



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:25 AM UTC

PDB ID : 4G1F / pdb_00004g1f
Title : Crystal Structure of human Dipeptidyl Peptidase IV in complex with a pyridopyrimidinedione analogue
Authors : Skene, R.J.; Gwaltney, S.L.
Deposited on : 2012-07-10
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

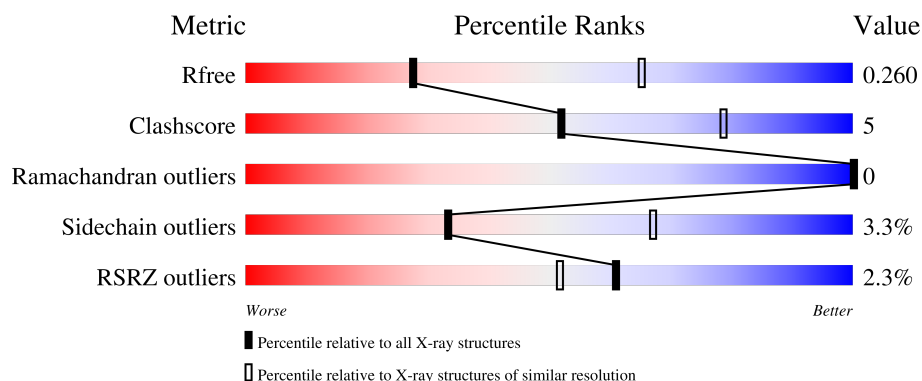
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	740	3% 85% 12% ..
1	B	740	2% 80% 16% ..
1	C	740	% 83% 14% ..
1	D	740	3% 82% 13% ..
2	E	2	50% 50%

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24443 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	724	Total	C	N	O	S	0	1	0
			5935	3812	977	1120	26			
1	B	727	Total	C	N	O	S	0	0	0
			5945	3818	977	1124	26			
1	C	722	Total	C	N	O	S	0	0	0
			5913	3798	972	1117	26			
1	D	715	Total	C	N	O	S	0	0	0
			5855	3762	964	1103	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.



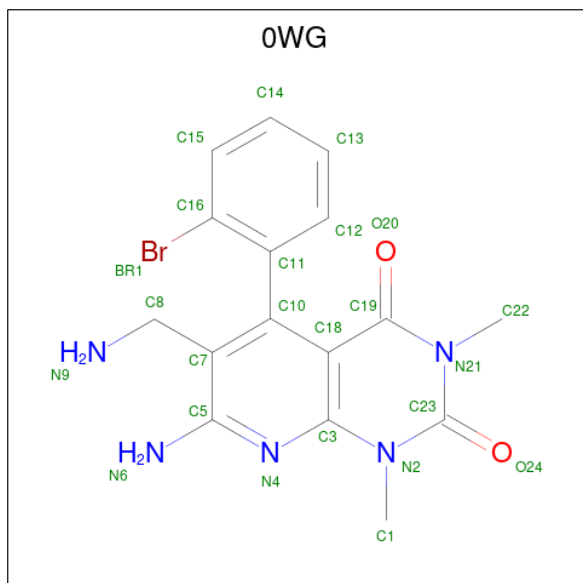
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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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 7-amino-6-(aminomethyl)-5-(2-bromophenyl)-1,3-dimethylpyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione (CCD ID: 0WG) (formula: $C_{16}H_{16}BrN_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			24	1	16	5	2		
3	B	1	Total	Br	C	N	O	0	0
			24	1	16	5	2		
3	C	1	Total	Br	C	N	O	0	0
			24	1	16	5	2		
3	D	1	Total	Br	C	N	O	0	0
			24	1	16	5	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	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		

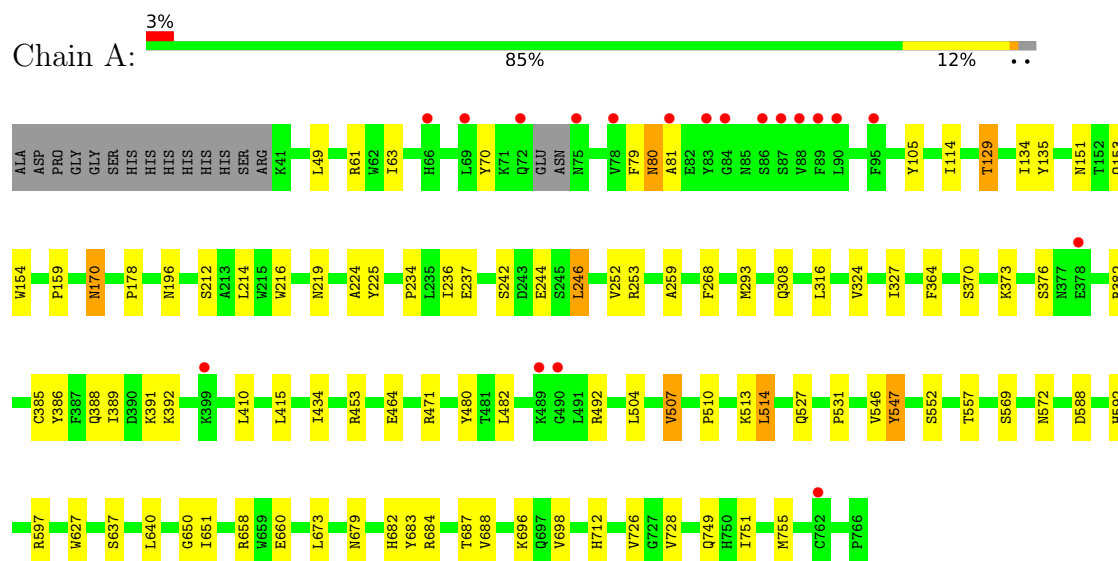
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total 115	O 115	0	0
5	B	112	Total 112	O 112	0	0
5	C	91	Total 91	O 91	0	0
5	D	73	Total 73	O 73	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

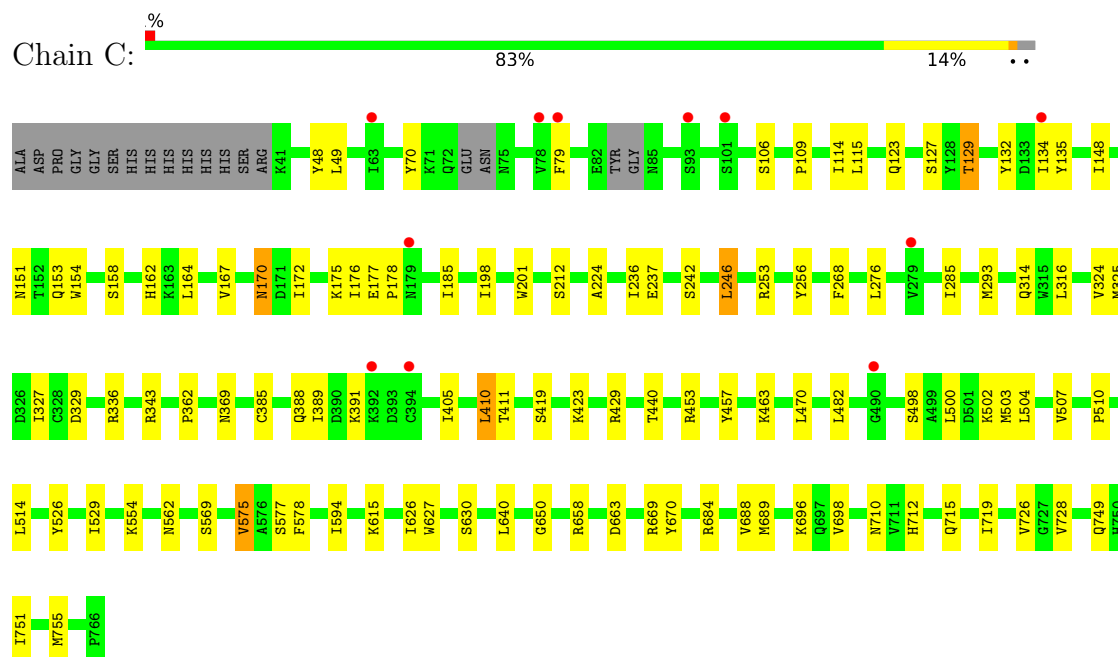
• Molecule 1: Dipeptidyl peptidase 4



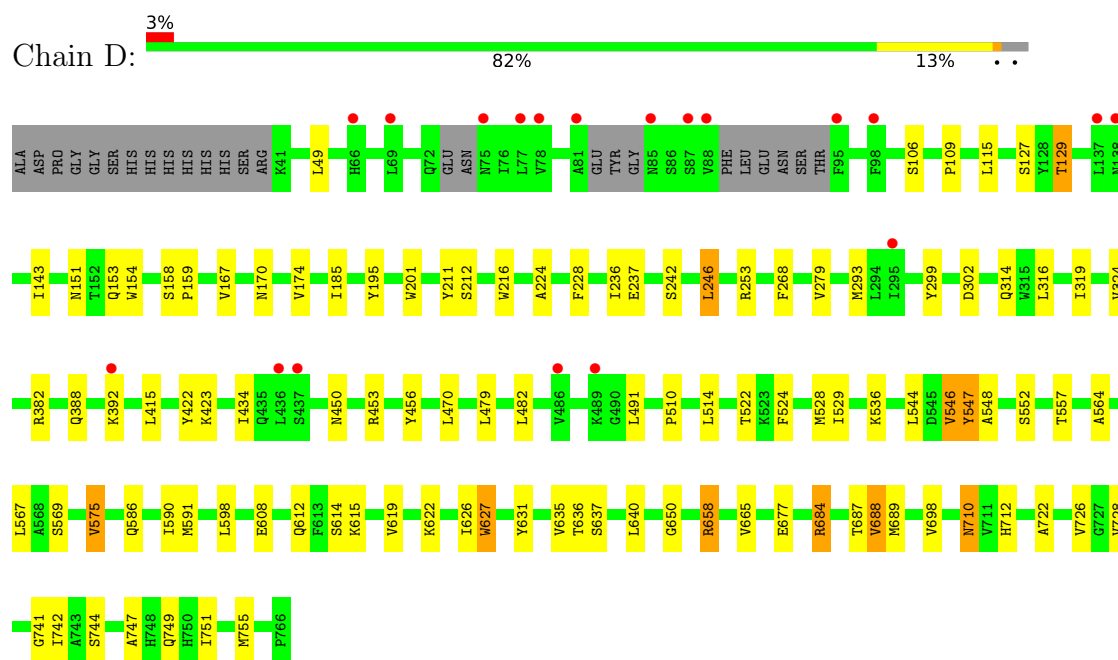
• Molecule 1: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



- Molecule 1: Dipeptidyl peptidase 4



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



- 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:  50% 50%

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:  100%

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	121.62Å 121.36Å 143.26Å 90.00° 114.63° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-2.90) 96.7 (40.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.207 , 0.259 0.207 , 0.260	Depositor DCC
R_{free} test set	4202 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24443	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, OWG

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	0.59	0/6111	0.74	0/8311
1	B	0.59	0/6116	0.76	5/8318 (0.1%)
1	C	0.59	0/6082	0.75	0/8270
1	D	0.60	0/6022	0.75	1/8187 (0.0%)
All	All	0.59	0/24331	0.75	6/33086 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	VAL	N-CA-C	5.53	116.08	108.12
1	B	547	TYR	N-CA-C	-5.35	104.95	112.12
1	B	96	ASP	N-CA-C	-5.30	106.95	113.41
1	D	546	VAL	N-CA-C	5.23	116.25	108.46
1	B	530	LEU	CA-C-N	5.23	123.47	119.66
1	B	530	LEU	C-N-CA	5.23	123.47	119.66

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	5935	0	5657	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5945	0	5658	76	0
1	C	5913	0	5638	61	0
1	D	5855	0	5587	54	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	24	0	16	0	0
3	B	24	0	16	1	0
3	C	24	0	16	1	0
3	D	24	0	16	0	0
4	A	56	0	52	0	0
4	B	56	0	52	0	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	115	0	0	1	0
5	B	112	0	0	0	0
5	C	91	0	0	0	0
5	D	73	0	0	0	0
All	All	24443	0	22885	241	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 5.

