



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:45 PM BST

PDB ID : 3O9V
Title : Crystal Structure of Human DPP4 Bound to TAK-986
Authors : Yano, J.K.; Aertgeerts, K.
Deposited on : 2010-08-04
Resolution : 2.75 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

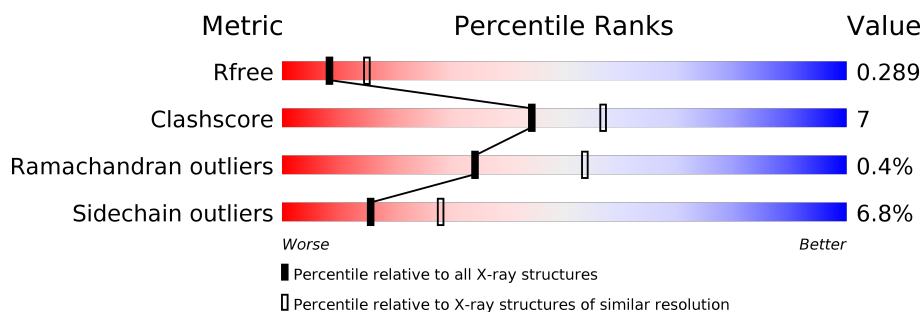
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



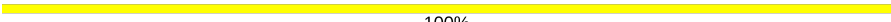
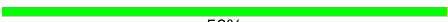
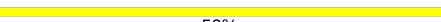
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	740	75% 21% ..
1	B	740	82% 15% ..
1	C	740	77% 20% ..
1	D	740	83% 14% ..
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	I	2	 50%  50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24702 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	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	D	727	Total	C	N	O	S	0	0	0
			5952	3821	981	1124	26			

There are 48 discrepancies between the modelled and reference sequences:

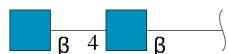
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
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.



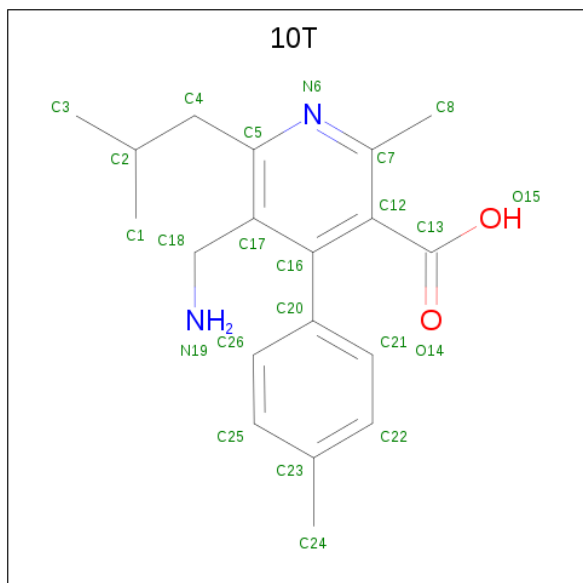
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

- Molecule 3 is 5-(aminomethyl)-2-methyl-4-(4-methylphenyl)-6-(2-methylpropyl)pyridine-3-carboxylic acid (three-letter code: 10T) (formula: $C_{19}H_{24}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	19	2	2		
3	B	1	Total	C	N	O	0	0
			23	19	2	2		
3	C	1	Total	C	N	O	0	0
			23	19	2	2		
3	D	1	Total	C	N	O	0	0
			23	19	2	2		

- 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	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total	O	0	0
			133	133		
5	B	123	Total	O	0	0
			123	123		

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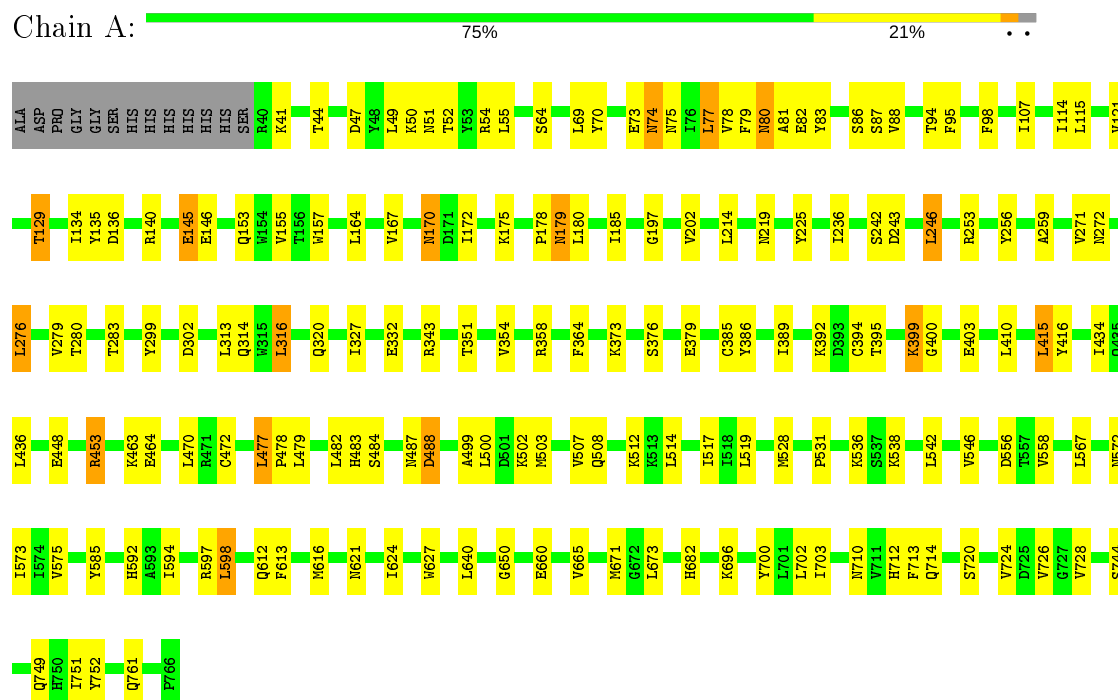
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	83	Total 83	O 83	0	0
5	D	112	Total 112	O 112	0	0

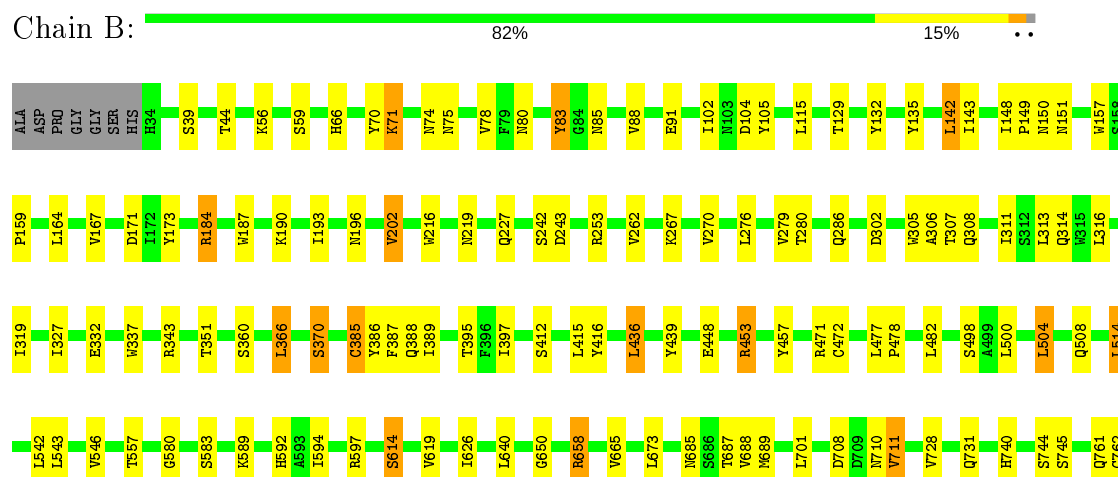
3 Residue-property plots

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



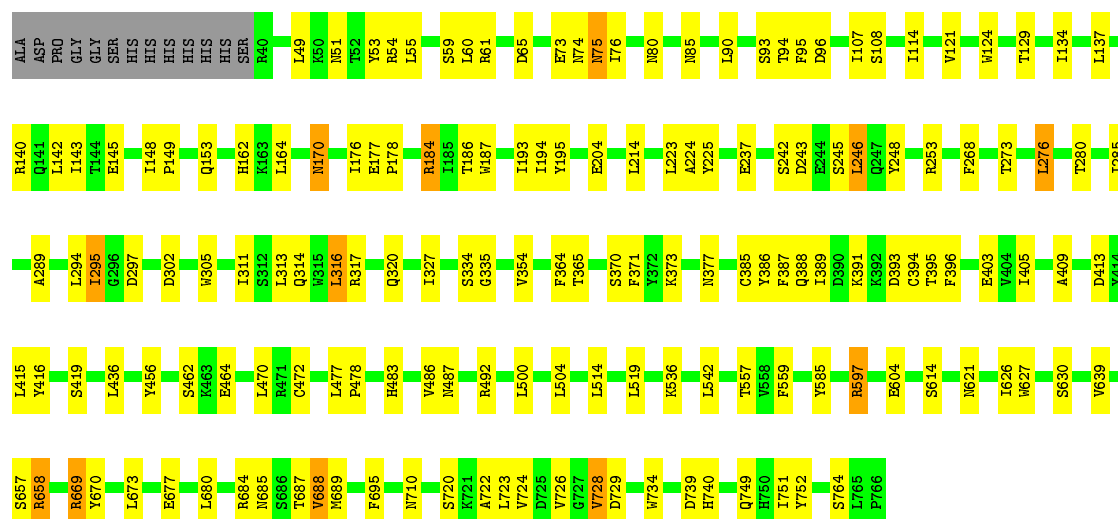
• Molecule 1: Dipeptidyl peptidase 4






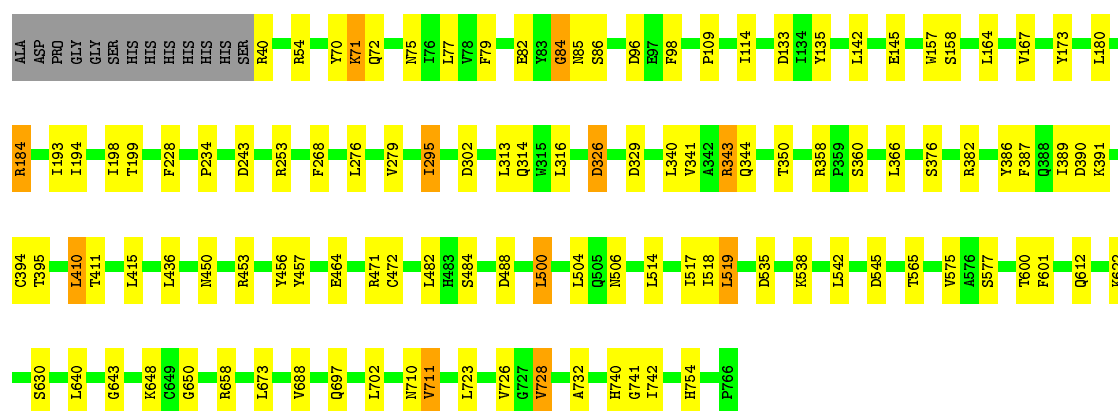
- Molecule 1: Dipeptidyl peptidase 4

Chain C:  77% 20% ..



- Molecule 1: Dipeptidyl peptidase 4

Chain D:  83% 14% ..



