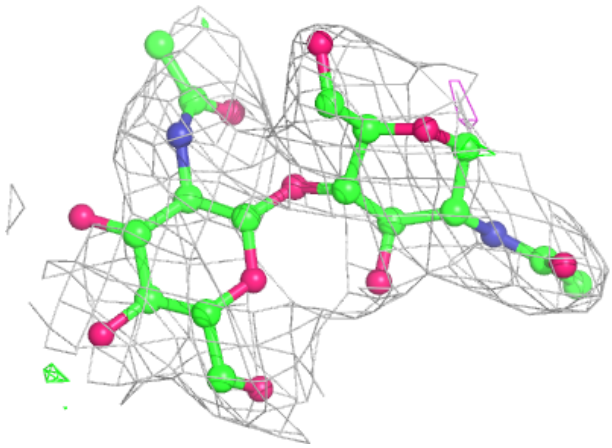


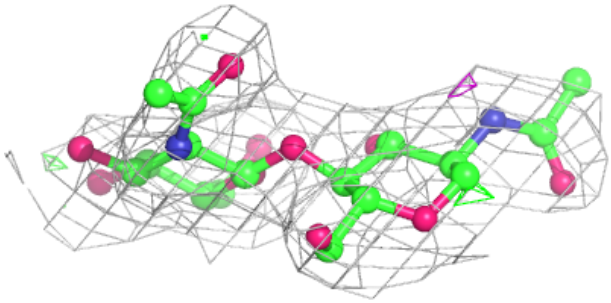


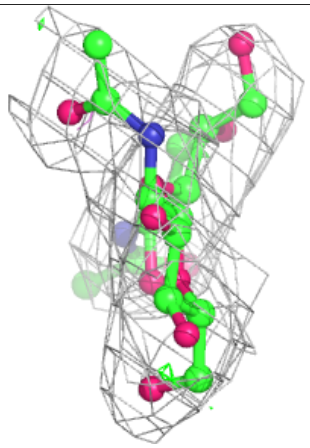


Electron density around Chain G:

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

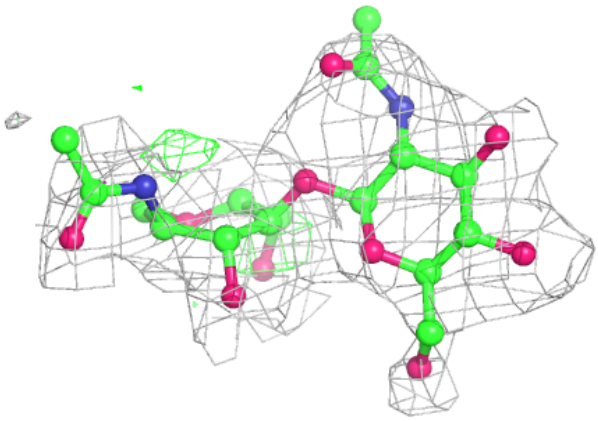


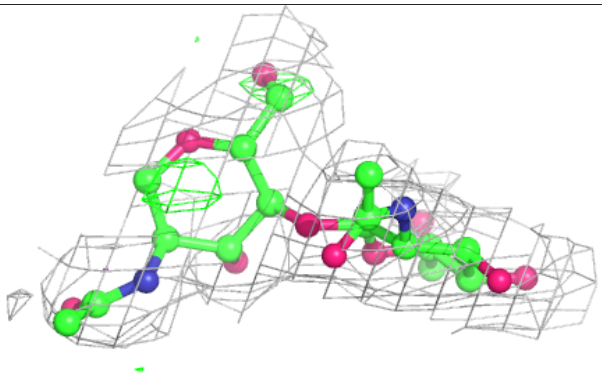


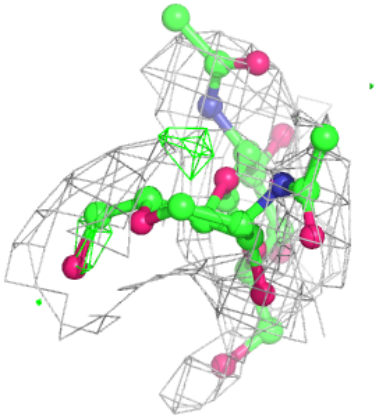


Electron density around Chain H:

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

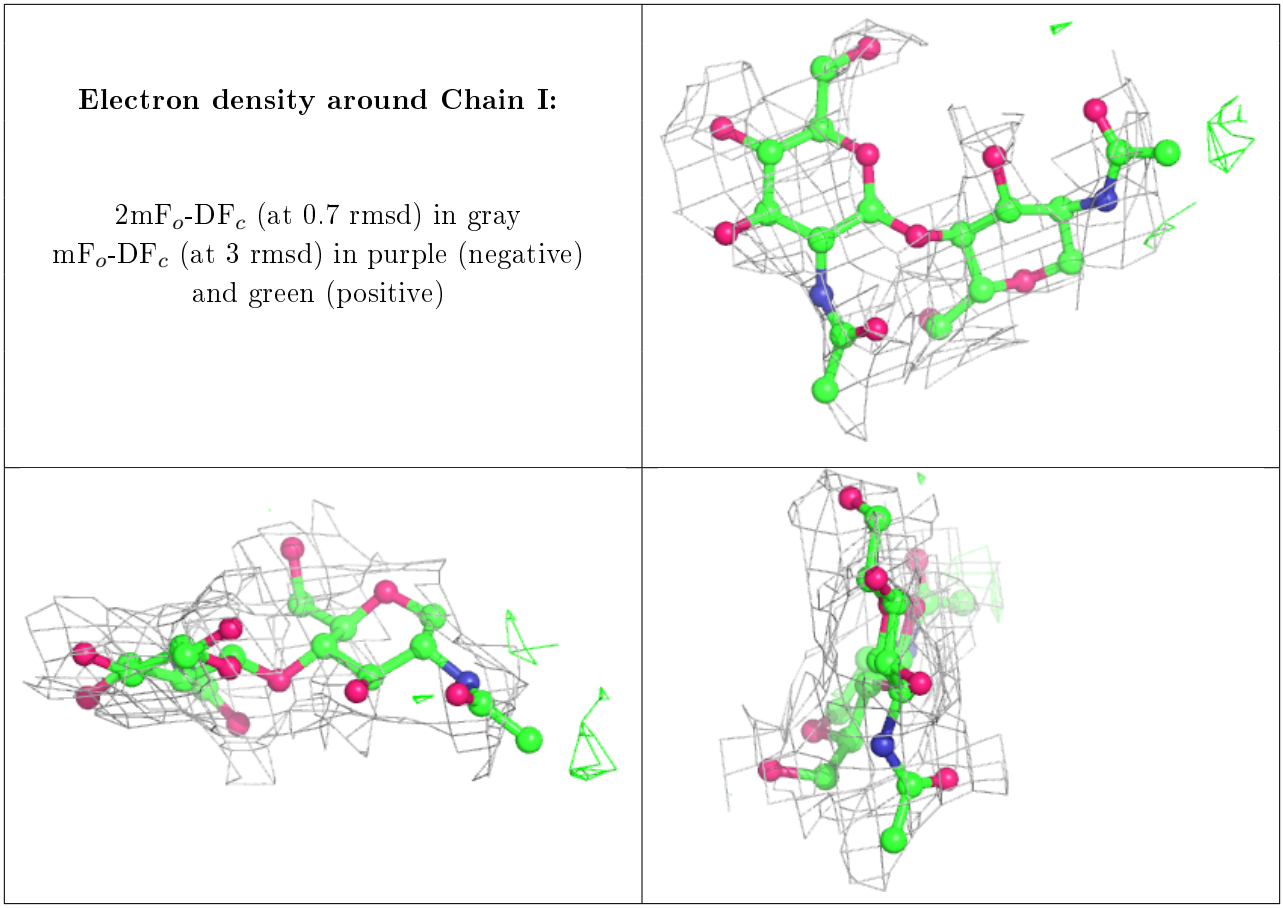






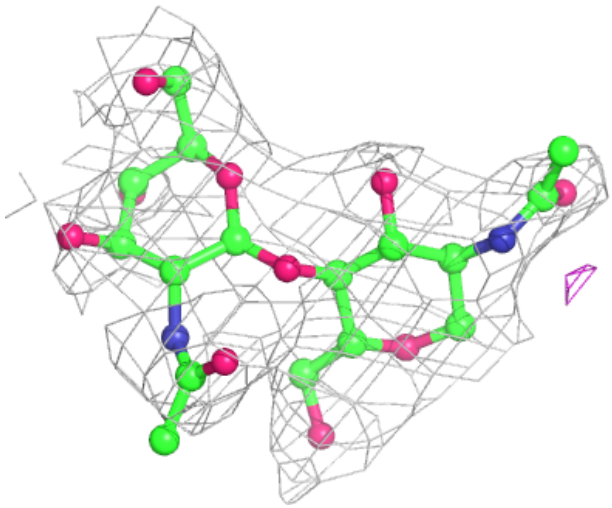
Electron density around Chain I:

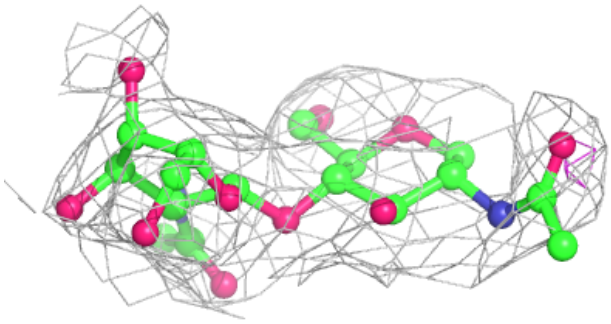
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain J:

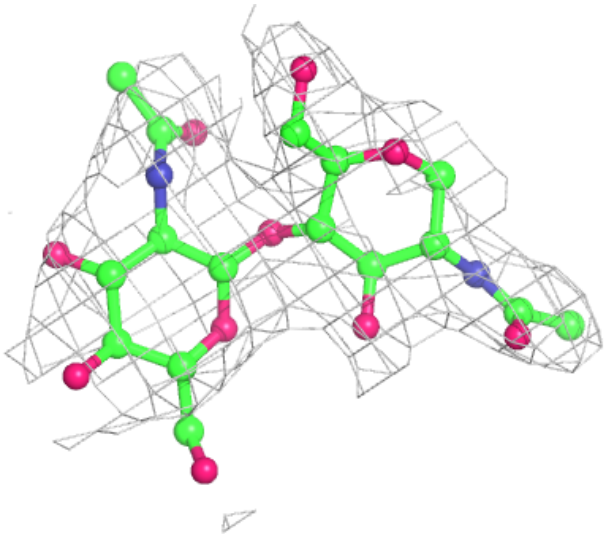
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

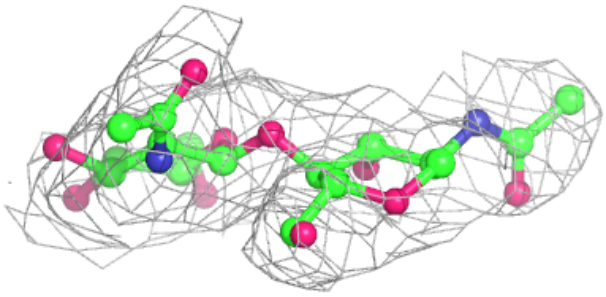


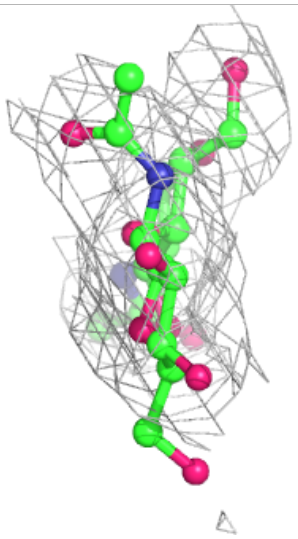


Electron density around Chain L:

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

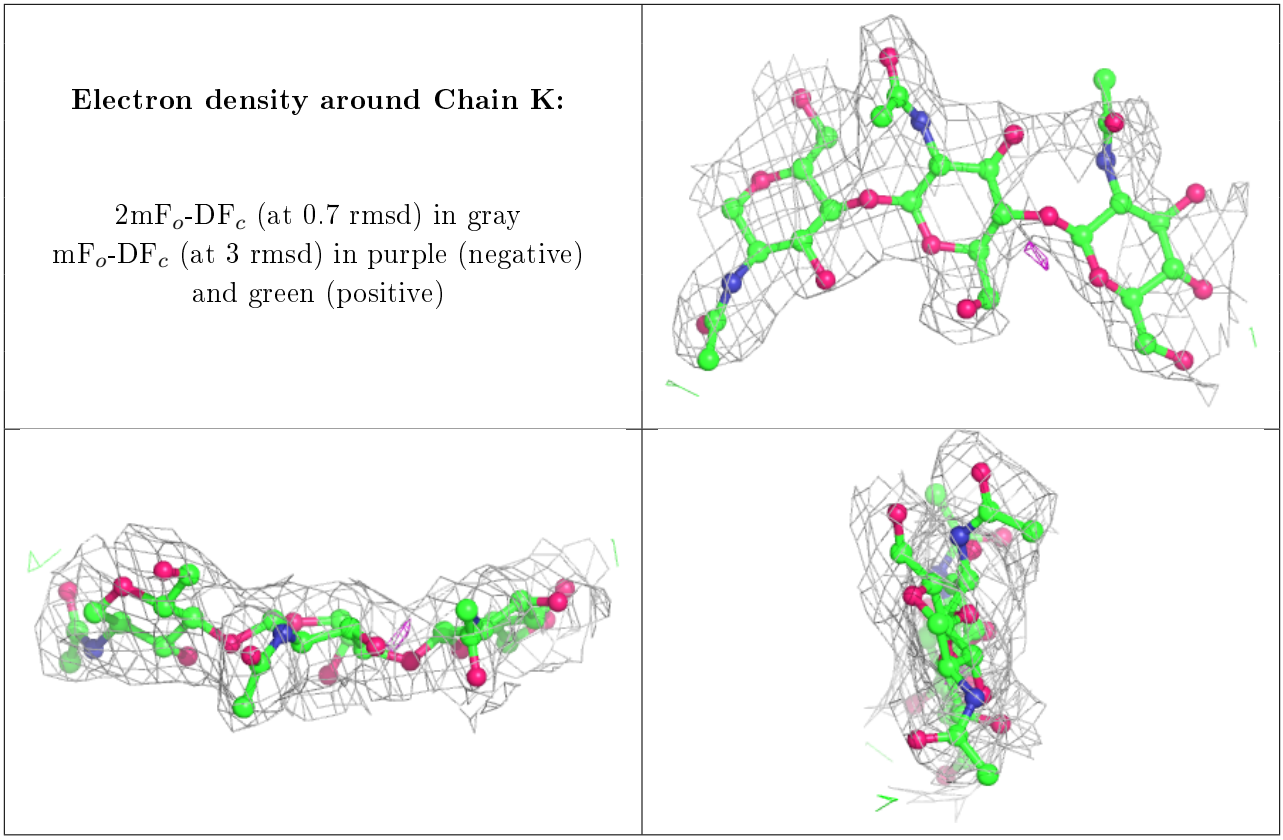






Electron density around Chain K:

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



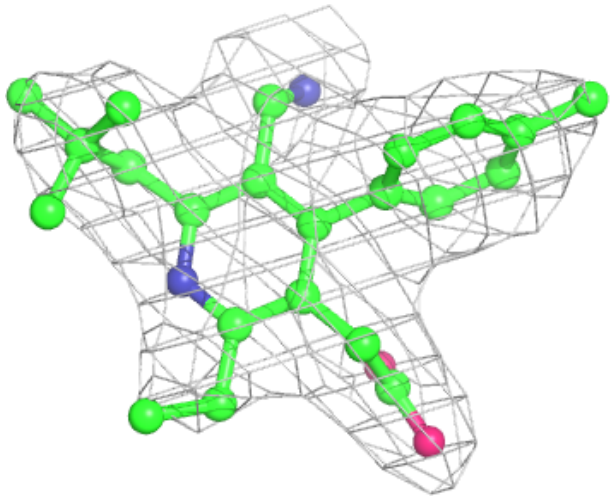
6.4 Ligands

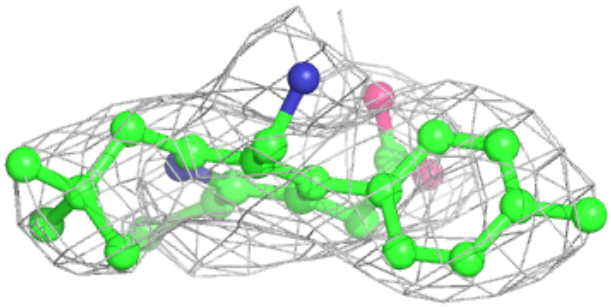
Unable to reproduce the depositors R factor - this section is therefore empty.