All (241) 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:684:ARG:HH21	1:D:684:ARG:HG3	1.25	0.97
1:B:63:ILE:HD11	1:B:69:LEU:HG	1.43	0.97
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.47	0.96
1:C:153:GLN:HE22	1:C:170:ASN:H	1.16	0.89
1:A:153:GLN:HE22	1:A:170:ASN:H	1.25	0.82
1:A:637:SER:HB3	1:A:688:VAL:HG21	1.65	0.79
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.65	0.79
1:B:153:GLN:HE22	1:B:170:ASN:H	1.30	0.78
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.68	0.76
1:D:153:GLN:HE22	1:D:170:ASN:H	1.34	0.75
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.68	0.75
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.70	0.74
1:B:640:LEU:HD21	1:B:650:GLY:HA3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HH11	1:A:61:ARG:HG3	1.55	0.68
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.22	0.68
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.76	0.67
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.75	0.67
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.77	0.67
1:C:129:THR:HG23	1:C:151:ASN:HA	1.75	0.66
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.44	0.65
1:D:684:ARG:HG3	1:D:684:ARG:NH2	2.01	0.65
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.63	0.63
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.80	0.63
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.81	0.63
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.81	0.63
1:C:201:TRP:HZ2	1:C:710:ASN:HA	1.64	0.62
1:C:751:ILE:HG12	1:C:755:MET:HE2	1.82	0.61
1:A:170:ASN:N	1:A:170:ASN:HD22	1.98	0.61
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.83	0.61
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.83	0.60
1:C:109:PRO:HG2	1:C:158:SER:O	2.02	0.59
1:D:453:ARG:HH21	1:D:479:LEU:HB2	1.69	0.58
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.83	0.58
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.85	0.58
1:D:129:THR:HG23	1:D:151:ASN:HA	1.86	0.58
1:B:637:SER:HB3	1:B:688:VAL:HG21	1.84	0.58
1:D:640:LEU:HB3	1:D:698:VAL:HG21	1.87	0.57
1:D:751:ILE:HG12	1:D:755:MET:HE2	1.87	0.57
1:C:201:TRP:CZ2	1:C:710:ASN:HA	2.38	0.57
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.87	0.57
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.87	0.57
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.87	0.57
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.86	0.57
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.86	0.57
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.70	0.56
1:B:109:PRO:HG2	1:B:158:SER:O	2.05	0.56
1:B:614:SER:HA	1:B:619:VAL:HB	1.87	0.56
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.88	0.56
1:B:681:ASP:O	1:B:685:ASN:HB2	2.07	0.55
1:D:174:VAL:HG23	1:D:185:ILE:HD11	1.88	0.55
1:B:630:SER:HB2	3:B:800:OWG:O20	2.06	0.54
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.90	0.54
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.89	0.54
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.90	0.54
1:C:658:ARG:HB2	1:C:689:MET:HE1	1.90	0.54
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.90	0.54
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.90	0.54
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.43	0.53
1:C:129:THR:HG21	1:C:151:ASN:HD22	1.72	0.53
1:D:637:SER:HB3	1:D:688:VAL:HG21	1.90	0.53
1:A:80:ASN:HD22	1:A:81:ALA:N	2.06	0.53
1:B:177:GLU:HB2	1:B:180:LEU:HD12	1.90	0.53
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.91	0.53
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.73	0.52
1:B:129:THR:HG23	1:B:151:ASN:HA	1.92	0.52
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.92	0.52
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.08	0.52
1:B:325:MET:HG2	1:B:345:HIS:HB2	1.92	0.52
1:D:109:PRO:HG2	1:D:158:SER:O	2.09	0.52
1:D:614:SER:HA	1:D:619:VAL:HB	1.92	0.52
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.92	0.52
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.45	0.52
1:D:564:ALA:HA	1:D:567:LEU:HD12	1.92	0.52
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.91	0.51
1:B:340:LEU:HD13	1:B:343:ARG:HE	1.74	0.51
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.92	0.51
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.92	0.51
1:C:293:MET:HE3	1:C:324:VAL:HG12	1.92	0.51
1:A:219:ASN:HB3	1:A:308:GLN:HE22	1.75	0.51
1:B:506:ASN:HB2	1:C:440:THR:HG23	1.93	0.51
1:C:164:LEU:HB3	1:C:175:LYS:HB2	1.93	0.51
1:D:546:VAL:HG12	1:D:627:TRP:O	2.11	0.51
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.92	0.51
1:D:684:ARG:HH21	1:D:684:ARG:CG	2.11	0.50
1:A:684:ARG:NH1	5:A:968:HOH:O	2.45	0.50
1:C:176:ILE:HD11	1:C:276:LEU:HD12	1.93	0.50
1:B:49:LEU:HB3	1:B:749:GLN:HG2	1.93	0.50
1:C:529:ILE:HB	1:C:575:VAL:HG13	1.94	0.50
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.77	0.50
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.95	0.49
1:C:498:SER:O	1:C:502:LYS:HG2	2.11	0.49
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.93	0.49
1:C:429:ARG:HB2	1:C:457:TYR:H	1.78	0.49
1:C:115:LEU:HD11	1:C:132:TYR:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:ASN:C	1:C:710:ASN:HD22	2.21	0.49
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.42	0.48
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.95	0.48
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.94	0.48
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.95	0.48
1:C:236:ILE:HG12	1:C:712:HIS:CD2	2.48	0.48
1:A:293:MET:HE3	1:A:324:VAL:HG12	1.95	0.48
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.95	0.48
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.44	0.48
1:D:453:ARG:NH2	1:D:479:LEU:HB2	2.29	0.48
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.95	0.48
1:B:751:ILE:HG12	1:B:755:MET:HE2	1.94	0.47
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.78	0.47
1:C:554:LYS:HB3	1:C:577:SER:HB3	1.96	0.47
1:C:626:ILE:O	1:C:650:GLY:HA2	2.14	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.97	0.47
1:C:148:ILE:HD11	1:C:164:LEU:HD21	1.96	0.47
1:D:415:LEU:HB3	1:D:434:ILE:HG23	1.97	0.47
1:B:453:ARG:HB2	1:B:476:GLY:HA3	1.96	0.47
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.97	0.47
1:D:684:ARG:NH2	1:D:684:ARG:CG	2.74	0.47
1:D:236:ILE:HG12	1:D:712:HIS:CD2	2.50	0.47
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.97	0.47
1:A:513:LYS:O	1:A:527:GLN:HA	2.15	0.47
1:D:689:MET:HG3	1:D:722:ALA:HB2	1.97	0.47
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.95	0.46
1:A:376:SER:HA	1:A:382:ARG:HA	1.96	0.46
1:C:167:VAL:HG11	1:C:198:ILE:HG12	1.98	0.46
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.97	0.46
1:C:640:LEU:HB3	1:C:698:VAL:HG21	1.96	0.46
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.98	0.46
1:B:273:THR:HA	1:B:276:LEU:HG	1.98	0.46
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.50	0.46
1:B:364:PHE:CE2	1:B:389:ILE:HD11	2.49	0.46
1:C:715:GLN:O	1:C:719:ILE:HG13	2.16	0.46
1:D:201:TRP:HZ2	1:D:710:ASN:HA	1.81	0.46
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.51	0.45
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.98	0.45
1:C:314:GLN:NE2	1:C:362:PRO:HD3	2.32	0.45
1:C:658:ARG:HH12	1:C:684:ARG:HE	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:HG23	1:A:151:ASN:HA	1.97	0.45
1:C:630:SER:HB2	3:C:800:OWG:O20	2.16	0.45
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.51	0.45
1:A:546:VAL:HG12	1:A:627:TRP:O	2.16	0.45
1:D:382:ARG:HH21	1:D:591:MET:HE1	1.81	0.45
1:D:741:GLY:O	1:D:742:ILE:C	2.59	0.45
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.99	0.45
1:B:550:PRO:HD2	1:B:666:TYR:OH	2.16	0.45
1:B:376:SER:HA	1:B:382:ARG:HA	1.98	0.44
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.99	0.44
1:C:134:ILE:HD13	1:C:178:PRO:HB3	1.99	0.44
1:B:659:TRP:HB3	1:B:667:THR:HG21	1.99	0.44
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.98	0.44
1:A:61:ARG:HH11	1:A:61:ARG:CG	2.28	0.44
1:A:327:ILE:HG12	1:A:389:ILE:HD12	2.00	0.44
1:B:514:LEU:HD22	1:B:525:TRP:HE3	1.82	0.44
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.98	0.44
1:B:472:CYS:O	1:B:478:PRO:HA	2.18	0.44
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.53	0.44
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.53	0.44
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.98	0.44
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.82	0.44
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.83	0.44
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.48	0.44
1:D:106:SER:HB3	1:D:115:LEU:HB3	2.00	0.44
1:A:751:ILE:O	1:A:755:MET:HG3	2.18	0.43
1:B:77:LEU:HD12	1:B:88:VAL:HG22	1.99	0.43
1:B:230:ASP:O	1:B:231:THR:C	2.61	0.43
1:A:244:GLU:HG3	1:B:689:MET:HE3	2.00	0.43
1:C:293:MET:CE	1:C:324:VAL:HG12	2.48	0.43
1:B:614:SER:HB2	1:B:621:ASN:HD22	1.83	0.43
1:D:293:MET:HE3	1:D:324:VAL:HG22	2.00	0.43
1:C:48:TYR:CE1	1:C:562:ASN:HA	2.53	0.43
1:B:148:ILE:HD11	1:B:164:LEU:HD21	2.01	0.43
1:B:135:TYR:HD1	1:B:142:LEU:HD13	1.84	0.43
1:A:236:ILE:HG12	1:A:712:HIS:CD2	2.54	0.43
1:C:162:HIS:NE2	1:C:177:GLU:OE1	2.51	0.43
1:C:49:LEU:HB3	1:C:749:GLN:HG2	2.00	0.43
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.54	0.43
1:A:696:LYS:HG3	1:A:728:VAL:HG22	2.01	0.42
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:TYR:CD2	1:D:552:SER:HB2	2.54	0.42
1:B:55:LEU:HD22	1:B:478:PRO:HG2	2.00	0.42
1:B:431:LEU:HD22	1:B:470:LEU:HD21	2.01	0.42
1:B:455:GLN:HB2	1:B:475:PRO:HD3	2.00	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.42
1:D:195:TYR:HB2	1:D:228:PHE:HB2	2.01	0.42
1:A:679:ASN:O	1:A:683:TYR:HD2	2.02	0.42
1:B:387:PHE:CD1	1:B:394:CYS:HB3	2.55	0.42
1:B:473:SER:HB3	1:B:558:VAL:HG13	2.00	0.42
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.55	0.42
1:A:170:ASN:O	1:A:196:ASN:HB2	2.19	0.42
1:A:370:SER:HB3	1:A:386:TYR:CE2	2.54	0.42
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.55	0.42
1:B:626:ILE:O	1:B:650:GLY:HA2	2.19	0.42
1:B:134:ILE:HG21	1:B:178:PRO:HB3	2.00	0.42
1:B:258:LYS:O	1:B:259:ALA:C	2.63	0.42
1:D:598:LEU:HG	1:D:631:TYR:OH	2.20	0.42
1:B:604:GLU:HA	1:B:607:ILE:HD12	2.02	0.41
1:B:72:GLN:HB2	1:B:75:ASN:HB2	2.01	0.41
1:B:195:TYR:HB2	1:B:228:PHE:HB2	2.02	0.41
1:C:123:GLN:HB3	1:C:127:SER:OG	2.21	0.41
1:C:170:ASN:N	1:C:170:ASN:HD22	2.18	0.41
1:C:172:ILE:HG22	1:C:185:ILE:HD12	2.02	0.41
1:C:285:ILE:HG21	1:C:336:ARG:HA	2.01	0.41
1:B:121:VAL:HB	1:B:129:THR:HB	2.00	0.41
1:C:500:LEU:HA	1:C:503:MET:HE2	2.01	0.41
1:D:608:GLU:O	1:D:612:GLN:HG2	2.19	0.41
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.54	0.41
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.55	0.41
1:D:153:GLN:NE2	1:D:167:VAL:HG12	2.35	0.41
1:B:214:LEU:HD23	1:B:225:TYR:HB3	2.03	0.41
1:B:363:HIS:HB3	1:B:410:LEU:HD22	2.03	0.41
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.83	0.41
1:B:372:TYR:OH	1:B:436:LEU:HG	2.20	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.21	0.41
1:C:70:TYR:HB3	1:C:79:PHE:CE1	2.55	0.41
1:C:410:LEU:HD22	1:C:411:THR:O	2.21	0.41
1:D:522:THR:HB	1:D:524:PHE:CE2	2.56	0.41
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.83	0.41
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.56	0.41
1:B:453:ARG:NH2	1:B:477:LEU:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:LEU:HD23	1:D:626:ILE:HD12	2.02	0.41
1:A:588:ASP:HB3	1:A:592:HIS:CD2	2.56	0.41
1:B:614:SER:HB2	1:B:621:ASN:ND2	2.36	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:C:369:ASN:O	1:C:389:ILE:HG12	2.21	0.41
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:D:744:SER:HB2	1:D:747:ALA:HB3	2.03	0.40
1:A:547:TYR:CD2	1:A:552:SER:HB2	2.56	0.40
1:B:153:GLN:HB3	1:B:211:TYR:CE1	2.57	0.40
1:B:475:PRO:HA	1:B:557:THR:O	2.20	0.40
1:B:741:GLY:O	1:B:742:ILE:C	2.63	0.40
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.04	0.40
1:A:170:ASN:N	1:A:170:ASN:ND2	2.69	0.40
1:B:343:ARG:HH21	1:B:389:ILE:HG21	1.87	0.40
1:B:547:TYR:CD1	1:B:547:TYR:C	2.99	0.40
1:C:423:LYS:HB3	1:C:423:LYS:HE2	1.91	0.40
1:D:299:TYR:CE1	1:D:665:VAL:HG22	2.57	0.40
1:D:548:ALA:HB3	1:D:635:VAL:HG21	2.02	0.40
1:A:504:LEU:HA	1:A:507:VAL:HG13	2.04	0.40
1:C:405:ILE:HG12	1:C:419:SER:HA	2.02	0.40
1:D:422:TYR:CE1	1:D:423:LYS:HE2	2.56	0.40
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.02	0.40
1:B:369:ASN:C	1:B:389:ILE:HD13	2.46	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	721/740 (97%)	679 (94%)	42 (6%)	0	100	100
1	B	723/740 (98%)	682 (94%)	41 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	716/740 (97%)	677 (95%)	39 (5%)	0	100	100
1	D	707/740 (96%)	665 (94%)	42 (6%)	0	100	100
All	All	2867/2960 (97%)	2703 (94%)	164 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	650/662 (98%)	633 (97%)	17 (3%)	40	73
1	B	650/662 (98%)	624 (96%)	26 (4%)	28	62
1	C	648/662 (98%)	629 (97%)	19 (3%)	37	71
1	D	641/662 (97%)	618 (96%)	23 (4%)	31	65
All	All	2589/2648 (98%)	2504 (97%)	85 (3%)	33	67