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

Chain E:  50% 50%



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

Chain F:  50% 50%

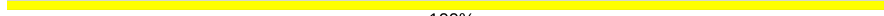
MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.17Å 122.89Å 144.91Å 90.00° 114.59° 90.00°	Depositor
Resolution (Å)	35.00 – 2.75 34.79 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-2.75) 98.7 (34.79-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.260 0.249 , 0.289	Depositor DCC
R_{free} test set	5026 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24702	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 10T

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	0.50	0/6129	0.63	0/8336
1	B	0.50	0/6190	0.61	0/8419
1	C	0.45	0/6129	0.59	1/8336 (0.0%)
1	D	0.49	0/6124	0.61	0/8329
All	All	0.49	0/24572	0.61	1/33420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	669	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5957	0	5676	91	0
1	B	6013	0	5715	69	0
1	C	5957	0	5677	89	0
1	D	5952	0	5672	64	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	2	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	23	0	23	0	0
3	B	23	0	23	0	0
3	C	23	0	23	1	0
3	D	23	0	23	1	0
4	A	28	0	26	0	0
4	B	56	0	52	1	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	133	0	0	3	0
5	B	123	0	0	4	0
5	C	83	0	0	2	0
5	D	112	0	0	3	0
All	All	24702	0	23087	310	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 (310) 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:518:ILE:O	1:D:519:LEU:HD13	1.66	0.96
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.53	0.88
1:A:153:GLN:HE22	1:A:170:ASN:H	1.22	0.88
1:A:399:LYS:HD2	1:A:400:GLY:N	1.94	0.83
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.65	0.78
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.68	0.76
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.19	0.73
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.36	0.72
1:C:153:GLN:HE22	1:C:170:ASN:H	1.36	0.71
1:A:77:LEU:HD12	1:A:88:VAL:HA	1.71	0.71
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.73	0.71
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.73	0.71
1:C:415:LEU:HB2	1:C:436:LEU:HD11	1.74	0.70
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.73	0.70
1:D:157:TRP:CZ3	1:D:164:LEU:HD21	2.26	0.69
1:D:391:LYS:HG2	5:D:839:HOH:O	1.92	0.69
1:D:517:ILE:HD13	1:D:612:GLN:HG3	1.74	0.69
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HD22	1:A:81:ALA:H	1.42	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.76	0.67
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.59	0.66
1:A:121:VAL:HB	1:A:129:THR:HG23	1.77	0.66
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.77	0.66
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.77	0.66
1:A:80:ASN:ND2	5:A:851:HOH:O	2.25	0.66
1:C:597:ARG:HD3	5:C:820:HOH:O	1.94	0.66
1:A:172:ILE:HG22	1:A:185:ILE:HD13	1.79	0.65
1:A:80:ASN:HD22	1:A:81:ALA:N	1.95	0.65
1:C:295:ILE:HD11	1:C:317:ARG:HE	1.62	0.64
1:B:59:SER:O	1:B:70:TYR:CD1	2.50	0.64
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.34	0.63
1:C:90:LEU:HD12	1:C:140:ARG:HH21	1.63	0.63
1:D:386:TYR:O	1:D:394:CYS:HB2	1.99	0.62
1:A:477:LEU:HD12	1:A:477:LEU:H	1.64	0.62
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.80	0.62
1:C:542:LEU:HD23	1:C:542:LEU:C	2.20	0.62
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.29	0.62
1:C:289:ALA:HB3	1:C:294:LEU:HD21	1.81	0.62
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.65	0.61
1:A:598:LEU:HB2	1:A:671:MET:SD	2.40	0.61
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.82	0.61
1:A:54:ARG:HD3	1:D:40:ARG:HH22	1.64	0.61
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.82	0.61
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.83	0.61
1:A:179:ASN:HD22	1:A:179:ASN:C	2.04	0.60
1:B:267:LYS:HG2	1:B:286:GLN:HE22	1.67	0.60
1:A:487:ASN:O	1:A:488:ASP:HB2	2.01	0.60
1:C:184:ARG:HD3	1:C:186:THR:O	2.01	0.60
1:D:157:TRP:CZ3	1:D:164:LEU:CD2	2.84	0.60
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.84	0.60
1:D:484:SER:O	1:D:488:ASP:HA	2.02	0.60
2:G:1:NAG:H62	2:G:2:NAG:HN2	1.67	0.60
2:G:1:NAG:H62	2:G:2:NAG:N2	2.16	0.59
1:D:295:ILE:HD13	1:D:295:ILE:O	2.02	0.59
1:A:170:ASN:N	1:A:170:ASN:HD22	2.01	0.59
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.83	0.59
1:A:399:LYS:HD2	1:A:400:GLY:H	1.65	0.59
1:A:453:ARG:NH2	1:A:477:LEU:O	2.36	0.59
1:A:594:ILE:HD12	1:A:594:ILE:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.38	0.58
1:C:170:ASN:N	1:C:170:ASN:HD22	2.01	0.58
1:C:121:VAL:HB	1:C:129:THR:HG22	1.85	0.58
1:D:366:LEU:HD23	1:D:366:LEU:O	2.04	0.58
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.39	0.57
1:B:370:SER:HG	1:B:386:TYR:HE2	1.52	0.57
1:C:114:ILE:HB	1:C:137:LEU:HD12	1.85	0.57
1:B:614:SER:HA	1:B:619:VAL:HB	1.87	0.57
1:D:723:LEU:HD22	1:D:728:VAL:HG11	1.86	0.57
1:B:542:LEU:HD23	1:B:542:LEU:C	2.24	0.57
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.87	0.57
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.87	0.56
1:A:484:SER:O	1:A:488:ASP:HA	2.05	0.56
1:A:134:ILE:HD13	1:A:178:PRO:HB3	1.86	0.56
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.88	0.56
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.88	0.56
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.87	0.55
1:D:389:ILE:HG22	1:D:390:ASP:OD1	2.06	0.55
1:A:500:LEU:HA	1:A:503:MET:HE3	1.88	0.55
1:D:366:LEU:HD23	1:D:366:LEU:C	2.27	0.55
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.55
1:B:397:ILE:HG22	1:B:439:TYR:CZ	2.41	0.54
1:C:415:LEU:CB	1:C:436:LEU:HD11	2.38	0.54
1:C:80:ASN:HB3	1:C:85:ASN:O	2.07	0.54
1:C:658:ARG:HG2	1:C:689:MET:CE	2.38	0.54
1:C:76:ILE:HD12	1:C:90:LEU:HD23	1.90	0.54
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.43	0.54
1:B:196:ASN:ND2	1:B:227:GLN:HG3	2.22	0.54
1:B:453:ARG:NH2	1:B:477:LEU:O	2.41	0.54
1:A:567:LEU:HD22	1:A:573:ILE:HD12	1.90	0.53
1:A:44:THR:HB	5:A:774:HOH:O	2.08	0.53
1:B:761:GLN:HG2	5:B:834:HOH:O	2.07	0.53
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.90	0.53
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.44	0.53
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.24	0.53
1:A:279:VAL:HG12	1:A:280:THR:HG23	1.91	0.52
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.91	0.52
1:B:242:SER:OG	1:B:243:ASP:N	2.43	0.52
1:A:499:ALA:O	1:A:503:MET:HE3	2.10	0.52
1:C:739:ASP:HB2	5:C:805:HOH:O	2.09	0.52
1:C:657:SER:HA	1:C:688:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG22	5:B:814:HOH:O	2.10	0.52
1:B:701:LEU:HD13	1:B:731:GLN:HB3	1.91	0.52
1:D:173:TYR:CE1	1:D:184:ARG:HG2	2.45	0.52
1:C:242:SER:OG	1:C:243:ASP:N	2.43	0.51
1:C:60:LEU:HD12	1:C:60:LEU:C	2.30	0.51
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.90	0.51
1:C:729:ASP:OD1	1:D:754:HIS:ND1	2.35	0.51
1:B:313:LEU:N	1:B:313:LEU:HD22	2.25	0.51
1:B:102:ILE:HD12	1:B:102:ILE:H	1.76	0.51
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.37	0.51
1:C:289:ALA:HB3	1:C:294:LEU:CD2	2.41	0.50
1:B:135:TYR:HD1	1:B:142:LEU:HD22	1.76	0.50
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.46	0.50
1:A:259:ALA:HB3	1:A:660:GLU:HA	1.93	0.50
1:A:594:ILE:CD1	1:A:594:ILE:C	2.79	0.50
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.92	0.50
1:B:415:LEU:HD23	1:B:415:LEU:C	2.31	0.50
1:C:214:LEU:HD22	1:C:223:LEU:HD11	1.93	0.50
1:C:316:LEU:HD13	1:C:320:GLN:HG2	1.92	0.50
1:B:83:TYR:N	1:B:83:TYR:CD2	2.79	0.50
1:A:47:ASP:HA	1:A:52:THR:OG1	2.11	0.50
1:D:542:LEU:C	1:D:542:LEU:HD23	2.32	0.50
1:A:64:SER:HA	1:A:463:LYS:HE2	1.92	0.50
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.41	0.50
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.42	0.50
1:C:734:TRP:CZ3	1:D:732:ALA:HB1	2.47	0.50
1:D:142:LEU:H	1:D:142:LEU:HD23	1.77	0.50
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.95	0.50
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.12	0.50
1:D:75:ASN:O	1:D:77:LEU:HD12	2.11	0.49
1:C:94:THR:HG22	1:C:95:PHE:CE1	2.48	0.49
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.26	0.49
1:A:720:SER:O	1:A:724:VAL:HG23	2.12	0.49
1:C:409:ALA:HB3	1:C:416:TYR:HB2	1.94	0.49
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.42	0.49
1:C:726:VAL:CG2	1:C:728:VAL:CG1	2.90	0.49
1:D:71:LYS:H	1:D:71:LYS:HD3	1.78	0.49
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.59	0.49
1:C:630:SER:HB2	1:C:740:HIS:NE2	2.28	0.49
1:C:142:LEU:HD12	1:C:143:ILE:N	2.28	0.49
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.48	0.49
1:A:386:TYR:O	1:A:394:CYS:HB2	2.13	0.48
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.95	0.48
1:B:279:VAL:HG23	1:B:280:THR:HG23	1.95	0.48
1:C:143:ILE:O	1:C:143:ILE:HG22	2.12	0.48
1:B:150:ASN:O	1:B:151:ASN:HB2	2.13	0.48
1:A:546:VAL:HG12	1:A:627:TRP:O	2.14	0.48
1:A:751:ILE:HG23	1:A:752:TYR:N	2.29	0.48
1:C:391:LYS:HE3	1:C:393:ASP:HB2	1.94	0.48
1:D:600:THR:OG1	1:D:601:PHE:N	2.46	0.48
1:A:153:GLN:NE2	1:A:167:VAL:HG12	2.29	0.48
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.95	0.48
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.43	0.47
1:C:626:ILE:HD13	1:C:639:VAL:HG11	1.96	0.47
1:B:305:TRP:CE2	1:B:311:ILE:HD12	2.48	0.47
1:C:370:SER:HG	1:C:386:TYR:HE2	1.61	0.47
1:C:657:SER:HA	1:C:688:VAL:HG13	1.96	0.47
1:A:272:ASN:O	1:A:276:LEU:HD13	2.13	0.47
1:D:199:THR:HA	1:D:228:PHE:CE2	2.50	0.47
1:D:410:LEU:HD22	1:D:411:THR:O	2.14	0.47
1:D:500:LEU:HD11	1:D:504:LEU:HD22	1.97	0.47
1:A:415:LEU:HD13	1:A:416:TYR:N	2.29	0.47
1:A:80:ASN:ND2	1:A:81:ALA:H	2.08	0.47
1:B:184:ARG:HD2	1:B:187:TRP:CZ2	2.48	0.47
1:C:658:ARG:HB3	1:C:687:THR:HG22	1.96	0.47
1:B:306:ALA:O	1:B:307:THR:HG23	2.14	0.47
1:C:93:SER:HA	1:C:96:ASP:HB3	1.97	0.47
1:A:512:LYS:NZ	1:A:558:VAL:O	2.48	0.47
3:C:1:10T:H18	3:C:1:10T:C21	2.44	0.47
1:C:54:ARG:O	1:C:500:LEU:HD22	2.15	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.97	0.46
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.96	0.46
1:C:124:TRP:HB2	1:C:204:GLU:OE1	2.15	0.46
1:A:613:PHE:O	1:A:616:MET:HB2	2.14	0.46
1:B:190:LYS:HG2	1:B:193:ILE:HD12	1.97	0.46
1:D:711:VAL:HG11	1:D:740:HIS:CE1	2.50	0.46
1:A:175:LYS:NZ	1:A:180:LEU:O	2.47	0.46
1:B:167:VAL:HA	1:B:171:ASP:O	2.15	0.46
1:B:415:LEU:HD23	1:B:416:TYR:N	2.30	0.46
1:C:377:ASN:HA	1:C:396:PHE:CZ	2.51	0.46
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ARG:HG2	1:B:689:MET:CE	2.46	0.46
1:C:472:CYS:O	1:C:478:PRO:HA	2.16	0.46
1:D:109:PRO:HG2	1:D:158:SER:O	2.14	0.46
1:A:107:ILE:HD11	1:A:114:ILE:HD12	1.98	0.46
1:A:343:ARG:HD2	1:A:389:ILE:CG2	2.45	0.46
1:A:472:CYS:O	1:A:478:PRO:HA	2.16	0.46
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.51	0.45
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.97	0.45
1:D:341:VAL:HG12	5:D:836:HOH:O	2.16	0.45
1:A:185:ILE:N	1:A:185:ILE:HD12	2.32	0.45
1:B:302:ASP:HB3	1:B:314:GLN:HE21	1.80	0.45
1:C:689:MET:HG3	1:C:722:ALA:HB2	1.99	0.45
1:D:741:GLY:O	1:D:742:ILE:C	2.54	0.45
1:B:44:THR:HB	5:B:819:HOH:O	2.16	0.45
1:B:542:LEU:HD23	1:B:543:LEU:N	2.31	0.45
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.99	0.45
1:D:376:SER:HA	1:D:382:ARG:HA	1.98	0.45
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.98	0.45
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.31	0.45
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.31	0.45
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.51	0.45
1:C:456:TYR:HB2	1:C:557:THR:OG1	2.17	0.45
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.52	0.45
1:C:148:ILE:HG23	1:C:149:PRO:HD2	1.98	0.45
1:D:279:VAL:O	1:D:279:VAL:HG12	2.16	0.45
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.47	0.45
1:C:405:ILE:HD12	1:C:585:TYR:CD2	2.52	0.45
1:B:306:ALA:O	1:B:307:THR:CG2	2.64	0.45
1:D:360:SER:HA	5:D:840:HOH:O	2.15	0.45
1:C:409:ALA:O	1:C:415:LEU:HD22	2.16	0.44
1:D:457:TYR:HA	1:D:471:ARG:O	2.18	0.44
1:D:456:TYR:O	1:D:472:CYS:HA	2.16	0.44
1:D:545:ASP:HB3	1:D:577:SER:OG	2.18	0.44
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.17	0.44
1:C:614:SER:HB2	1:C:621:ASN:OD1	2.17	0.44
3:D:1:10T:C21	3:D:1:10T:H18	2.47	0.44
1:C:65:ASP:HA	1:C:462:SER:HB2	1.99	0.44
1:A:512:LYS:HA	1:A:528:MET:O	2.18	0.44
1:B:351:THR:OG1	1:B:592:HIS:CD2	2.71	0.44
1:B:71:LYS:HA	1:B:75:ASN:O	2.18	0.44
1:C:658:ARG:HG2	1:C:689:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:HB3	1:B:308:GLN:HE22	1.83	0.44
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.99	0.44
1:D:84:GLY:O	1:D:86:SER:N	2.46	0.44
1:B:85:ASN:OD1	4:B:851:NAG:H82	2.18	0.43
1:A:172:ILE:HD11	1:A:197:GLY:HA3	1.99	0.43
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.99	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.53	0.43
1:C:75:ASN:N	1:C:75:ASN:OD1	2.51	0.43
1:A:316:LEU:HD21	1:A:354:VAL:CG1	2.48	0.43
1:B:88:VAL:HG11	1:B:91:GLU:HG3	1.99	0.43
1:A:79:PHE:HA	1:A:86:SER:HB3	1.99	0.43
1:A:713:PHE:O	1:A:714:GLN:C	2.57	0.43
1:C:364:PHE:CD2	1:C:371:PHE:HB3	2.53	0.43
1:C:720:SER:O	1:C:724:VAL:HG23	2.19	0.43
1:B:580:GLY:O	1:B:583:SER:OG	2.31	0.43
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.34	0.43
1:A:316:LEU:HD21	1:A:354:VAL:HG12	2.00	0.43
1:D:711:VAL:CG1	1:D:740:HIS:ND1	2.81	0.43
1:B:104:ASP:OD1	1:B:105:TYR:N	2.52	0.42
1:C:176:ILE:HG22	1:C:177:GLU:HG2	2.01	0.42
1:C:370:SER:OG	1:C:386:TYR:HE2	2.02	0.42
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.54	0.42
1:A:512:LYS:HE2	1:A:556:ASP:O	2.18	0.42
1:B:39:SER:HB3	1:B:508:GLN:HG3	2.01	0.42
1:A:145:GLU:O	1:A:146:GLU:HB2	2.18	0.42
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.54	0.42
1:D:711:VAL:HG12	1:D:740:HIS:CE1	2.53	0.42
1:D:702:LEU:O	1:D:732:ALA:HA	2.20	0.42
1:A:107:ILE:CD1	1:A:114:ILE:HD12	2.49	0.42
1:A:136:ASP:O	1:A:140:ARG:N	2.53	0.42
1:A:219:ASN:ND2	5:A:767:HOH:O	2.51	0.42
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.82	0.42
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.42
1:B:500:LEU:O	1:B:504:LEU:HD22	2.20	0.42
1:B:78:VAL:HG13	1:B:78:VAL:O	2.20	0.42
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.20	0.42
1:A:597:ARG:NH1	1:A:682:HIS:HB2	2.34	0.42
1:B:135:TYR:CD1	1:B:142:LEU:HD22	2.54	0.42
1:B:542:LEU:HD23	1:B:543:LEU:C	2.40	0.42
1:D:366:LEU:CD2	1:D:366:LEU:C	2.87	0.42
1:D:518:ILE:HG22	1:D:519:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD23	1:A:77:LEU:O	2.18	0.42
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.02	0.42
1:C:751:ILE:HG23	1:C:752:TYR:N	2.35	0.42
1:D:70:TYR:CE2	1:D:79:PHE:HB2	2.55	0.42
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.55	0.42
1:B:708:ASP:OD1	1:B:740:HIS:HA	2.20	0.42
1:C:134:ILE:HD13	1:C:178:PRO:HB3	2.02	0.41
1:C:76:ILE:HB	1:C:90:LEU:HB3	2.00	0.41
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.85	0.41
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.55	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.21	0.41
1:C:680:LEU:O	1:C:684:ARG:HG3	2.20	0.41
1:D:622:LYS:O	1:D:648:LYS:HD2	2.21	0.41
1:B:115:LEU:HD11	1:B:132:TYR:HB3	2.01	0.41
1:A:487:ASN:O	1:A:488:ASP:CB	2.68	0.41
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.41
1:B:83:TYR:H	1:B:83:TYR:HD2	1.62	0.41
1:A:179:ASN:HD22	1:A:180:LEU:N	2.19	0.41
1:B:457:TYR:HA	1:B:471:ARG:O	2.21	0.41
1:C:53:TYR:HB3	1:C:500:LEU:HD11	2.02	0.41
1:D:167:VAL:HG11	1:D:198:ILE:HG12	2.03	0.41
1:D:54:ARG:O	1:D:500:LEU:HD22	2.20	0.41
1:B:319:ILE:HD12	1:B:319:ILE:H	1.86	0.41
1:C:248:TYR:OH	1:D:234:PRO:HG2	2.21	0.41
1:C:486:VAL:HG13	1:C:487:ASN:OD1	2.20	0.41
1:B:148:ILE:HG23	1:B:149:PRO:HD2	2.02	0.41
1:C:195:TYR:CD1	1:C:195:TYR:N	2.89	0.41
1:C:285:ILE:HG13	1:C:335:GLY:O	2.21	0.41
1:C:387:PHE:CE1	1:C:394:CYS:HB3	2.56	0.41
1:C:695:PHE:CD1	1:C:723:LEU:HD21	2.55	0.41
1:C:248:TYR:CZ	1:D:234:PRO:HG2	2.55	0.40
1:D:535:ASP:HB3	1:D:538:LYS:HD2	2.03	0.40
1:B:366:LEU:O	1:B:366:LEU:HD22	2.20	0.40
1:C:415:LEU:HD13	1:C:415:LEU:C	2.42	0.40
1:C:55:LEU:HD21	1:C:559:PHE:HE2	1.85	0.40
1:C:162:HIS:NE2	1:C:177:GLU:OE1	2.52	0.40
1:C:542:LEU:HD23	1:C:542:LEU:O	2.22	0.40
1:D:326:ASP:OD2	1:D:344:GLN:HG2	2.21	0.40
1:A:214:LEU:HD23	1:A:225:TYR:HB3	2.02	0.40
1:A:621:ASN:HA	1:A:624:ILE:HD11	2.04	0.40
1:B:370:SER:HB3	5:B:856:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ARG:HB3	1:B:687:THR:HG22	2.03	0.40
1:C:107:ILE:HG22	1:C:108:SER:O	2.21	0.40
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.04	0.40
1:D:500:LEU:CD1	1:D:504:LEU:HD22	2.52	0.40
1:B:744:SER:O	1:B:745:SER:C	2.60	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%)	679 (94%)	42 (6%)	4 (1%)	25	42
1	B	731/740 (99%)	692 (95%)	37 (5%)	2 (0%)	41	60
1	C	725/740 (98%)	679 (94%)	42 (6%)	4 (1%)	25	42
1	D	725/740 (98%)	675 (93%)	47 (6%)	3 (0%)	34	53
All	All	2906/2960 (98%)	2725 (94%)	168 (6%)	13 (0%)	34	53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
1	A	488	ASP
1	C	73	GLU
1	D	82	GLU
1	A	74	ASN
1	C	334	SER
1	B	74	ASN
1	A	508	GLN
1	C	297	ASP
1	D	85	ASN