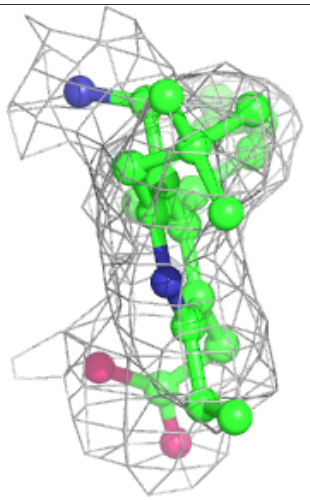
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 01T C 1:

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

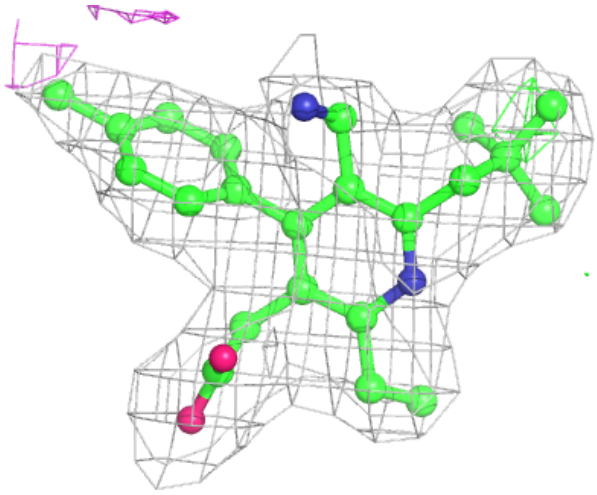


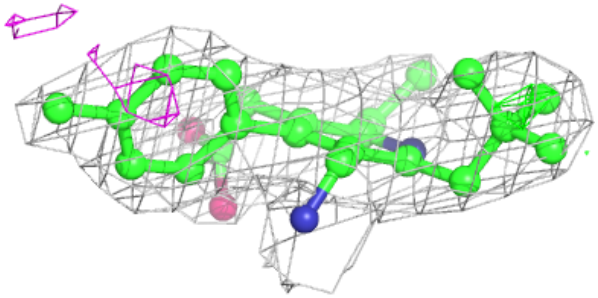


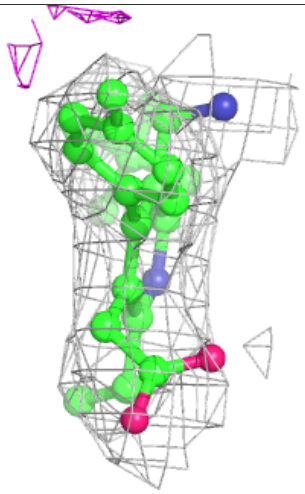


Electron density around 01T D 1:

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

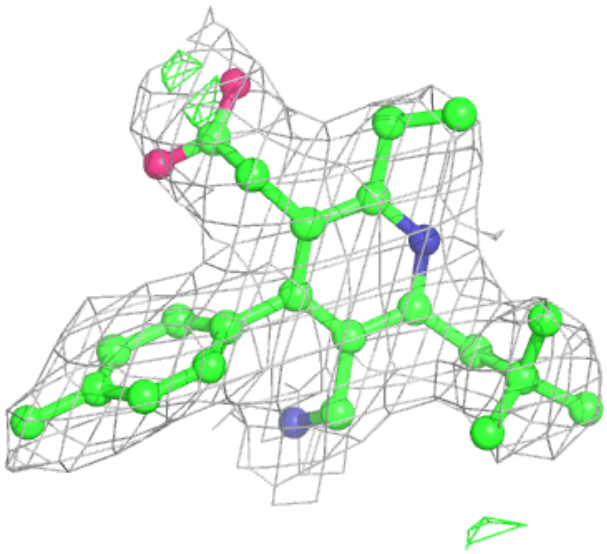


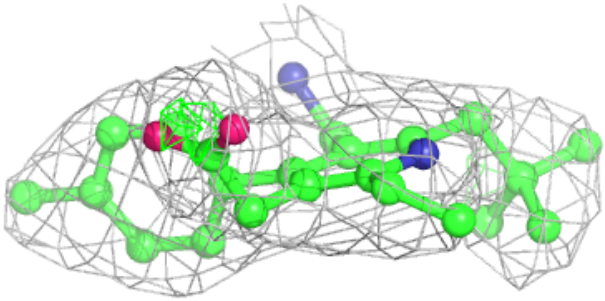


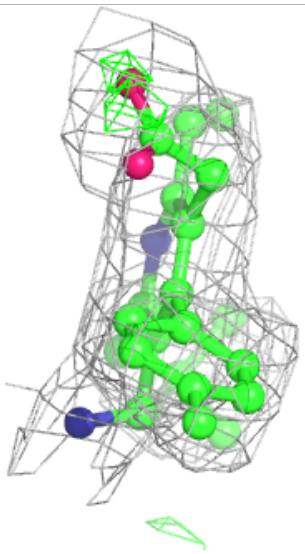


Electron density around 01T B 1:

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

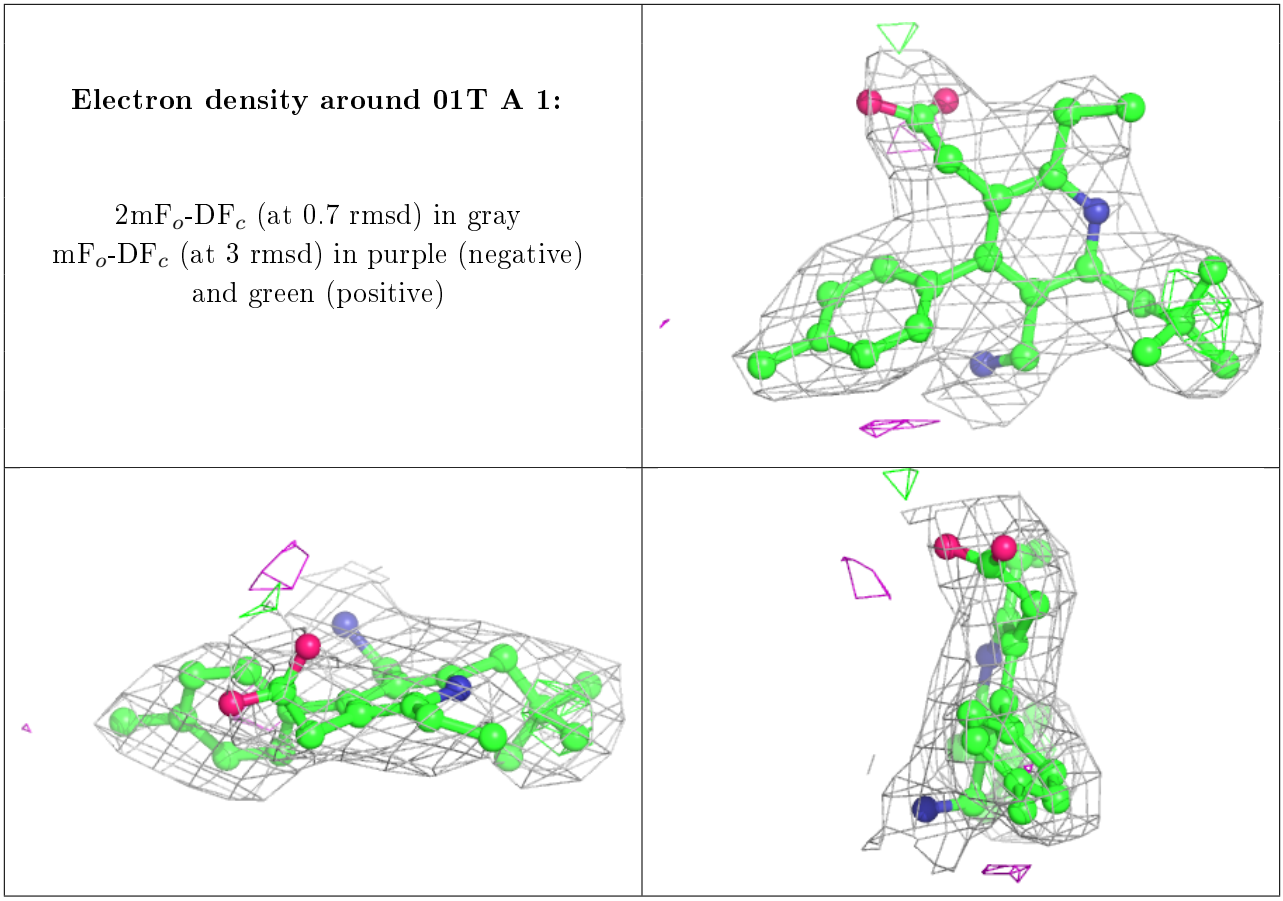






Electron density around 01T A 1:

$2mF_o$-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

Unable to reproduce the depositors R factor - this section is therefore empty.