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	80	ASN
1	A	129	THR
1	A	170	ASN
1	A	246	LEU
1	A	316	LEU
1	A	373	LYS
1	A	385	CYS
1	A	392	LYS
1	A	453	ARG
1	A	464	GLU
1	A	482	LEU
1	A	492	ARG
1	A	507	VAL

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Mol	Chain	Res	Type
1	A	514	LEU
1	A	547	TYR
1	A	673	LEU
1	B	41	LYS
1	B	57	LEU
1	B	75	ASN
1	B	77	LEU
1	B	143	ILE
1	B	179	ASN
1	B	246	LEU
1	B	316	LEU
1	B	325	MET
1	B	366	LEU
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	482	LEU
1	B	506	ASN
1	B	514	LEU
1	B	547	TYR
1	B	575	VAL
1	B	594	ILE
1	B	621	ASN
1	B	640	LEU
1	B	688	VAL
1	B	710	ASN
1	C	129	THR
1	C	170	ASN
1	C	246	LEU
1	C	316	LEU
1	C	329	ASP
1	C	385	CYS
1	C	410	LEU
1	C	453	ARG
1	C	463	LYS
1	C	470	LEU
1	C	482	LEU
1	C	504	LEU
1	C	507	VAL

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Mol	Chain	Res	Type
1	C	514	LEU
1	C	575	VAL
1	C	594	ILE
1	C	615	LYS
1	C	627	TRP
1	C	688	VAL
1	D	129	THR
1	D	143	ILE
1	D	246	LEU
1	D	279	VAL
1	D	316	LEU
1	D	319	ILE
1	D	388	GLN
1	D	392	LYS
1	D	450	ASN
1	D	470	LEU
1	D	514	LEU
1	D	528	MET
1	D	536	LYS
1	D	547	TYR
1	D	575	VAL
1	D	615	LYS
1	D	622	LYS
1	D	627	TRP
1	D	658	ARG
1	D	677	GLU
1	D	684	ARG
1	D	688	VAL
1	D	710	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	123	GLN
1	A	151	ASN
1	A	153	GLN
1	A	170	ASN
1	A	227	GLN
1	A	338	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	430	ASN
1	A	450	ASN
1	A	505	GLN
1	A	508	GLN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	A	748	HIS
1	B	72	GLN
1	B	75	ASN
1	B	80	ASN
1	B	141	GLN
1	B	151	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	338	ASN
1	B	344	GLN
1	B	430	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	527	GLN
1	B	572	ASN
1	B	592	HIS
1	B	595	ASN
1	B	710	ASN
1	C	85	ASN
1	C	112	GLN
1	C	141	GLN
1	C	151	ASN
1	C	153	GLN
1	C	170	ASN
1	C	196	ASN
1	C	227	GLN
1	C	344	GLN
1	C	369	ASN
1	C	383	HIS
1	C	435	GLN
1	C	505	GLN

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Mol	Chain	Res	Type
1	C	527	GLN
1	C	572	ASN
1	C	606	GLN
1	C	697	GLN
1	C	710	ASN
1	C	749	GLN
1	D	85	ASN
1	D	123	GLN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	338	ASN
1	D	506	ASN
1	D	508	GLN
1	D	527	GLN
1	D	606	GLN
1	D	697	GLN
1	D	710	ASN

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	2,1	14,14,15	0.54	0	17,19,21	0.77	0
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.78	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.54	0	17,19,21	0.95	1 (5%)
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.79	0
2	NAG	G	1	2,1	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
2	NAG	G	2	2	14,14,15	0.48	0	17,19,21	0.70	0
2	NAG	H	1	2,1	14,14,15	0.63	0	17,19,21	0.88	1 (5%)
2	NAG	H	2	2	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.51	0	17,19,21	1.09	1 (5%)
2	NAG	I	2	2	14,14,15	0.49	0	17,19,21	1.04	1 (5%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	3.02	116.23	112.19
2	I	1	NAG	C1-O5-C5	3.00	116.20	112.19
2	I	2	NAG	C1-O5-C5	2.96	116.16	112.19
2	H	2	NAG	C1-O5-C5	2.50	115.54	112.19
2	H	1	NAG	C4-C3-C2	2.41	114.55	111.02
2	E	2	NAG	C1-O5-C5	2.34	115.32	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	2.10	114.99	112.19

There are no chirality outliers.