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Mol	Chain	Res	Type
1	B	478	PRO
1	C	295	ILE
1	D	84	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	652/662 (98%)	597 (92%)	55 (8%)	11	19
1	B	658/662 (99%)	615 (94%)	43 (6%)	17	30
1	C	652/662 (98%)	611 (94%)	41 (6%)	18	31
1	D	651/662 (98%)	613 (94%)	38 (6%)	20	35
All	All	2613/2648 (99%)	2436 (93%)	177 (7%)	16	28

All (177) 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	73	GLU
1	A	74	ASN
1	A	75	ASN
1	A	77	LEU
1	A	78	VAL
1	A	80	ASN
1	A	82	GLU
1	A	83	TYR
1	A	87	SER
1	A	94	THR
1	A	129	THR
1	A	145	GLU
1	A	170	ASN
1	A	179	ASN
1	A	202	VAL

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Mol	Chain	Res	Type
1	A	243	ASP
1	A	246	LEU
1	A	256	TYR
1	A	271	VAL
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	358	ARG
1	A	373	LYS
1	A	376	SER
1	A	379	GLU
1	A	385	CYS
1	A	392	LYS
1	A	395	THR
1	A	399	LYS
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	477	LEU
1	A	482	LEU
1	A	502	LYS
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	536	LYS
1	A	538	LYS
1	A	542	LEU
1	A	575	VAL
1	A	598	LEU
1	A	673	LEU
1	A	710	ASN
1	A	744	SER
1	A	761	GLN
1	B	56	LYS
1	B	66	HIS
1	B	71	LYS
1	B	80	ASN
1	B	83	TYR

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Mol	Chain	Res	Type
1	B	129	THR
1	B	142	LEU
1	B	143	ILE
1	B	184	ARG
1	B	202	VAL
1	B	262	VAL
1	B	276	LEU
1	B	316	LEU
1	B	332	GLU
1	B	360	SER
1	B	366	LEU
1	B	370	SER
1	B	385	CYS
1	B	388	GLN
1	B	395	THR
1	B	412	SER
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	472	CYS
1	B	482	LEU
1	B	498	SER
1	B	504	LEU
1	B	514	LEU
1	B	546	VAL
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	614	SER
1	B	658	ARG
1	B	665	VAL
1	B	673	LEU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	B	711	VAL
1	B	728	VAL
1	B	762	CYS
1	C	51	ASN
1	C	59	SER
1	C	61	ARG
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	75	ASN
1	C	145	GLU
1	C	164	LEU
1	C	170	ASN
1	C	184	ARG
1	C	245	SER
1	C	246	LEU
1	C	276	LEU
1	C	280	THR
1	C	313	LEU
1	C	316	LEU
1	C	354	VAL
1	C	365	THR
1	C	373	LYS
1	C	385	CYS
1	C	388	GLN
1	C	395	THR
1	C	413	ASP
1	C	419	SER
1	C	464	GLU
1	C	477	LEU
1	C	492	ARG
1	C	504	LEU
1	C	514	LEU
1	C	519	LEU
1	C	536	LYS
1	C	597	ARG
1	C	604	GLU
1	C	627	TRP
1	C	658	ARG
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	C	728	VAL
1	C	764	SER
1	D	71	LYS
1	D	72	GLN
1	D	96	ASP
1	D	98	PHE
1	D	133	ASP

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Mol	Chain	Res	Type
1	D	145	GLU
1	D	180	LEU
1	D	184	ARG
1	D	243	ASP
1	D	276	LEU
1	D	295	ILE
1	D	316	LEU
1	D	326	ASP
1	D	329	ASP
1	D	343	ARG
1	D	350	THR
1	D	358	ARG
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	436	LEU
1	D	450	ASN
1	D	453	ARG
1	D	464	GLU
1	D	482	LEU
1	D	500	LEU
1	D	506	ASN
1	D	514	LEU
1	D	519	LEU
1	D	565	THR
1	D	575	VAL
1	D	630	SER
1	D	658	ARG
1	D	673	LEU
1	D	688	VAL
1	D	710	ASN
1	D	711	VAL
1	D	728	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	179	ASN
1	A	430	ASN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	A	761	GLN
1	B	38	HIS
1	B	80	ASN
1	B	119	ASN
1	B	169	ASN
1	B	196	ASN
1	B	286	GLN
1	B	338	ASN
1	B	388	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	74	ASN
1	C	123	GLN
1	C	138	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	455	GLN
1	C	572	ASN
1	C	685	ASN
1	C	710	ASN
1	C	731	GLN
1	D	92	ASN
1	D	123	GLN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	344	GLN
1	D	430	ASN
1	D	685	ASN
1	D	694	ASN
1	D	697	GLN
1	D	710	ASN