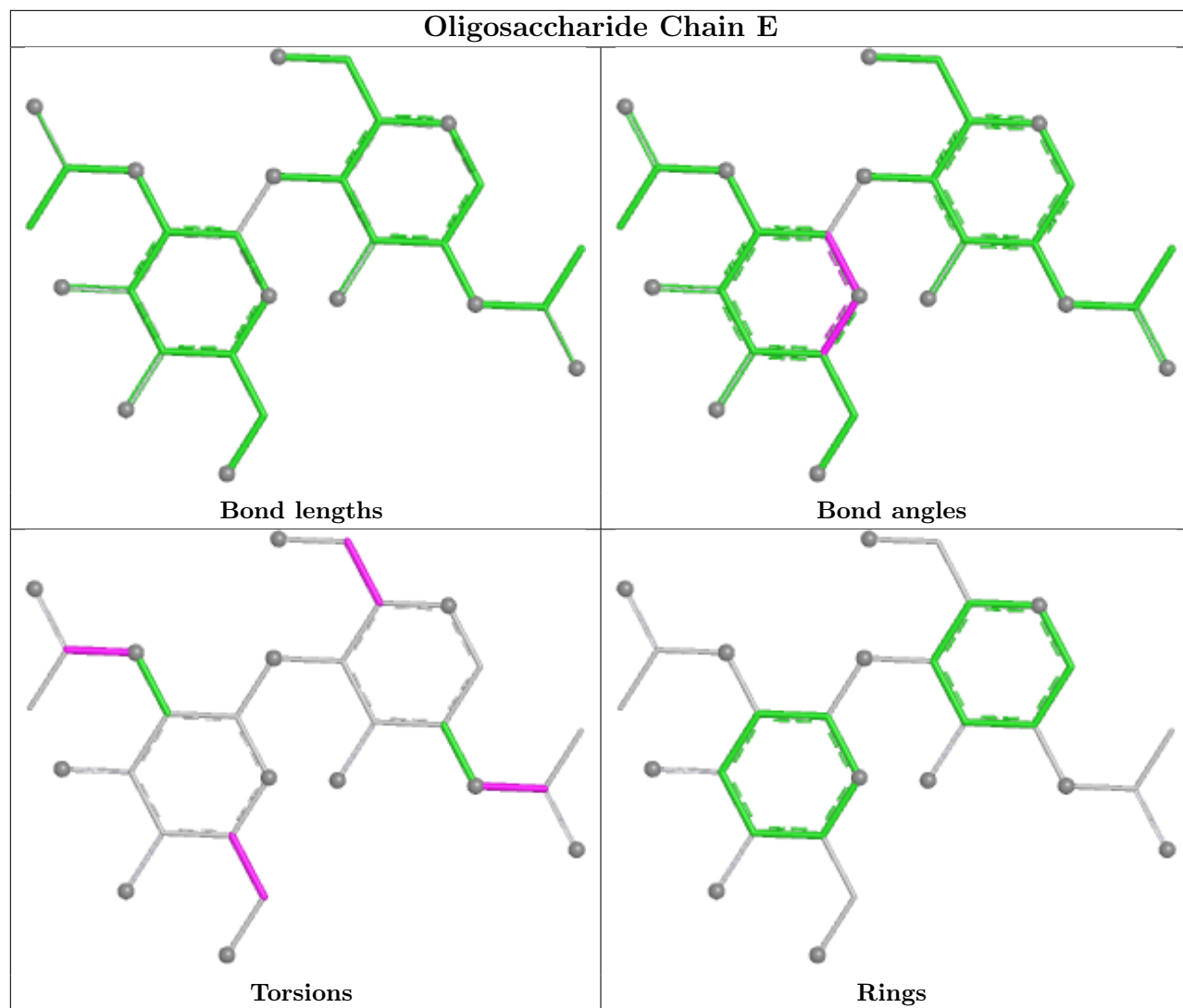
All (30) torsion outliers are listed below:

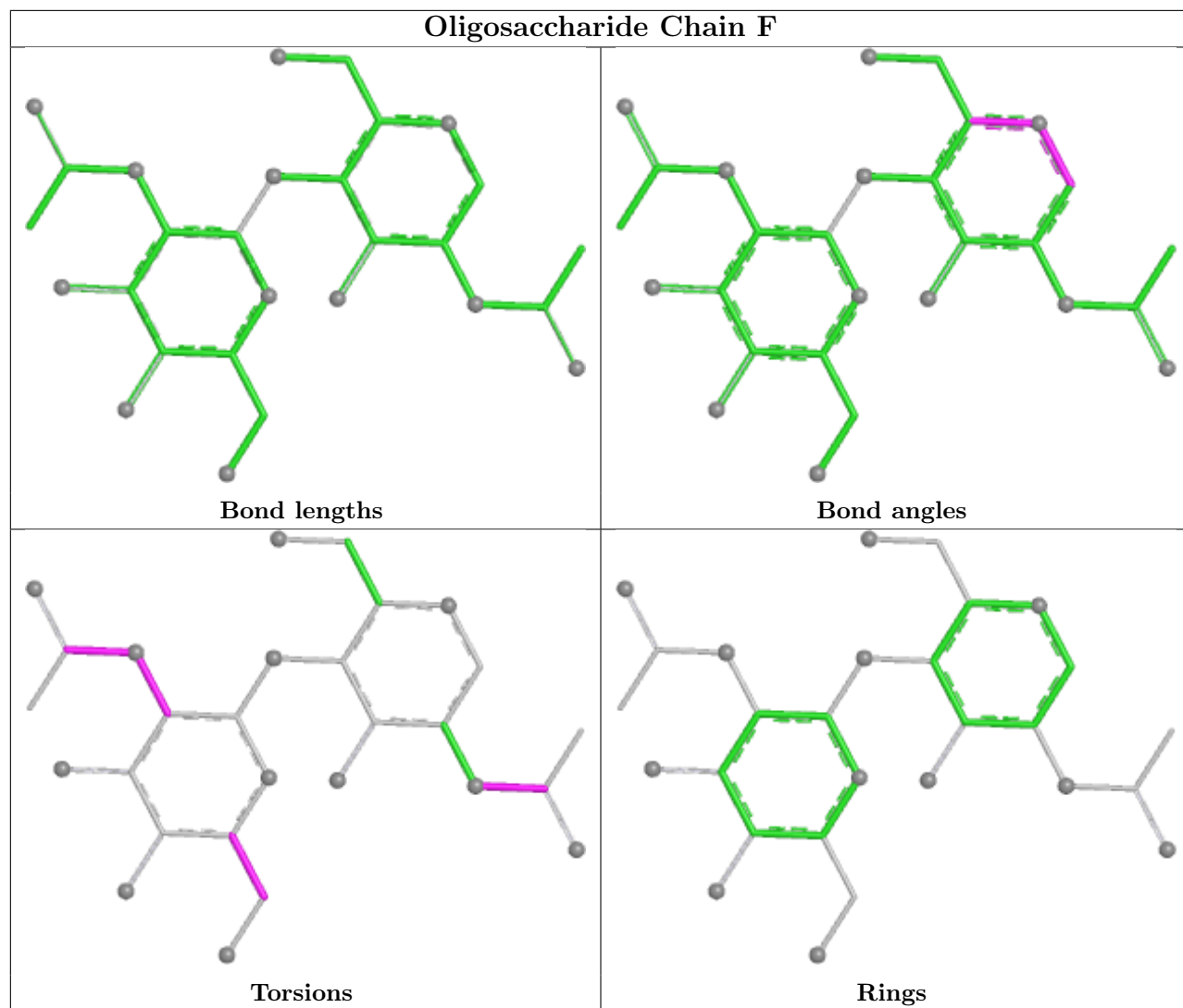
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6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

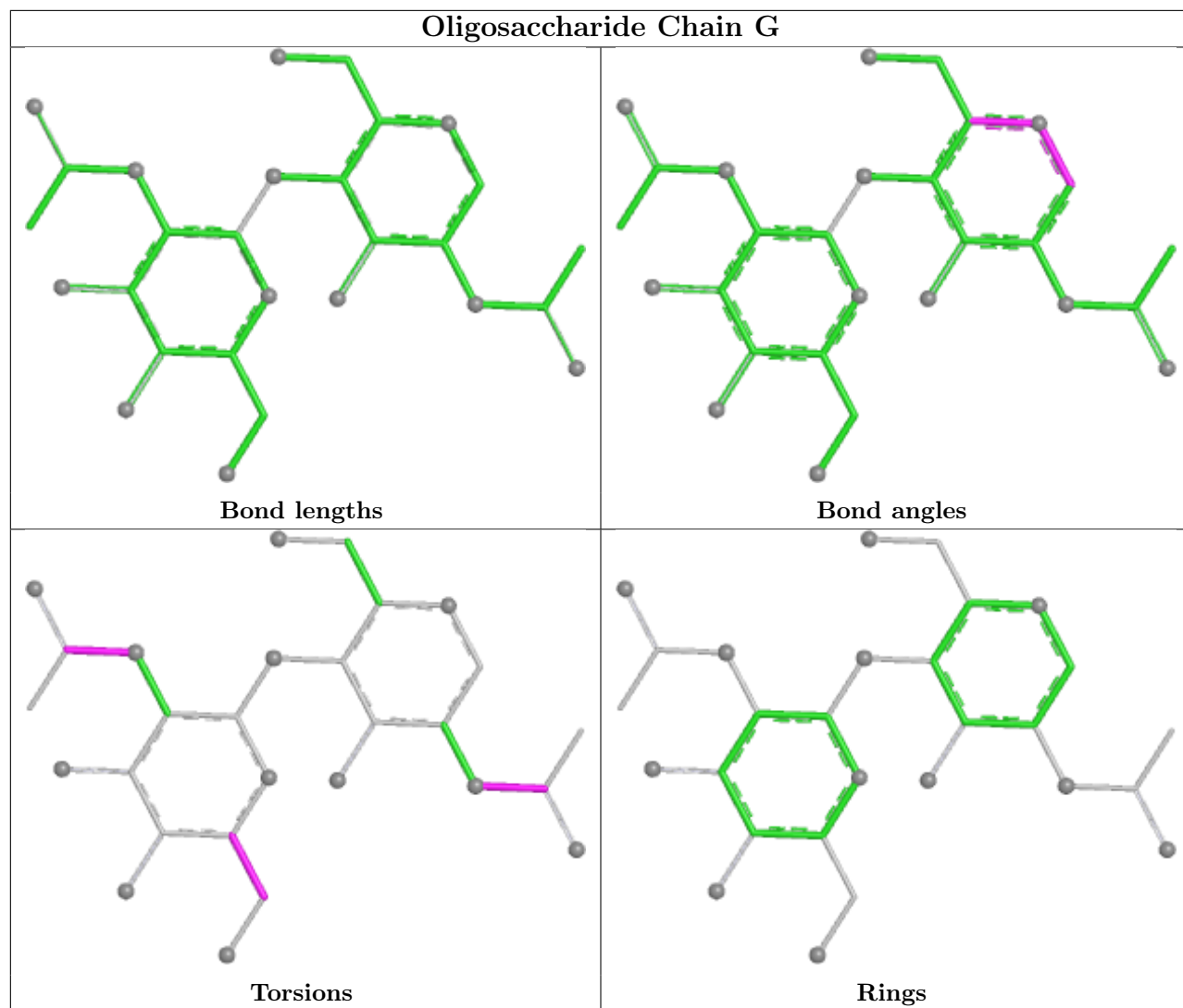
There are no ring outliers.

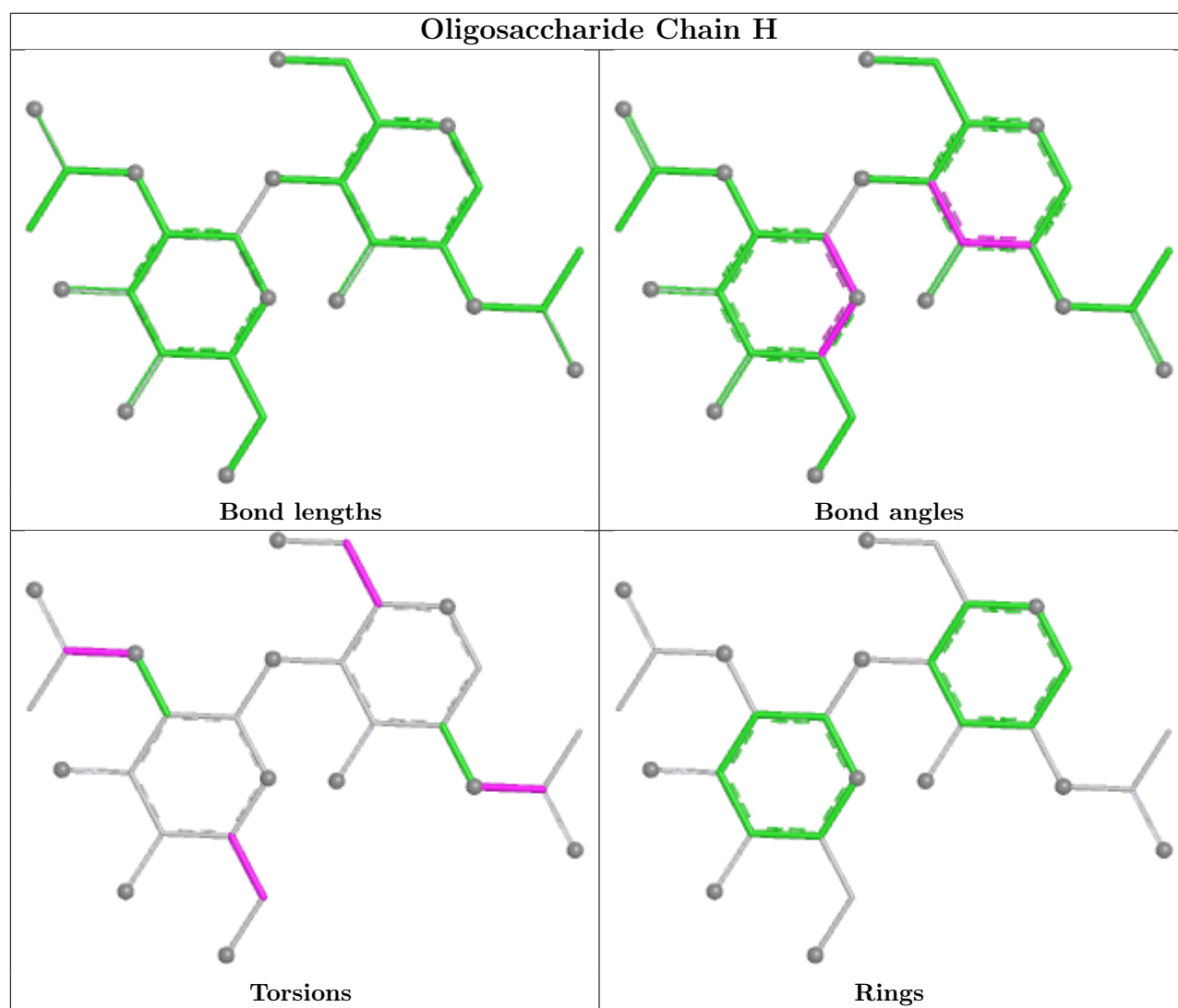
No monomer is involved in short contacts.

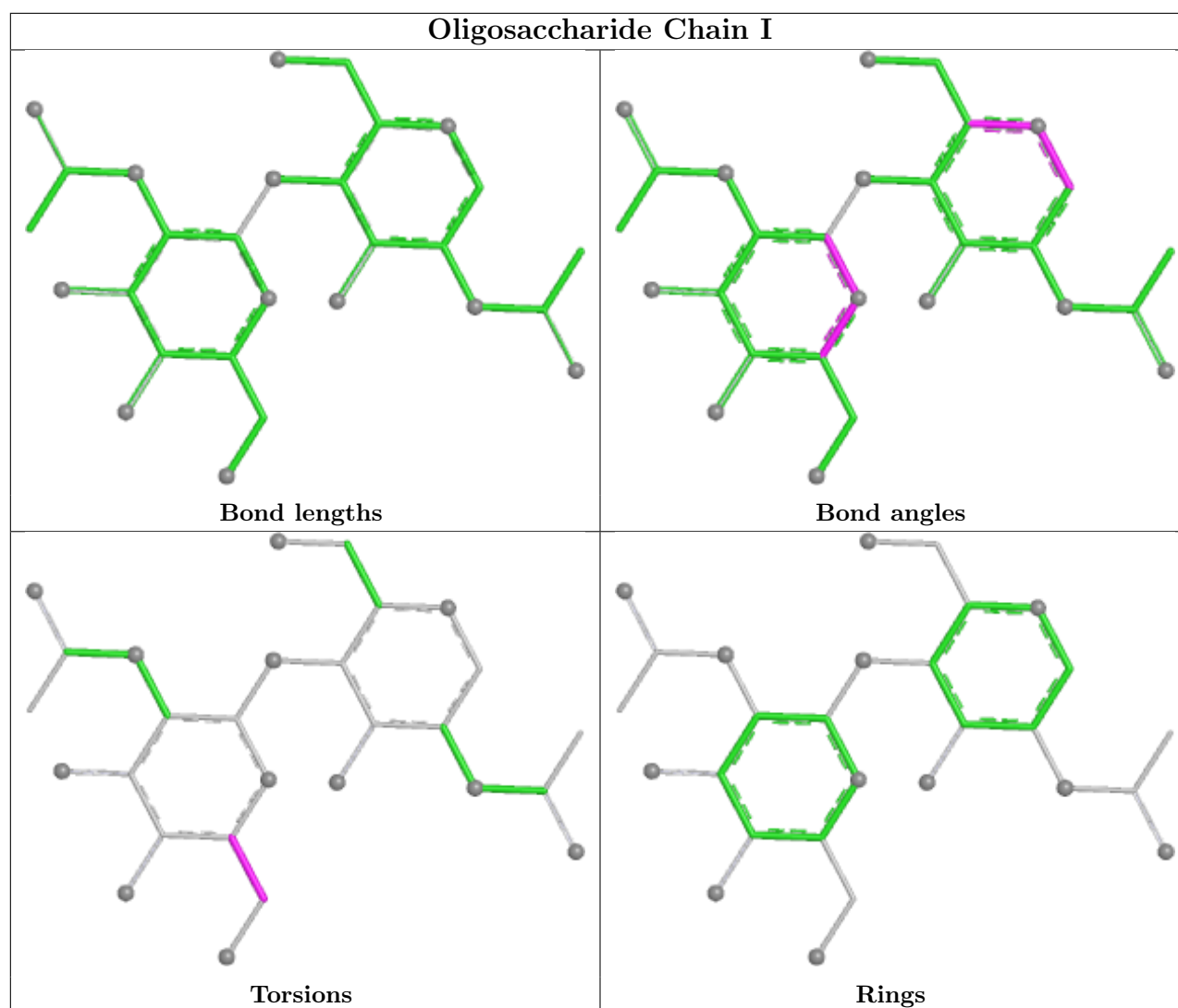
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











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	$\# Z > 2$
3	OWG	A	800	-	26,26,26	0.93	1 (3%)	36,39,39	2.43	9 (25%)
4	NAG	A	802	1	14,14,15	0.47	0	17,19,21	1.05	1 (5%)
4	NAG	B	802	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	806	1	14,14,15	0.45	0	17,19,21	1.17	1 (5%)
4	NAG	D	801	1	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
4	NAG	A	808	1	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
4	NAG	A	801	1	14,14,15	0.45	0	17,19,21	1.05	1 (5%)
4	NAG	B	803	1	14,14,15	0.47	0	17,19,21	0.60	0
3	0WG	B	800	-	26,26,26	0.94	0	36,39,39	2.41	10 (27%)
4	NAG	C	802	1	14,14,15	0.54	0	17,19,21	0.59	0
4	NAG	C	801	1	14,14,15	0.46	0	17,19,21	1.50	1 (5%)
4	NAG	D	804	1	14,14,15	0.63	0	17,19,21	1.13	2 (11%)
3	0WG	C	800	-	26,26,26	0.95	1 (3%)	36,39,39	2.33	12 (33%)
4	NAG	A	803	1	14,14,15	0.58	0	17,19,21	1.23	1 (5%)
4	NAG	B	801	1	14,14,15	0.63	0	17,19,21	1.30	2 (11%)
3	0WG	D	800	-	26,26,26	0.98	1 (3%)	36,39,39	2.33	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0WG	A	800	-	-	0/5/6/6	0/3/3/3
4	NAG	A	802	1	-	2/6/23/26	0/1/1/1
4	NAG	B	802	1	-	2/6/23/26	0/1/1/1
4	NAG	B	806	1	-	4/6/23/26	0/1/1/1
4	NAG	D	801	1	-	2/6/23/26	0/1/1/1
4	NAG	A	808	1	-	2/6/23/26	0/1/1/1
4	NAG	A	801	1	-	4/6/23/26	0/1/1/1
4	NAG	B	803	1	-	2/6/23/26	0/1/1/1
3	0WG	B	800	-	-	0/5/6/6	0/3/3/3
4	NAG	C	802	1	-	4/6/23/26	0/1/1/1
4	NAG	C	801	1	-	1/6/23/26	0/1/1/1
4	NAG	D	804	1	-	5/6/23/26	0/1/1/1
3	0WG	C	800	-	-	0/5/6/6	0/3/3/3
4	NAG	A	803	1	-	0/6/23/26	0/1/1/1
4	NAG	B	801	1	-	2/6/23/26	0/1/1/1
3	0WG	D	800	-	-	0/5/6/6	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	800	OWG	C23-N2	-2.40	1.35	1.38
3	C	800	OWG	C23-N2	-2.20	1.35	1.38
3	A	800	OWG	C23-N2	-2.20	1.35	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	OWG	N21-C23-N2	8.32	122.81	116.98
3	A	800	OWG	N21-C23-N2	7.99	122.58	116.98
3	D	800	OWG	N21-C23-N2	7.97	122.57	116.98
3	B	800	OWG	N21-C23-N2	7.81	122.45	116.98
3	B	800	OWG	C19-N21-C23	-6.11	120.85	125.60
3	A	800	OWG	C19-N21-C23	-5.99	120.94	125.60
3	D	800	OWG	C19-N21-C23	-5.97	120.96	125.60
3	C	800	OWG	C19-N21-C23	-5.67	121.19	125.60
4	C	801	NAG	C1-O5-C5	5.56	119.64	112.19
3	A	800	OWG	C10-C11-C16	-4.52	118.35	122.56
3	A	800	OWG	O24-C23-N2	-4.46	118.32	122.10
3	C	800	OWG	O24-C23-N2	-4.20	118.53	122.10
3	D	800	OWG	O24-C23-N2	-4.05	118.66	122.10
4	A	808	NAG	C1-O5-C5	3.88	117.39	112.19
3	B	800	OWG	O24-C23-N2	-3.76	118.91	122.10
4	A	803	NAG	C4-C3-C2	3.60	116.29	111.02
3	B	800	OWG	C10-C11-C16	-3.60	119.21	122.56
3	A	800	OWG	C8-C7-C5	-3.43	119.08	122.56
3	C	800	OWG	C10-C11-C16	-3.39	119.40	122.56
4	A	802	NAG	C1-O5-C5	3.36	116.69	112.19
3	B	800	OWG	C8-C7-C5	-3.28	119.23	122.56
4	B	806	NAG	C1-O5-C5	3.28	116.58	112.19
3	D	800	OWG	C10-C11-C16	-3.16	119.62	122.56
4	A	801	NAG	C1-O5-C5	2.97	116.17	112.19
4	D	801	NAG	C1-O5-C5	2.92	116.10	112.19
4	B	801	NAG	C1-O5-C5	2.83	115.98	112.19
4	B	801	NAG	C4-C3-C2	2.83	115.17	111.02
4	D	804	NAG	C2-N2-C7	2.79	126.63	122.90
3	D	800	OWG	C8-C7-C5	-2.78	119.74	122.56
3	D	800	OWG	C18-C19-N21	2.78	119.26	115.75
3	B	800	OWG	C18-C19-N21	2.76	119.24	115.75
3	B	800	OWG	N4-C3-N2	2.70	120.89	117.41
4	B	802	NAG	C1-O5-C5	2.63	115.72	112.19
3	A	800	OWG	C1-N2-C23	2.58	120.01	117.34
3	C	800	OWG	C8-C7-C5	-2.57	119.95	122.56
3	C	800	OWG	N4-C3-N2	2.56	120.71	117.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	800	0WG	N4-C3-N2	2.53	120.68	117.41
3	A	800	0WG	C18-C19-N21	2.48	118.89	115.75
3	C	800	0WG	C1-N2-C23	2.47	119.89	117.34
3	A	800	0WG	N4-C3-N2	2.42	120.53	117.41
3	B	800	0WG	C5-N4-C3	2.30	122.85	116.99
3	B	800	0WG	C1-N2-C23	2.27	119.69	117.34
3	D	800	0WG	C3-C18-C19	-2.25	117.11	119.05
4	D	804	NAG	C1-O5-C5	2.25	115.20	112.19
3	B	800	0WG	C18-C3-N4	-2.23	119.86	123.53
3	C	800	0WG	C18-C19-N21	2.19	118.52	115.75
3	C	800	0WG	C18-C3-N4	-2.17	119.95	123.53
3	C	800	0WG	C5-N4-C3	2.17	122.51	116.99
3	D	800	0WG	C5-N4-C3	2.15	122.47	116.99
3	D	800	0WG	C18-C3-N4	-2.14	120.00	123.53
3	C	800	0WG	C15-C16-C11	-2.08	119.48	121.70
3	A	800	0WG	C5-N4-C3	2.07	122.25	116.99
3	C	800	0WG	C3-N2-C23	-2.03	120.34	122.22