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Mol	Chain	Res	Type
1	D	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	0.60	0	17,19,21	0.94	1 (5%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.82	0
2	NAG	F	1	1,2	14,14,15	0.60	0	17,19,21	1.22	1 (5%)
2	NAG	F	2	2	14,14,15	0.68	0	17,19,21	0.98	0
2	NAG	G	1	1,2	14,14,15	0.83	1 (7%)	17,19,21	1.29	3 (17%)
2	NAG	G	2	2	14,14,15	0.51	0	17,19,21	1.61	3 (17%)
2	NAG	H	1	1,2	14,14,15	0.53	0	17,19,21	1.28	2 (11%)
2	NAG	H	2	2	14,14,15	0.35	0	17,19,21	1.28	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.58	0	17,19,21	1.43	3 (17%)
2	NAG	I	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	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	-2.04	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	O5-C1-C2	-4.07	104.87	111.29
2	F	1	NAG	C1-O5-C5	3.60	117.06	112.19
2	G	2	NAG	C1-C2-N2	3.58	116.61	110.49
2	I	1	NAG	C3-C4-C5	3.23	116.00	110.24
2	H	2	NAG	C1-O5-C5	2.98	116.23	112.19
2	H	1	NAG	O5-C1-C2	-2.71	107.02	111.29
2	G	1	NAG	C1-O5-C5	2.67	115.80	112.19
2	H	2	NAG	O4-C4-C5	2.59	115.72	109.30
2	G	1	NAG	O5-C5-C6	-2.57	103.17	107.20
2	G	1	NAG	O5-C1-C2	-2.55	107.26	111.29
2	I	1	NAG	C4-C3-C2	2.52	114.71	111.02
2	G	2	NAG	C4-C3-C2	-2.50	107.35	111.02
2	H	1	NAG	O3-C3-C4	-2.43	104.73	110.35
2	I	1	NAG	O5-C1-C2	-2.23	107.76	111.29
2	E	1	NAG	O5-C1-C2	-2.01	108.12	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2

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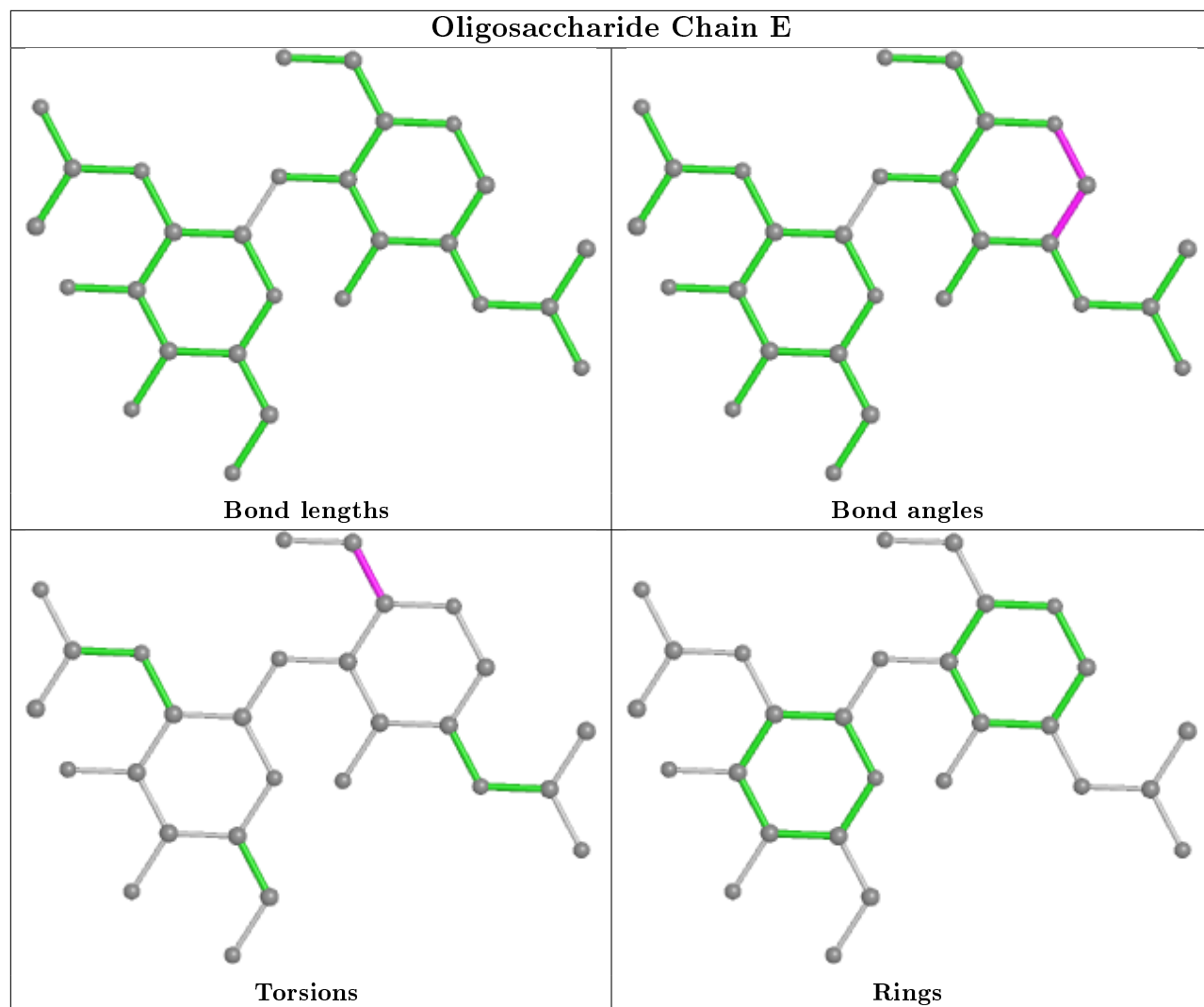
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6

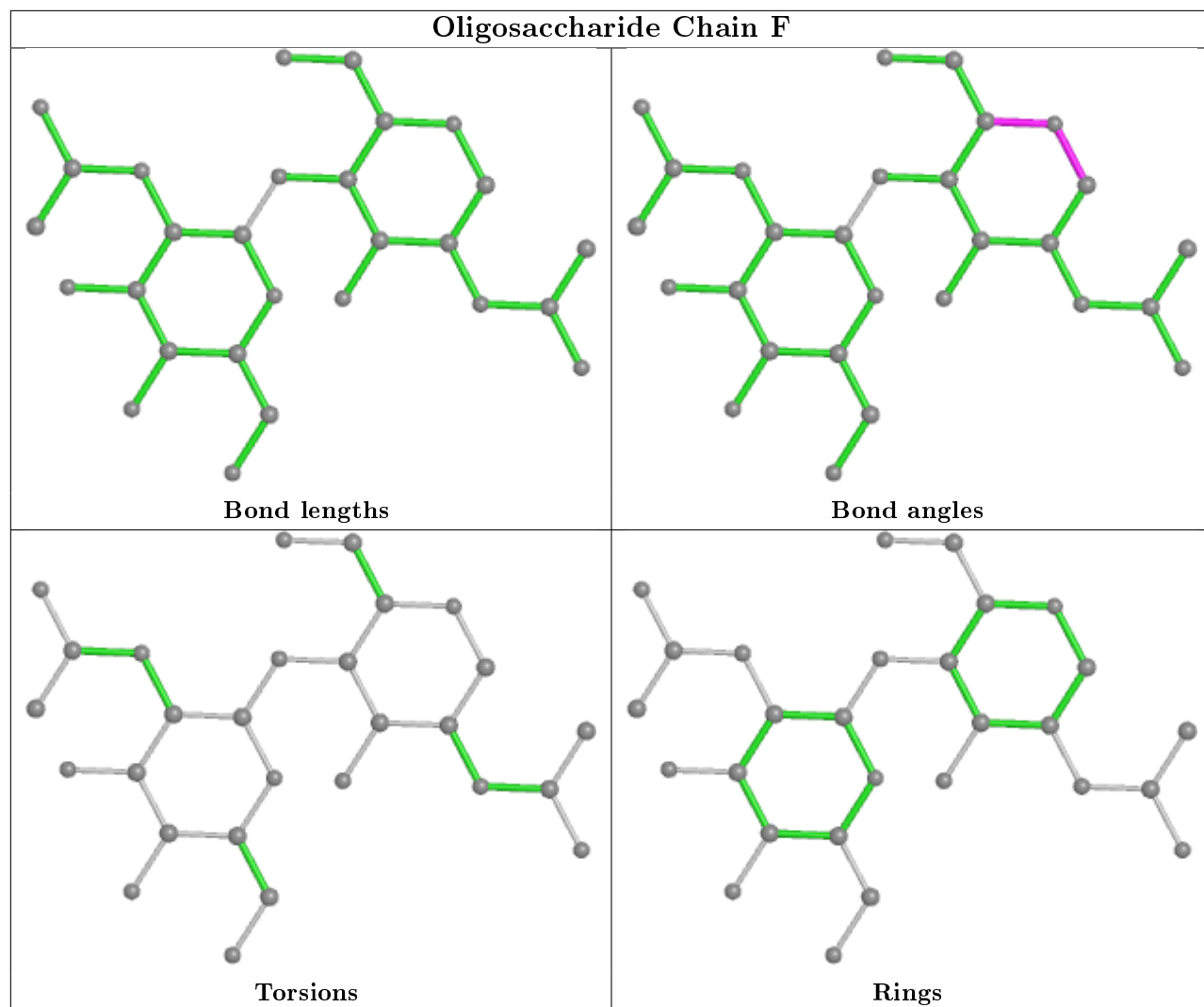
There are no ring outliers.

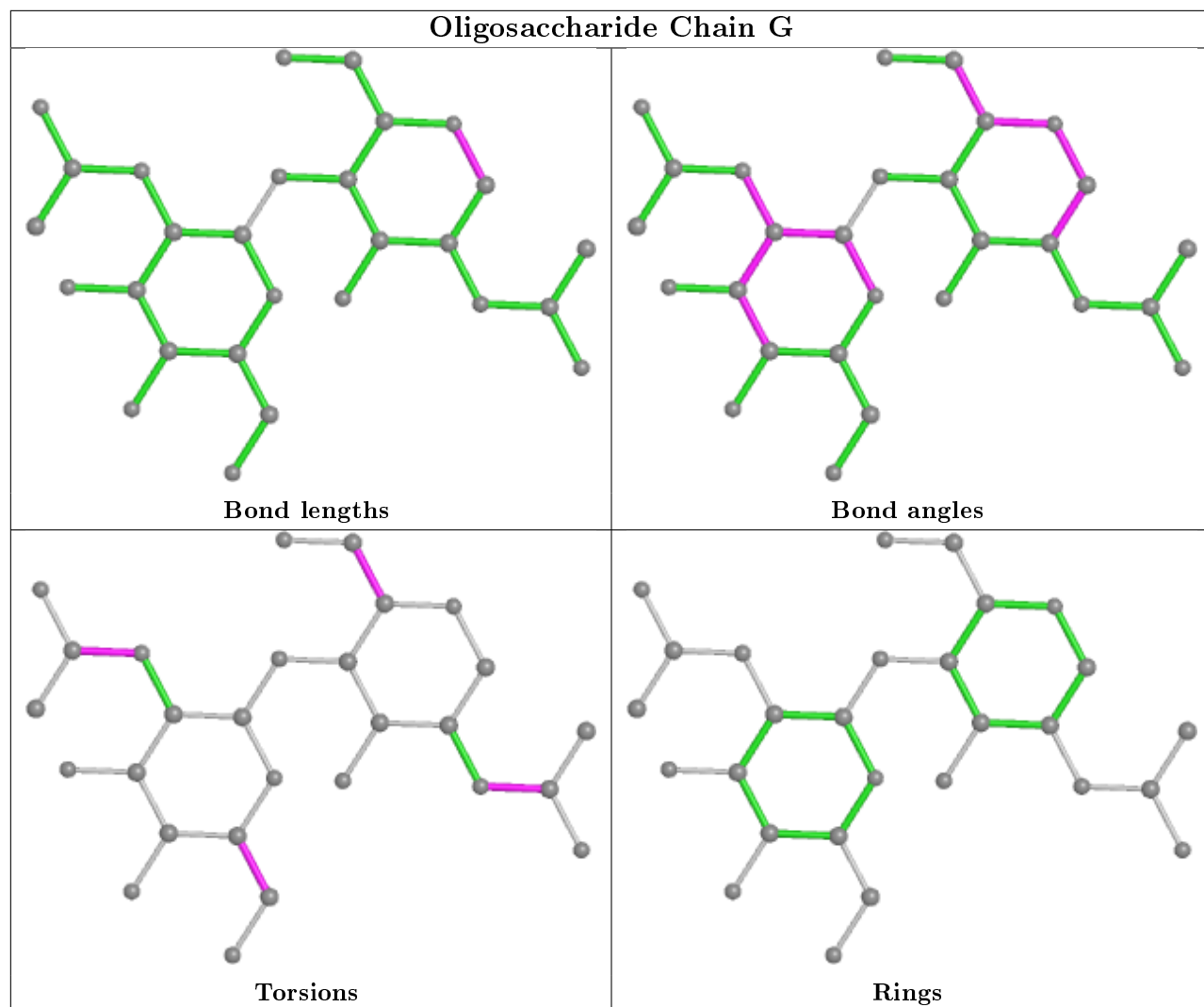
2 monomers are involved in 2 short contacts:

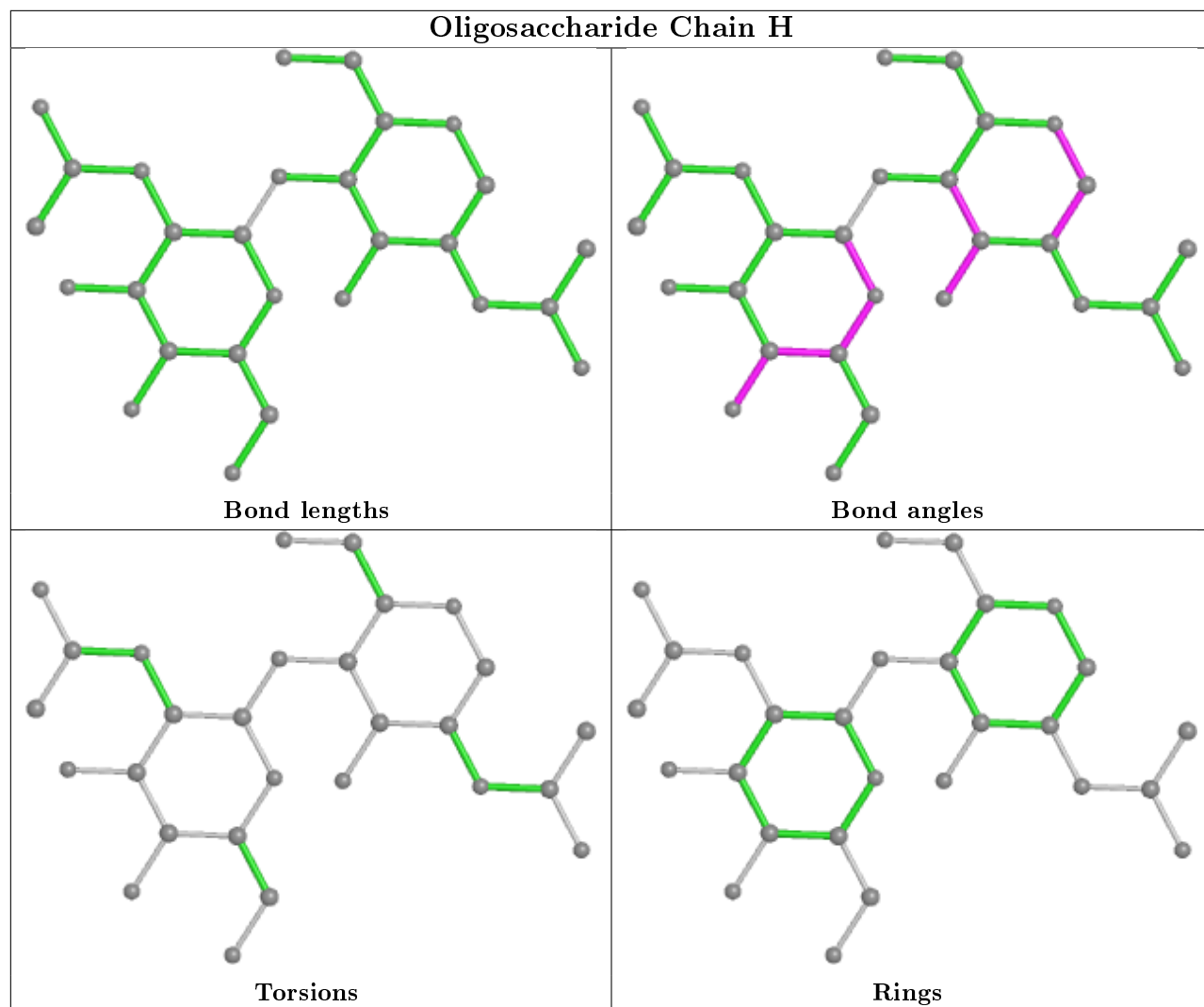
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0
2	G	2	NAG	2	0

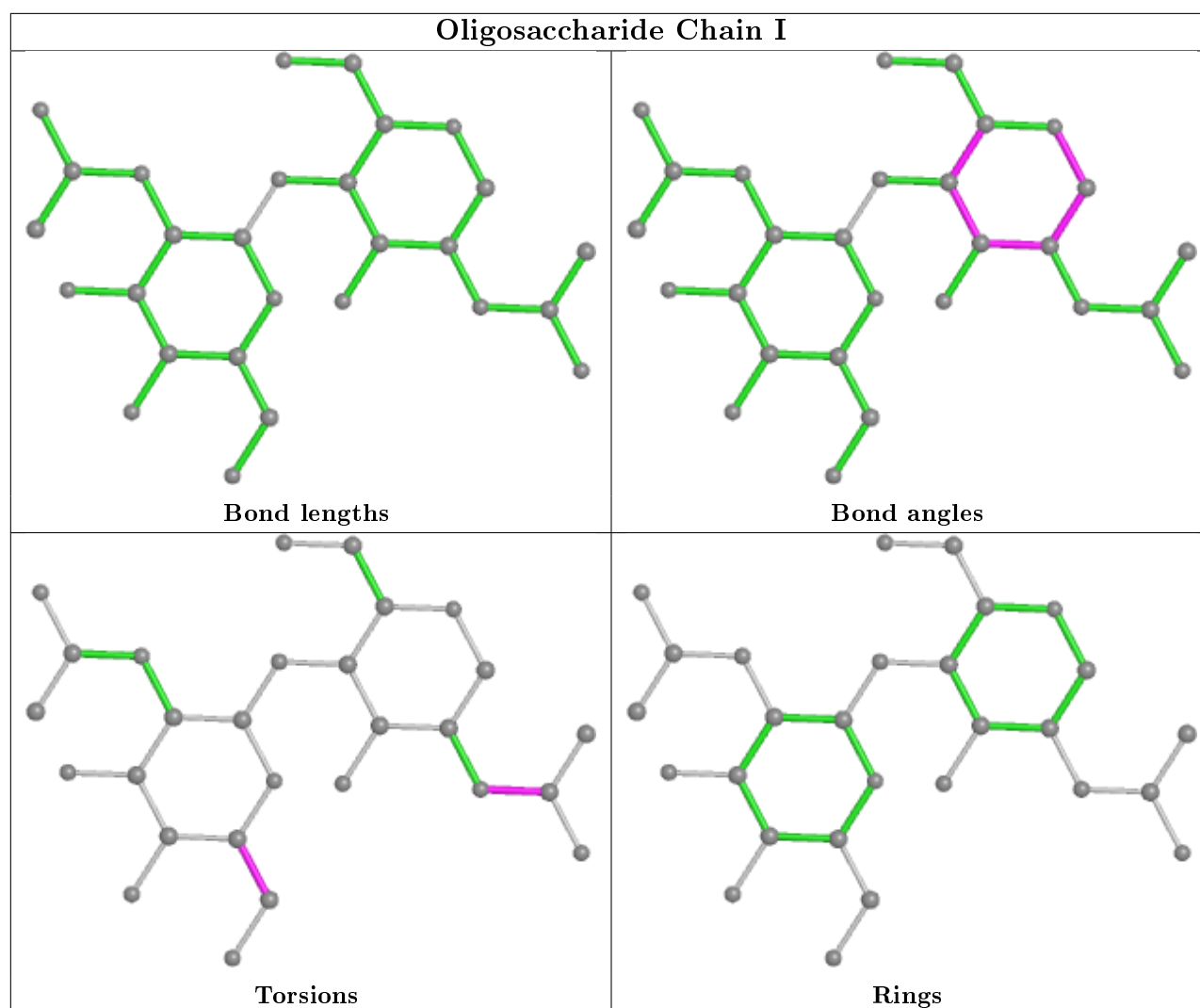
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

14 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	A	1501	1	14,14,15	0.57	0	17,19,21	1.86	3 (17%)
4	NAG	D	2811	1	14,14,15	0.70	0	17,19,21	1.22	2 (11%)
3	10T	B	1	-	22,24,24	0.87	1 (4%)	26,34,34	1.65	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	10T	A	1	-	22,24,24	0.90	1 (4%)	26,34,34	1.48	3 (11%)
3	10T	D	1	-	22,24,24	0.83	1 (4%)	26,34,34	1.80	4 (15%)
3	10T	C	1	-	22,24,24	0.94	1 (4%)	26,34,34	1.61	4 (15%)
4	NAG	C	1501	1	14,14,15	0.55	0	17,19,21	1.71	3 (17%)
4	NAG	D	1501	1	14,14,15	0.53	0	17,19,21	1.42	1 (5%)
4	NAG	B	1501	1	14,14,15	0.48	0	17,19,21	1.49	2 (11%)
4	NAG	B	851	1	14,14,15	0.57	0	17,19,21	1.74	4 (23%)
4	NAG	C	2811	1	14,14,15	0.75	0	17,19,21	1.64	3 (17%)
4	NAG	B	2811	1	14,14,15	0.58	0	17,19,21	1.20	2 (11%)
4	NAG	B	2191	1	14,14,15	0.72	0	17,19,21	1.19	1 (5%)
4	NAG	A	3211	1	14,14,15	0.61	0	17,19,21	1.04	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2811	1	-	4/6/23/26	0/1/1/1
3	10T	B	1	-	-	0/9/14/14	0/2/2/2
3	10T	A	1	-	-	1/9/14/14	0/2/2/2
3	10T	D	1	-	-	0/9/14/14	0/2/2/2
3	10T	C	1	-	-	1/9/14/14	0/2/2/2
4	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1501	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	851	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2191	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3211	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	10T	C12-C13	3.38	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	10T	C12-C13	3.30	1.50	1.47
3	B	1	10T	C12-C13	3.17	1.50	1.47
3	D	1	10T	C12-C13	2.72	1.50	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1501	NAG	C1-O5-C5	5.19	119.22	112.19
3	D	1	10T	C12-C7-N6	-5.19	118.70	122.39
4	D	1501	NAG	C1-O5-C5	5.13	119.14	112.19
4	A	1501	NAG	C1-O5-C5	4.95	118.90	112.19
4	B	1501	NAG	C1-O5-C5	4.91	118.85	112.19
3	C	1	10T	C12-C7-N6	-4.55	119.15	122.39
3	A	1	10T	C12-C7-N6	-4.30	119.33	122.39
3	B	1	10T	C12-C7-N6	-4.24	119.37	122.39
3	D	1	10T	C17-C5-N6	-4.23	119.92	123.49
3	C	1	10T	C17-C5-N6	-4.22	119.93	123.49
4	B	851	NAG	O5-C5-C6	4.11	113.64	107.20
4	C	2811	NAG	O5-C5-C6	3.98	113.44	107.20
3	A	1	10T	C17-C5-N6	-3.78	120.30	123.49
4	B	851	NAG	C4-C3-C2	3.70	116.45	111.02
4	D	2811	NAG	C1-O5-C5	3.60	117.08	112.19
4	B	2811	NAG	C1-O5-C5	3.60	117.07	112.19
3	B	1	10T	C17-C5-N6	-3.54	120.50	123.49
3	D	1	10T	C7-N6-C5	3.54	122.83	118.99
4	C	2811	NAG	C4-C3-C2	3.47	116.10	111.02
3	B	1	10T	C16-C12-C13	-3.46	116.47	120.00
4	A	1501	NAG	C4-C3-C2	-3.34	106.12	111.02
4	B	2191	NAG	C1-O5-C5	3.30	116.66	112.19
3	C	1	10T	C7-N6-C5	3.21	122.47	118.99
3	A	1	10T	C7-N6-C5	3.05	122.30	118.99
3	D	1	10T	C8-C7-N6	2.85	120.90	116.49
4	C	2811	NAG	C2-N2-C7	2.69	126.73	122.90
3	B	1	10T	C8-C7-N6	2.65	120.59	116.49
4	C	1501	NAG	O5-C5-C6	2.55	111.19	107.20
4	B	851	NAG	C1-C2-N2	-2.39	106.41	110.49
4	B	851	NAG	C1-O5-C5	2.36	115.38	112.19
4	B	2811	NAG	O5-C5-C6	2.25	110.73	107.20
4	A	3211	NAG	C1-O5-C5	2.24	115.23	112.19
3	B	1	10T	C7-N6-C5	2.20	121.37	118.99
4	A	1501	NAG	O5-C5-C6	2.17	110.61	107.20
3	C	1	10T	C8-C7-N6	2.14	119.80	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1501	NAG	O5-C5-C6	2.08	110.47	107.20
4	C	1501	NAG	O7-C7-N2	2.03	125.69	121.95
4	D	2811	NAG	C4-C3-C2	2.02	113.98	111.02
4	A	3211	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (32) torsion outliers are listed below:

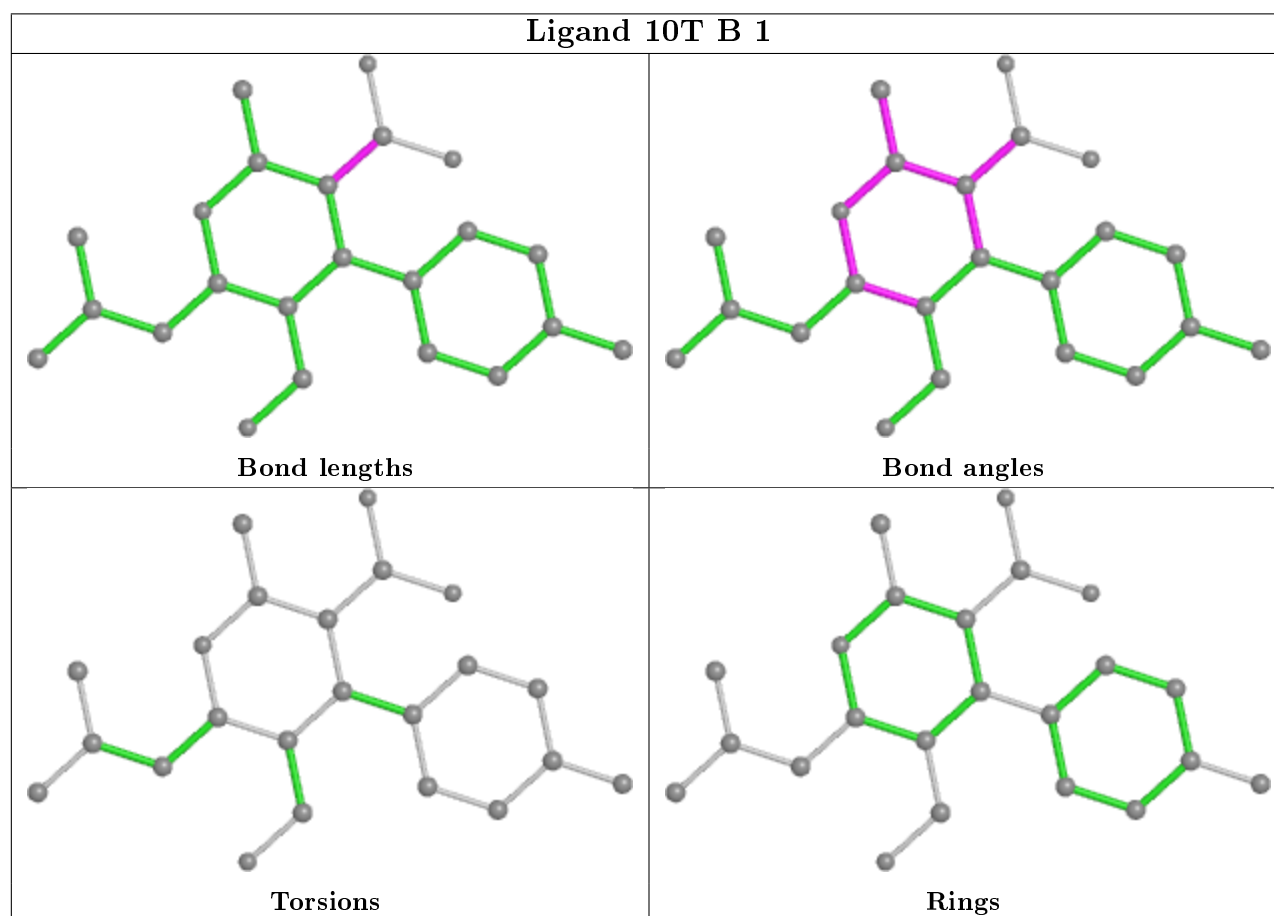
Mol	Chain	Res	Type	Atoms
4	A	1501	NAG	O7-C7-N2-C2
3	A	1	10T	C16-C17-C18-N19
4	B	851	NAG	C8-C7-N2-C2
4	B	851	NAG	O7-C7-N2-C2
4	A	1501	NAG	C8-C7-N2-C2
4	B	851	NAG	O5-C5-C6-O6
4	D	2811	NAG	C8-C7-N2-C2
4	B	2811	NAG	C8-C7-N2-C2
4	B	2191	NAG	C8-C7-N2-C2
4	B	2191	NAG	O7-C7-N2-C2
4	B	851	NAG	C4-C5-C6-O6
4	D	2811	NAG	O7-C7-N2-C2
4	B	2811	NAG	O7-C7-N2-C2
4	A	1501	NAG	C4-C5-C6-O6
4	C	2811	NAG	C4-C5-C6-O6
4	A	3211	NAG	O5-C5-C6-O6
4	A	1501	NAG	O5-C5-C6-O6
4	C	2811	NAG	O5-C5-C6-O6
4	D	1501	NAG	O5-C5-C6-O6
4	D	1501	NAG	C4-C5-C6-O6
4	A	3211	NAG	C4-C5-C6-O6
4	B	1501	NAG	C4-C5-C6-O6
4	D	2811	NAG	C4-C5-C6-O6
4	D	1501	NAG	C8-C7-N2-C2
4	D	2811	NAG	O5-C5-C6-O6
4	D	1501	NAG	O7-C7-N2-C2
4	C	1501	NAG	C8-C7-N2-C2
4	B	1501	NAG	O5-C5-C6-O6
4	C	1501	NAG	O7-C7-N2-C2
3	C	1	10T	C3-C2-C4-C5
4	A	3211	NAG	C8-C7-N2-C2
4	A	3211	NAG	O7-C7-N2-C2

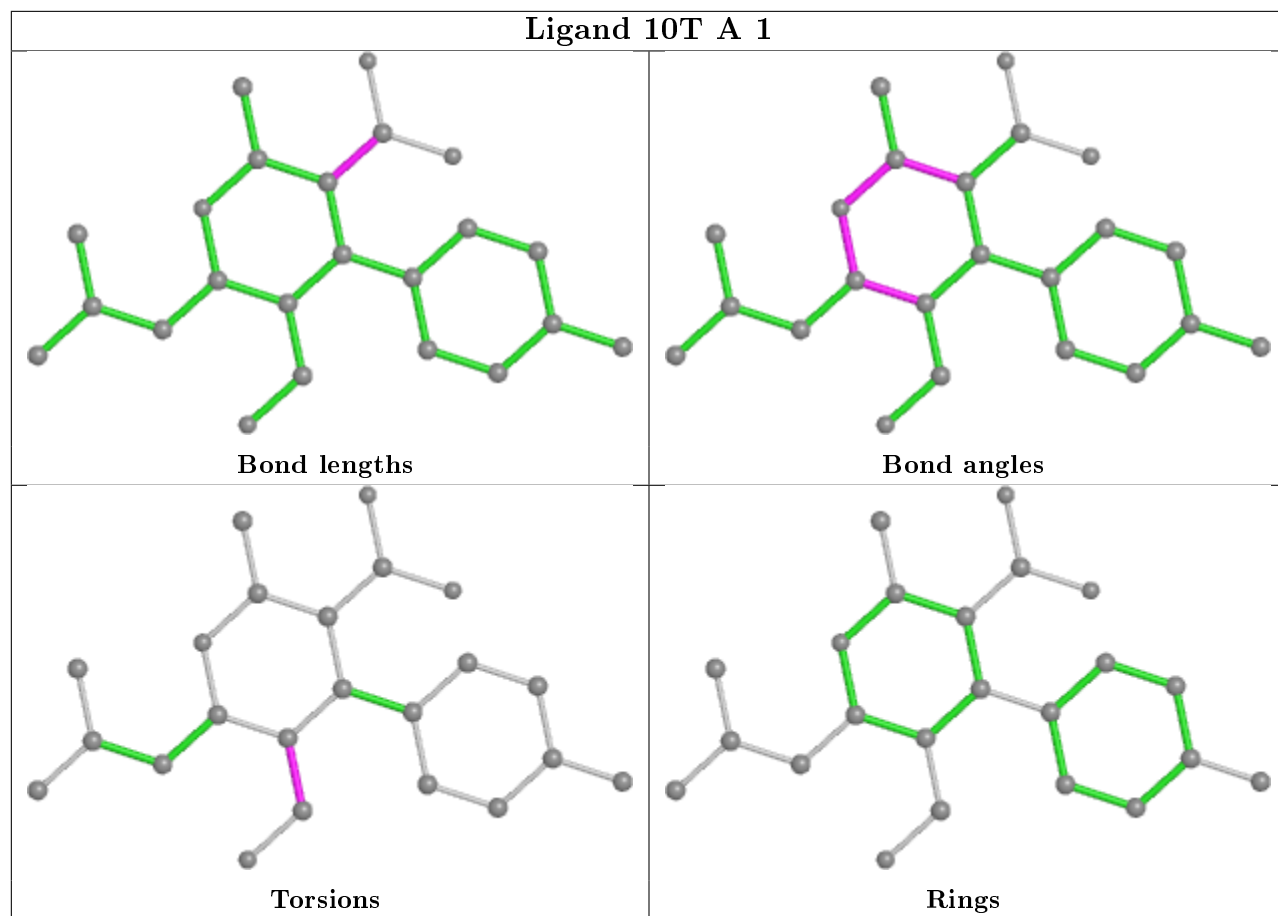
There are no ring outliers.

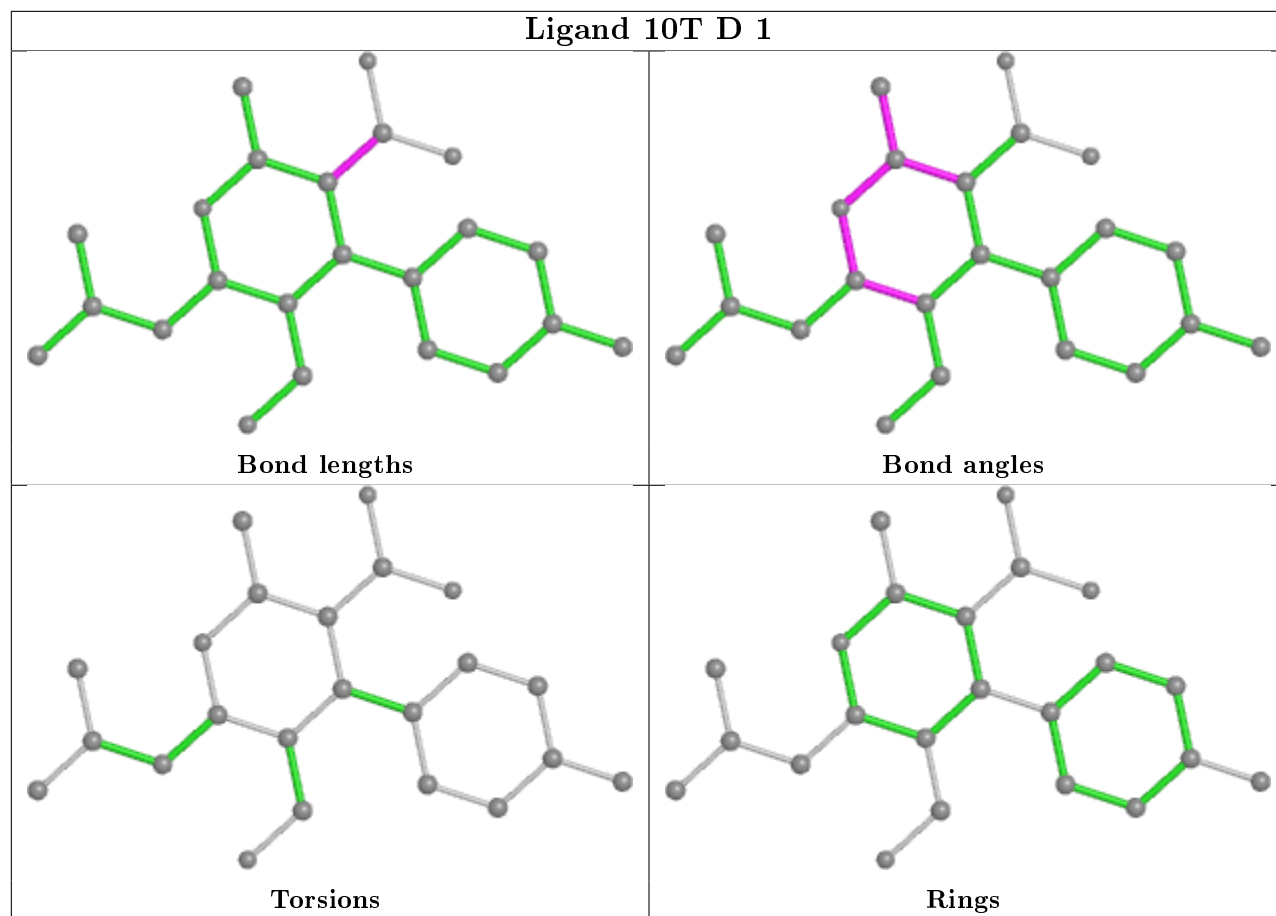
3 monomers are involved in 3 short contacts:

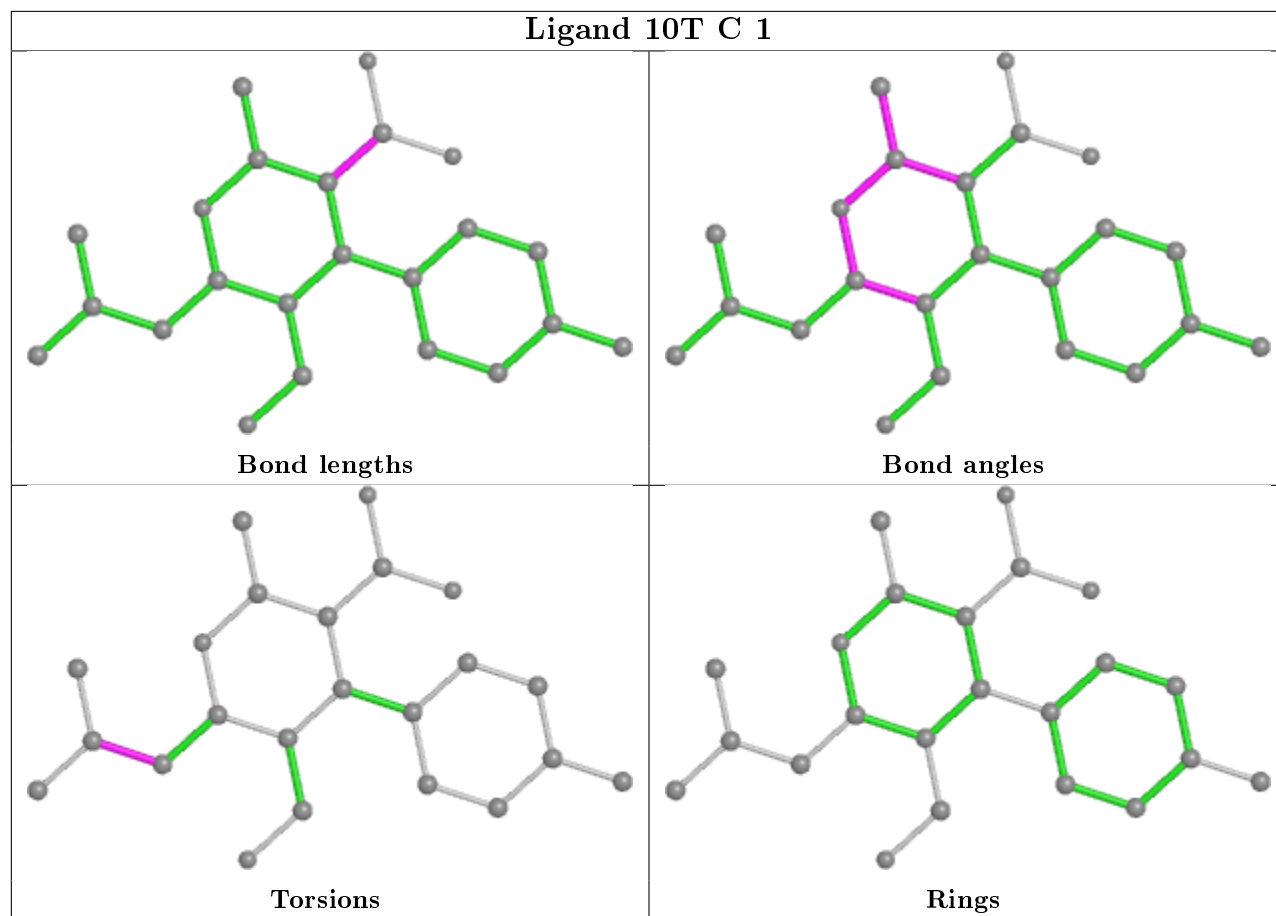
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	10T	1	0
3	C	1	10T	1	0
4	B	851	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.









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 ⓘ

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

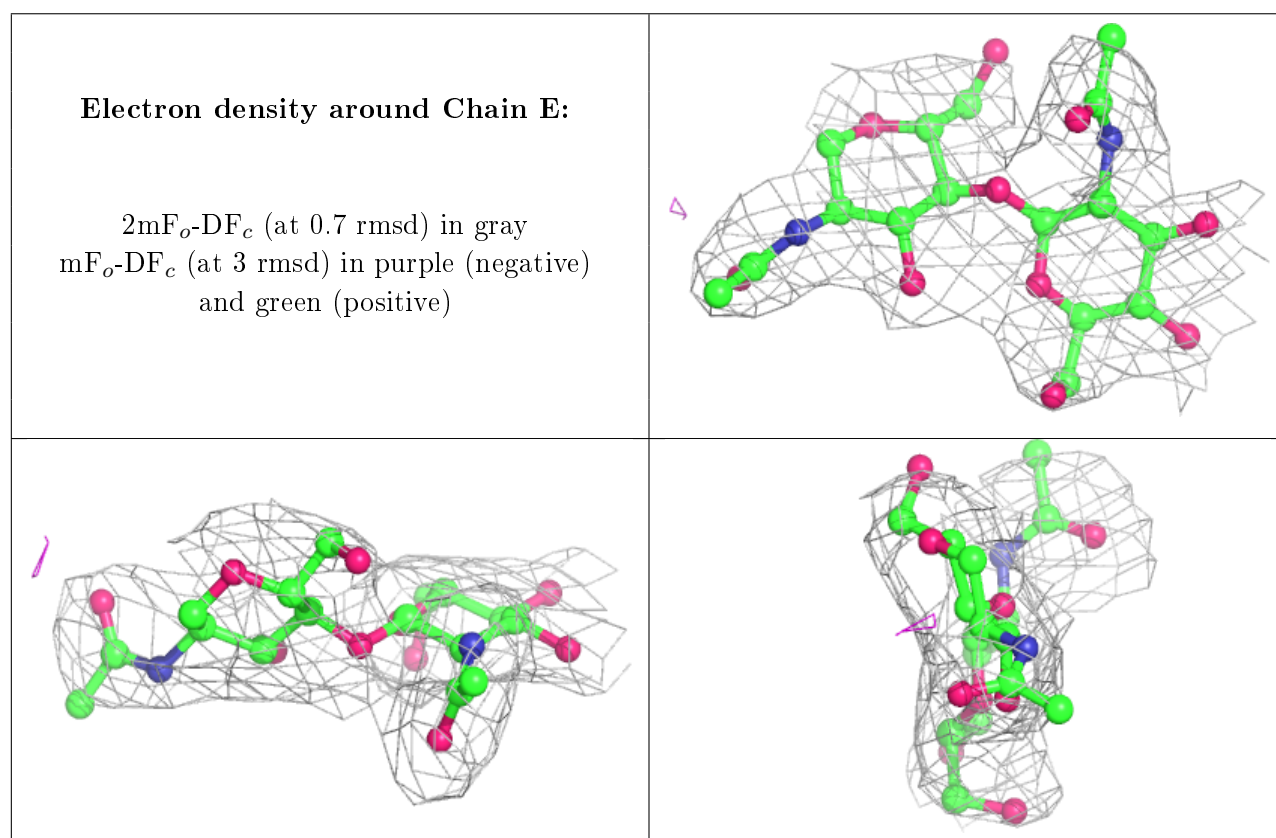
6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

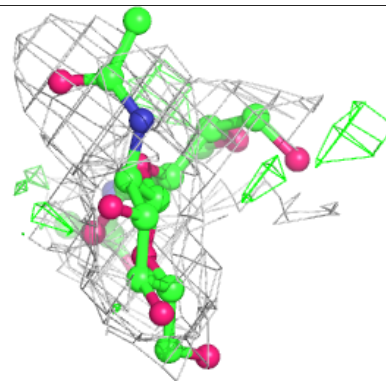
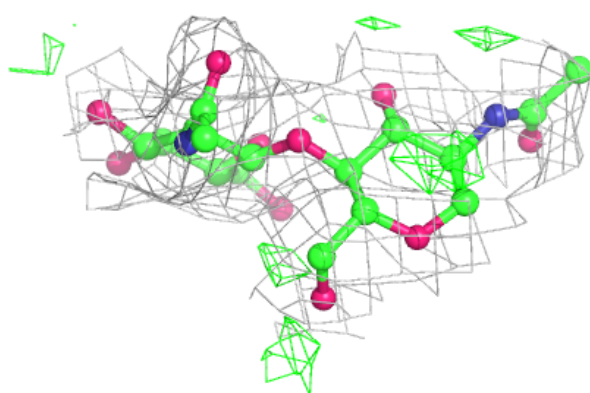
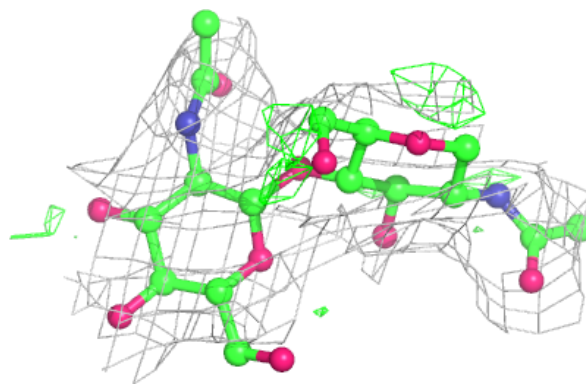
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

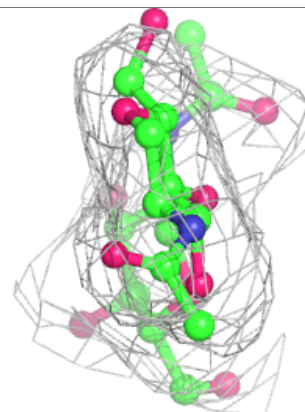
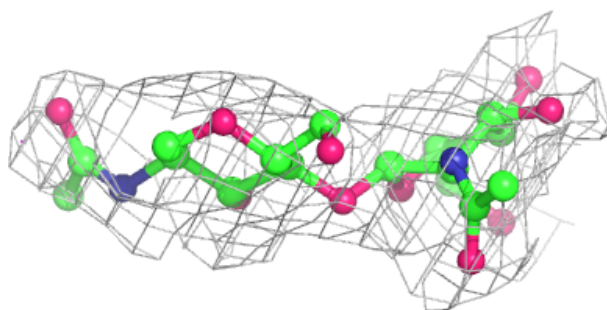
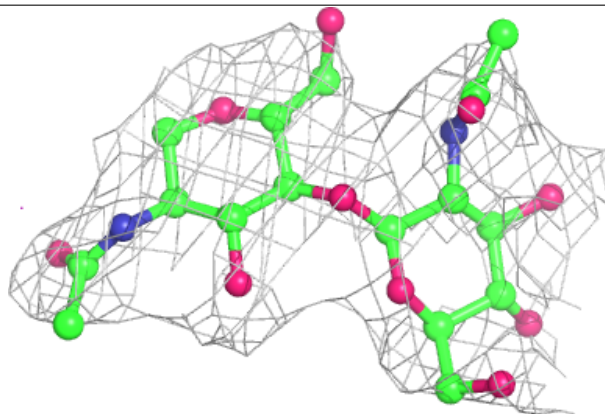


Electron density around Chain F:

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

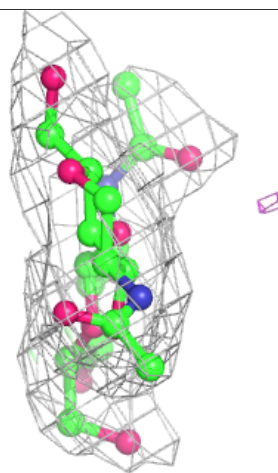
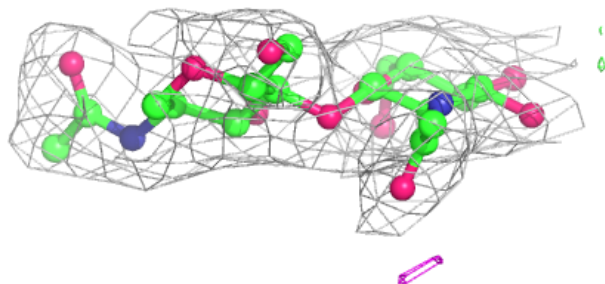
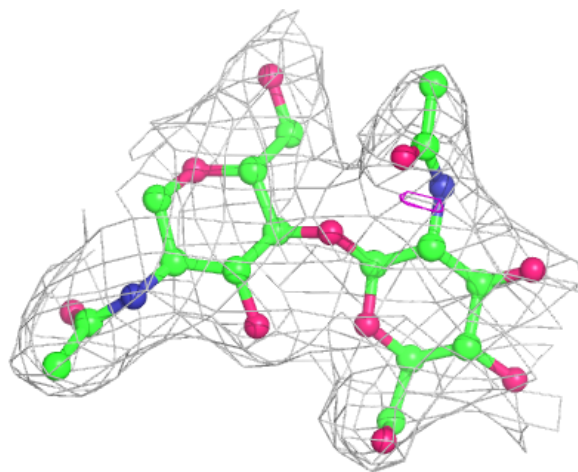
**Electron density around Chain G:**