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	802	NAG	C8-C7-N2-C2
4	A	802	NAG	O7-C7-N2-C2
4	B	801	NAG	C8-C7-N2-C2
4	B	801	NAG	O7-C7-N2-C2
4	B	806	NAG	C8-C7-N2-C2
4	B	806	NAG	O7-C7-N2-C2
4	D	804	NAG	C3-C2-N2-C7
4	D	804	NAG	C8-C7-N2-C2
4	D	804	NAG	O7-C7-N2-C2
4	B	803	NAG	C8-C7-N2-C2
4	B	803	NAG	O7-C7-N2-C2
4	D	804	NAG	O5-C5-C6-O6
4	D	801	NAG	O5-C5-C6-O6
4	A	801	NAG	O5-C5-C6-O6
4	C	802	NAG	C8-C7-N2-C2
4	C	802	NAG	O7-C7-N2-C2
4	A	808	NAG	O5-C5-C6-O6
4	D	801	NAG	C4-C5-C6-O6

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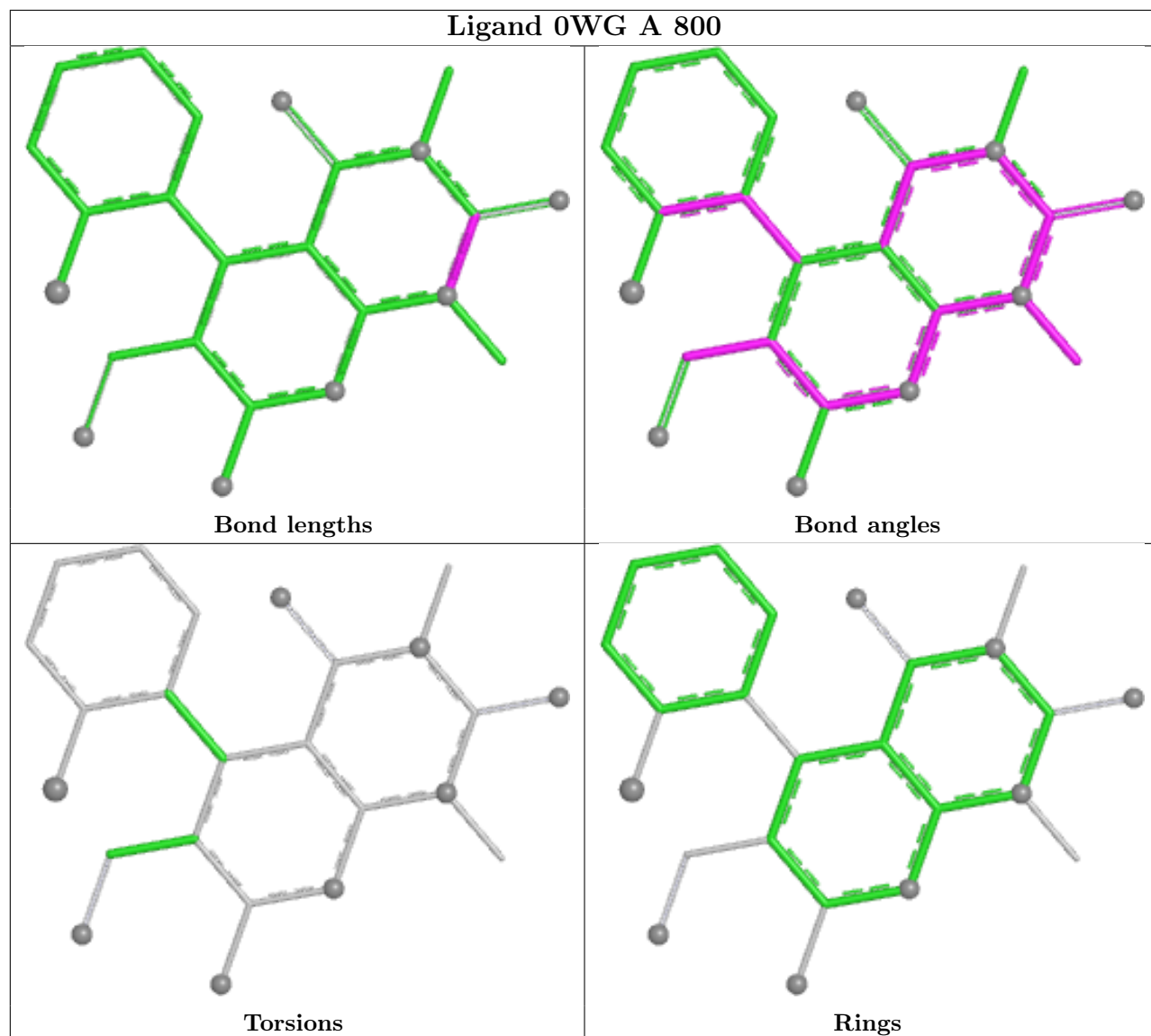
Mol	Chain	Res	Type	Atoms
4	B	802	NAG	C4-C5-C6-O6
4	B	806	NAG	C4-C5-C6-O6
4	D	804	NAG	C4-C5-C6-O6
4	B	802	NAG	O5-C5-C6-O6
4	C	801	NAG	O5-C5-C6-O6
4	B	806	NAG	O5-C5-C6-O6
4	C	802	NAG	C4-C5-C6-O6
4	A	801	NAG	C4-C5-C6-O6
4	A	808	NAG	C4-C5-C6-O6
4	C	802	NAG	O5-C5-C6-O6

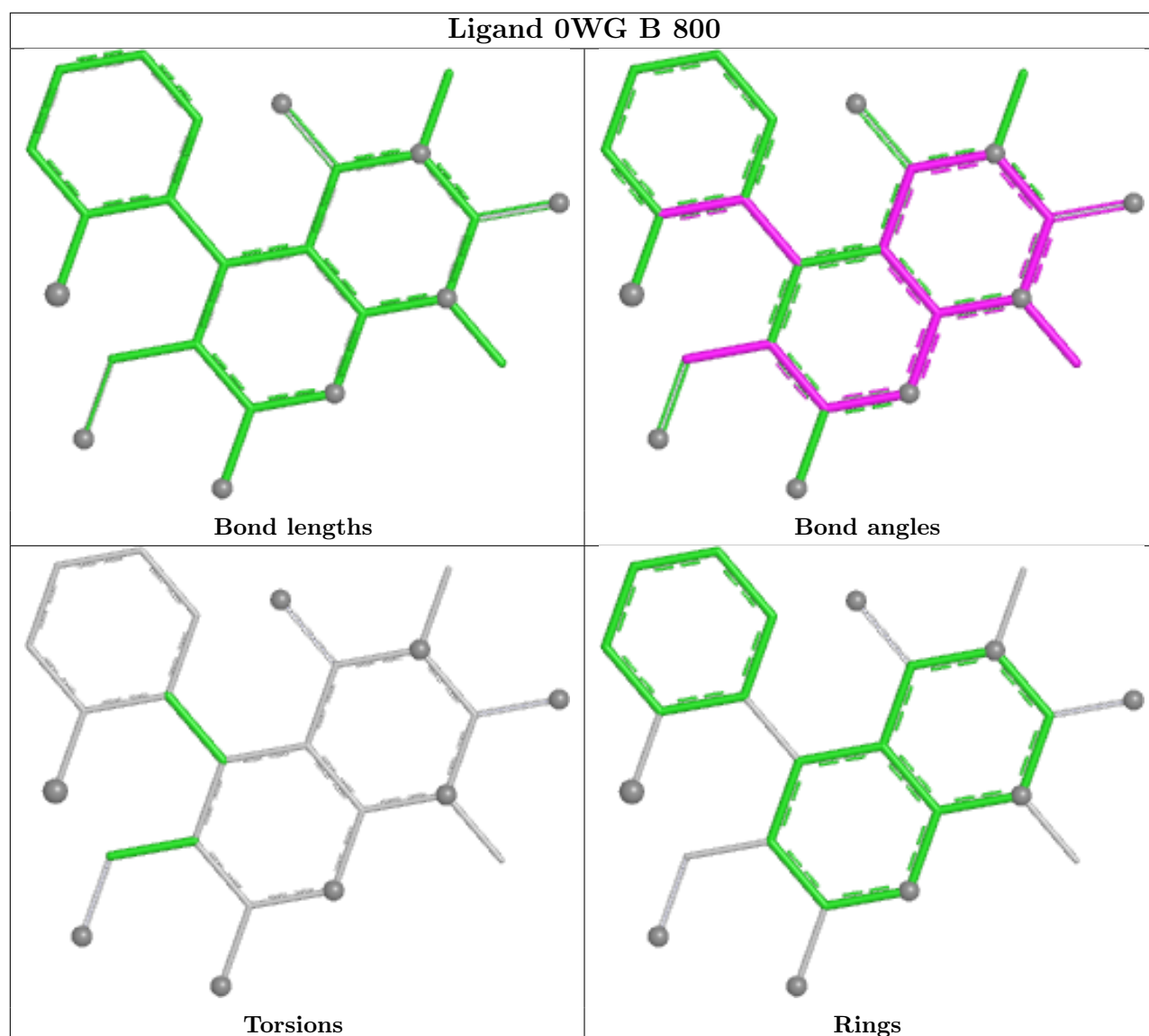
There are no ring outliers.

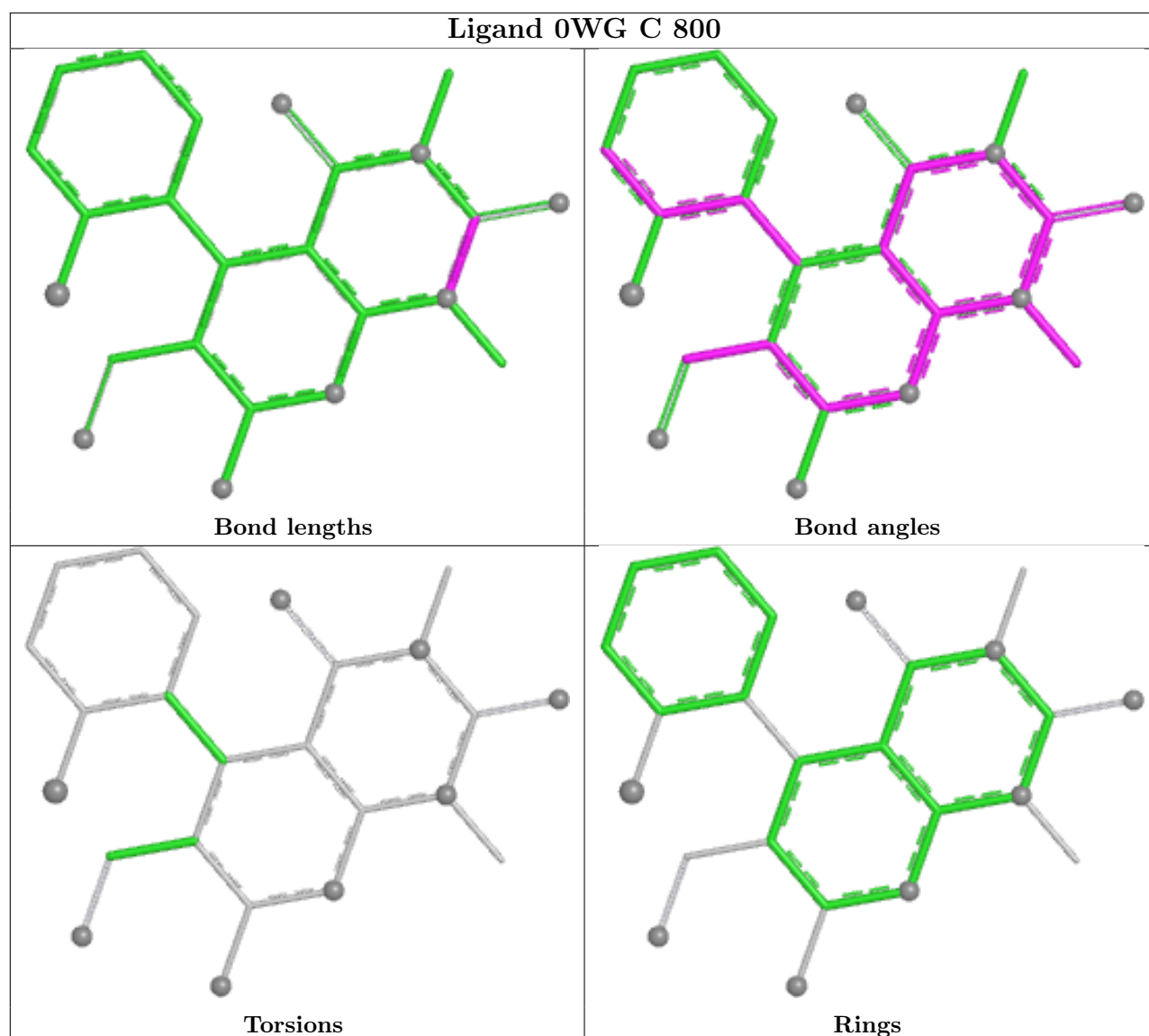
2 monomers are involved in 2 short contacts:

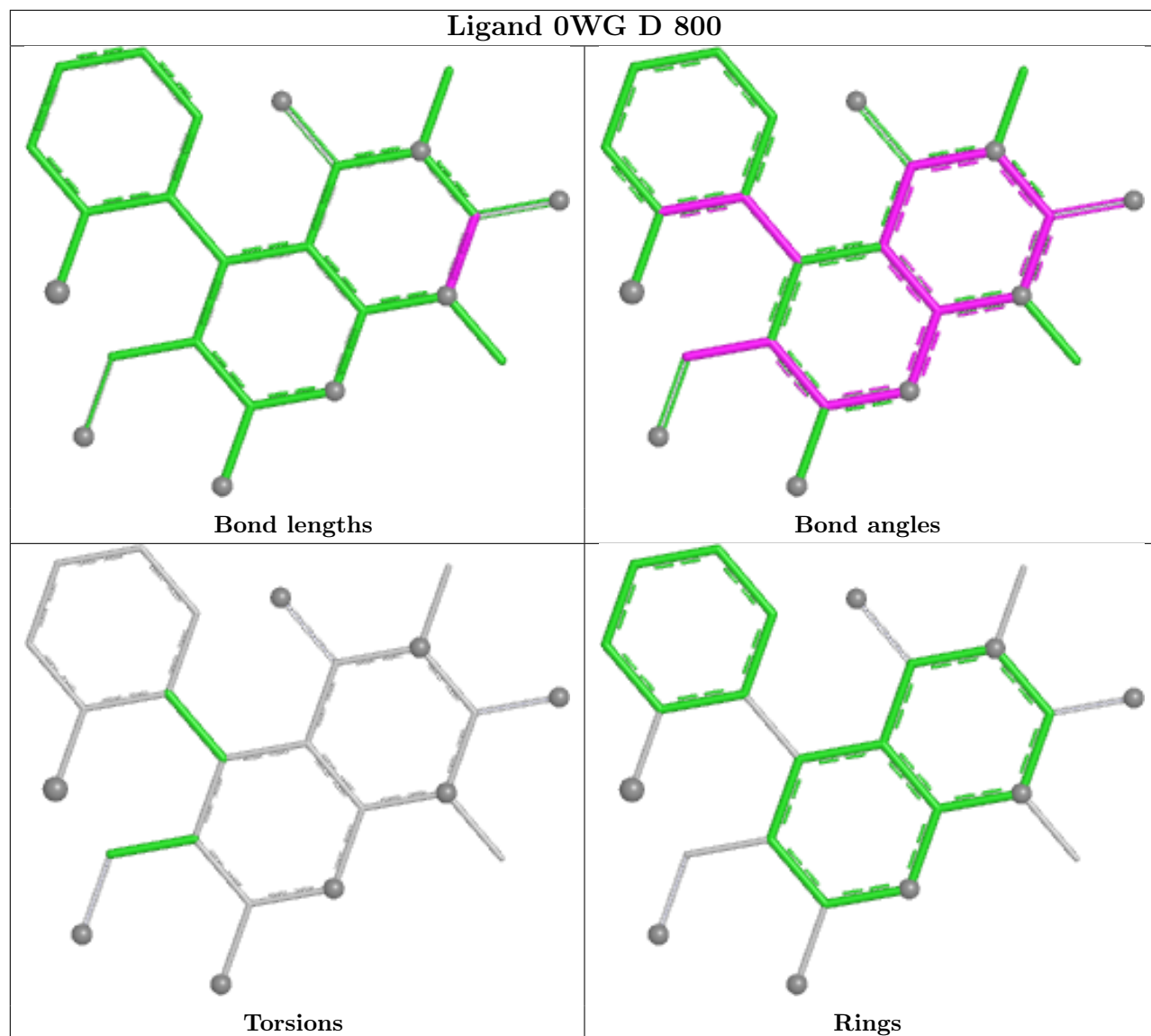
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	0WG	1	0
3	C	800	0WG	1	0

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	724/740 (97%)	0.07	19 (2%)	57 48	16, 38, 82, 108	1 (0%)
1	B	727/740 (98%)	0.04	18 (2%)	58 48	17, 37, 67, 117	0
1	C	722/740 (97%)	0.15	11 (1%)	72 64	18, 43, 86, 118	0
1	D	715/740 (96%)	0.28	19 (2%)	56 47	18, 49, 90, 128	0
All	All	2888/2960 (97%)	0.13	67 (2%)	61 52	16, 41, 84, 128	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	ALA	5.1
1	B	81	ALA	4.8
1	D	88	VAL	4.8
1	D	95	PHE	4.4
1	B	70	TYR	4.1
1	B	83	TYR	3.5
1	B	78	VAL	3.4
1	D	85	ASN	3.3
1	A	87	SER	3.1
1	D	77	LEU	3.1
1	D	78	VAL	2.9
1	A	489	LYS	2.9
1	B	84	GLY	2.9
1	C	279	VAL	2.9
1	C	394	CYS	2.9
1	D	137	LEU	2.9
1	A	84	GLY	2.8
1	B	38	HIS	2.7
1	B	89	PHE	2.7
1	A	90	LEU	2.7
1	C	490	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	89	PHE	2.6
1	D	489	LYS	2.6
1	D	392	LYS	2.5
1	C	79	PHE	2.5
1	D	87	SER	2.5
1	A	399	LYS	2.5
1	C	93	SER	2.5
1	D	295	ILE	2.4
1	A	88	VAL	2.4
1	D	436	LEU	2.4
1	D	486	VAL	2.4
1	A	72	GLN	2.4
1	D	75	ASN	2.4
1	B	766	PRO	2.4
1	A	86	SER	2.3
1	A	66	HIS	2.3
1	D	66	HIS	2.3
1	B	79	PHE	2.2
1	A	69	LEU	2.2
1	B	75	ASN	2.2
1	B	489	LYS	2.2
1	A	83	TYR	2.2
1	A	75	ASN	2.2
1	C	63	ILE	2.2
1	D	138	ASN	2.2
1	B	65	ASP	2.2
1	C	392	LYS	2.2
1	C	78	VAL	2.1
1	A	95	PHE	2.1
1	D	98	PHE	2.1
1	A	762	CYS	2.1
1	D	437	SER	2.1
1	B	72	GLN	2.1
1	A	81	ALA	2.1
1	B	342	ALA	2.1
1	B	87	SER	2.1
1	A	78	VAL	2.1
1	B	85	ASN	2.1
1	C	179	ASN	2.0
1	D	69	LEU	2.0
1	A	490	GLY	2.0
1	A	378	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	101	SER	2.0
1	C	134	ILE	2.0
1	B	82	GLU	2.0
1	B	88	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