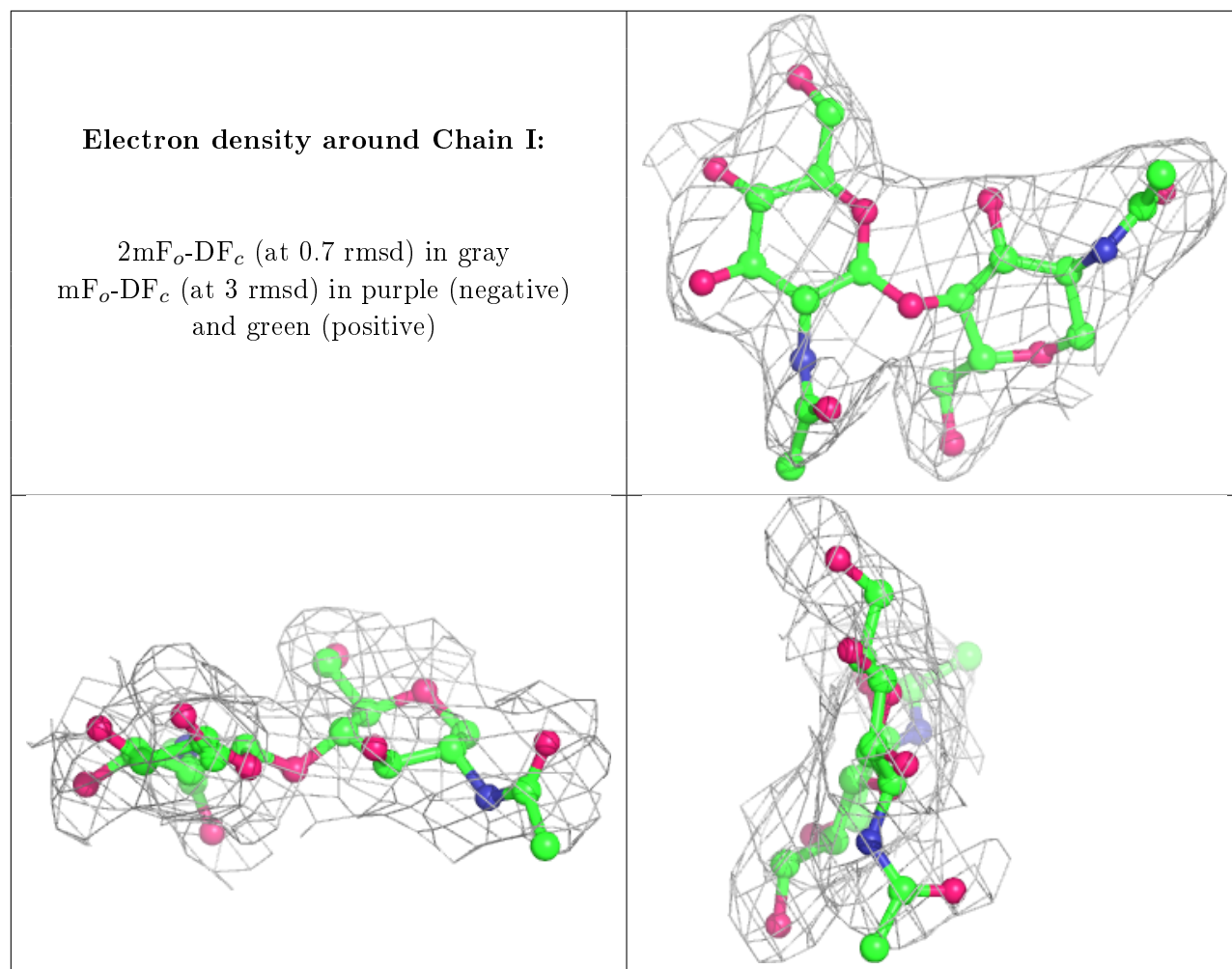
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





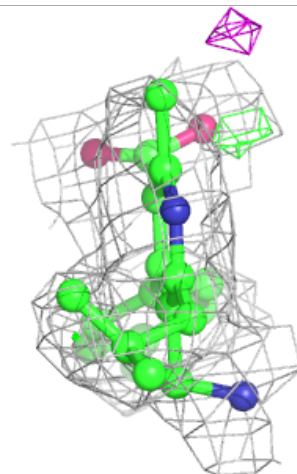
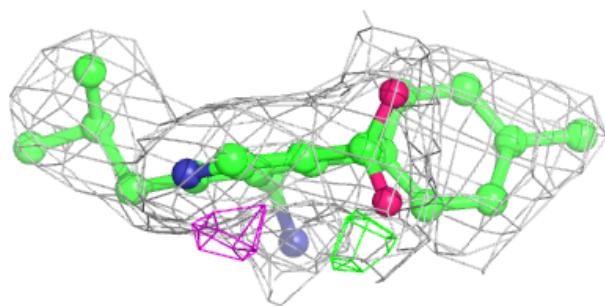
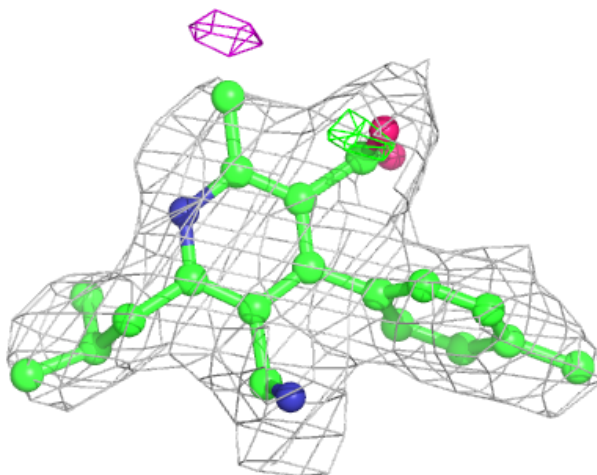
6.4 Ligands [i](#)

Unable to reproduce the depositor's 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.

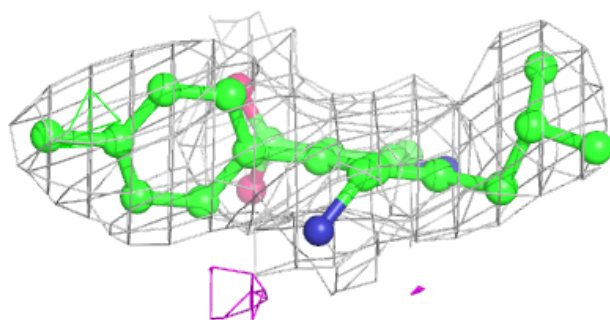
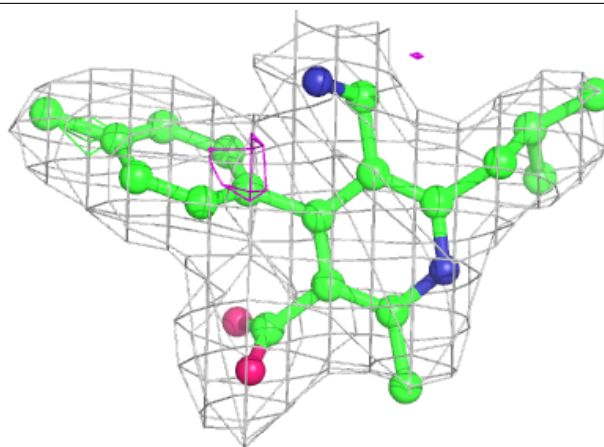
Electron density around 10T B 1:

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



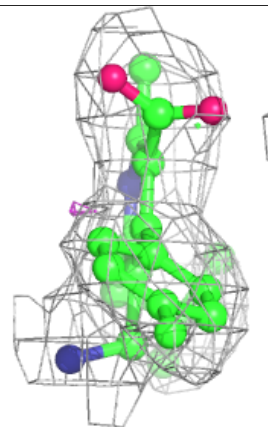
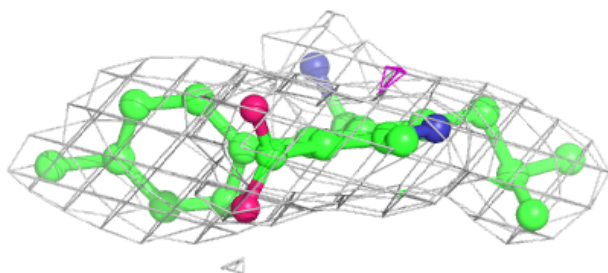
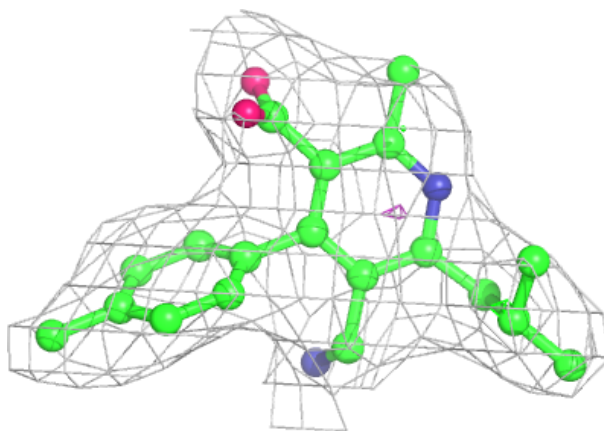
Electron density around 10T A 1:

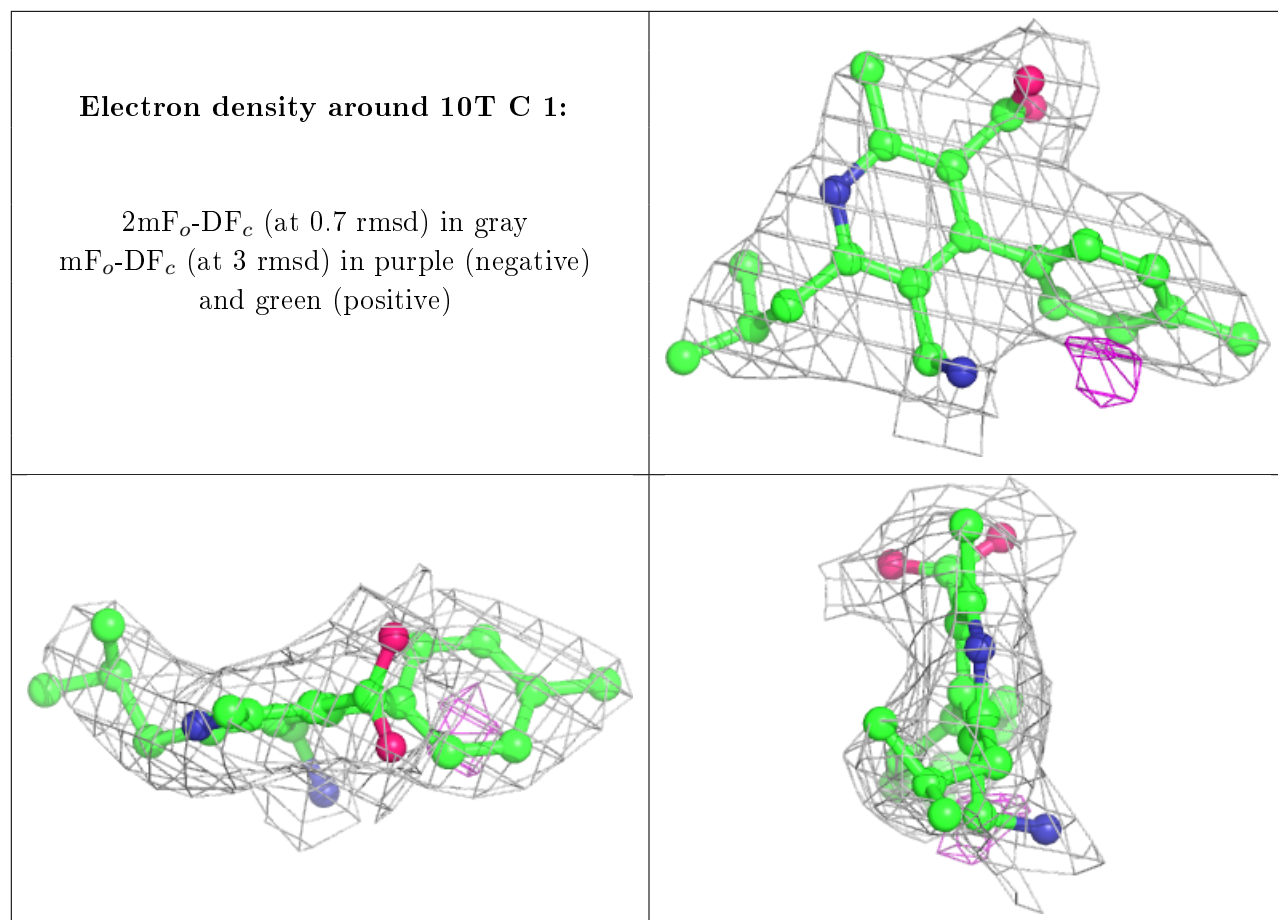
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 10T 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)





6.5 Other polymers [i](#)

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