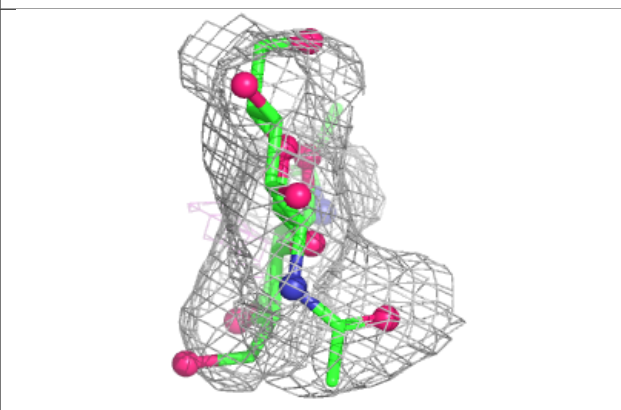
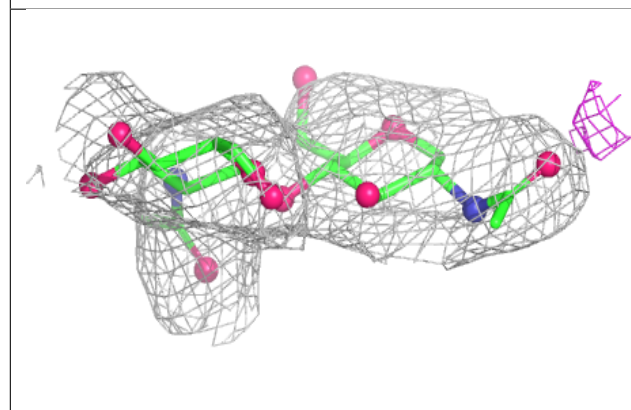
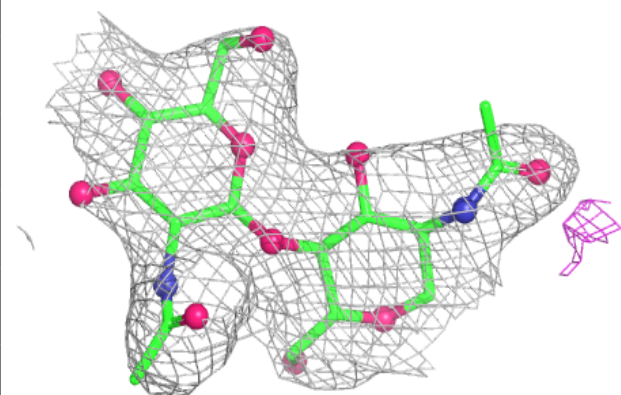
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	2	14/15	0.59	0.15	76,85,86,87	0
2	NAG	F	1	14/15	0.62	0.15	67,75,80,82	0
2	NAG	G	2	14/15	0.64	0.17	74,83,88,88	0
2	NAG	F	2	14/15	0.80	0.14	78,82,92,97	0
2	NAG	E	2	14/15	0.82	0.12	53,61,64,66	0
2	NAG	I	2	14/15	0.82	0.12	53,56,60,60	0
2	NAG	H	1	14/15	0.84	0.11	42,50,61,68	0
2	NAG	E	1	14/15	0.89	0.11	46,52,57,57	0
2	NAG	I	1	14/15	0.91	0.08	37,41,42,49	0
2	NAG	G	1	14/15	0.91	0.10	47,54,62,66	0

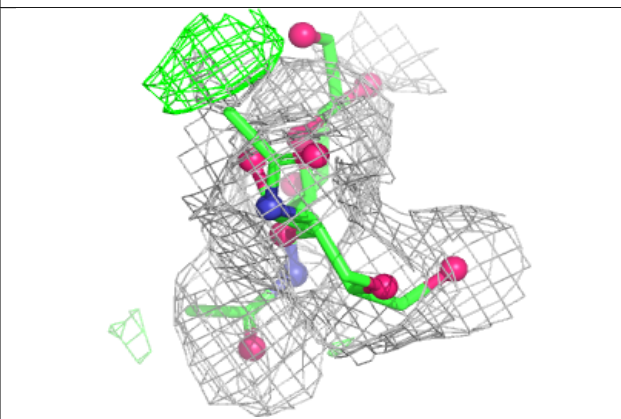
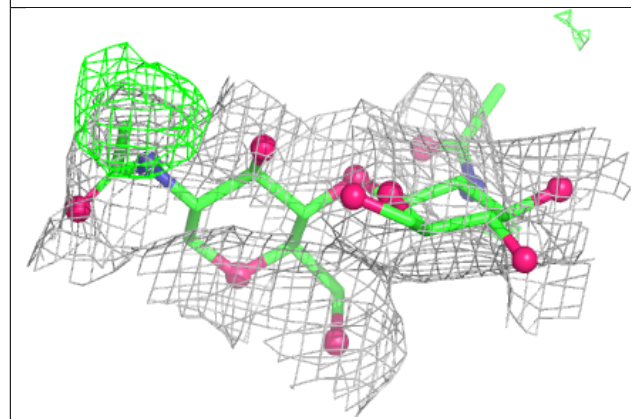
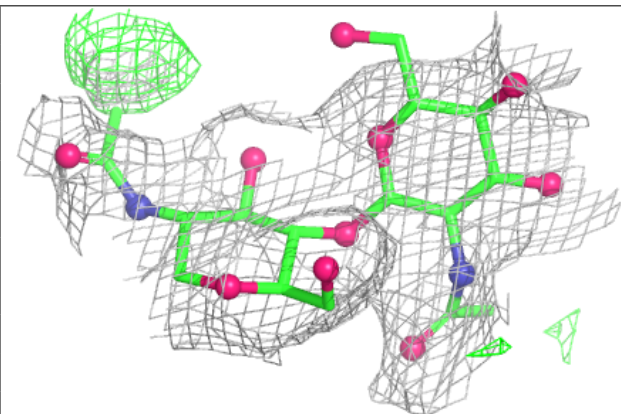
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

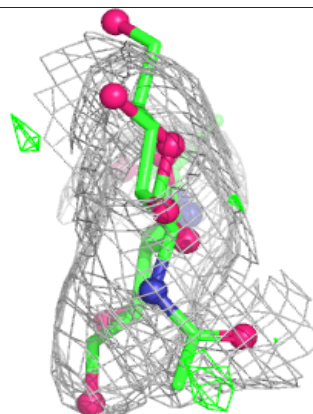
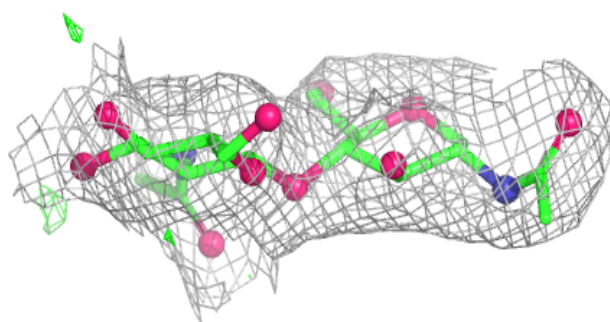
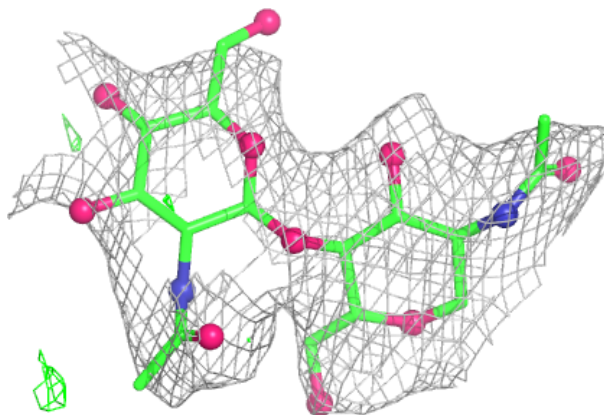
**Electron density around Chain F:**

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



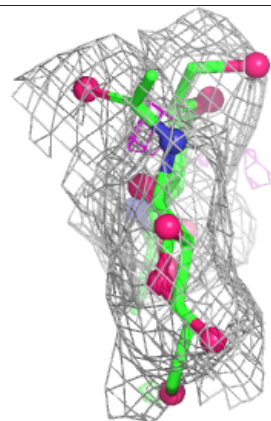
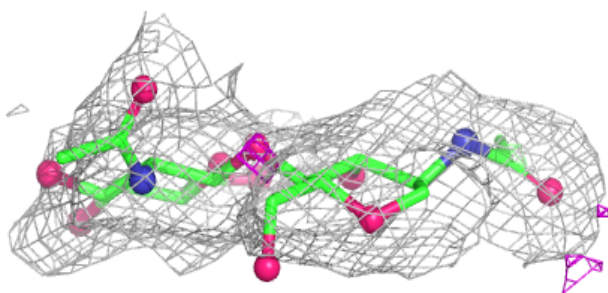
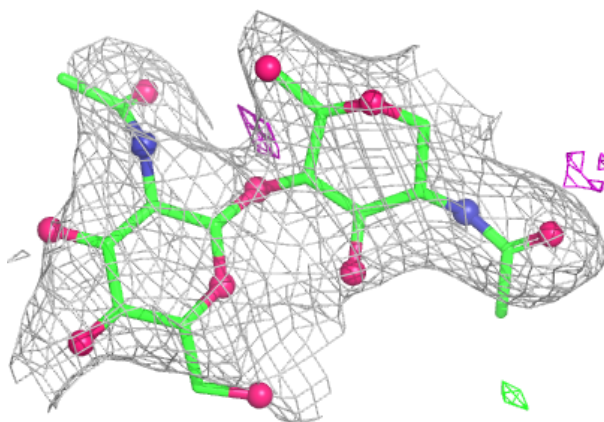
Electron density around Chain G:

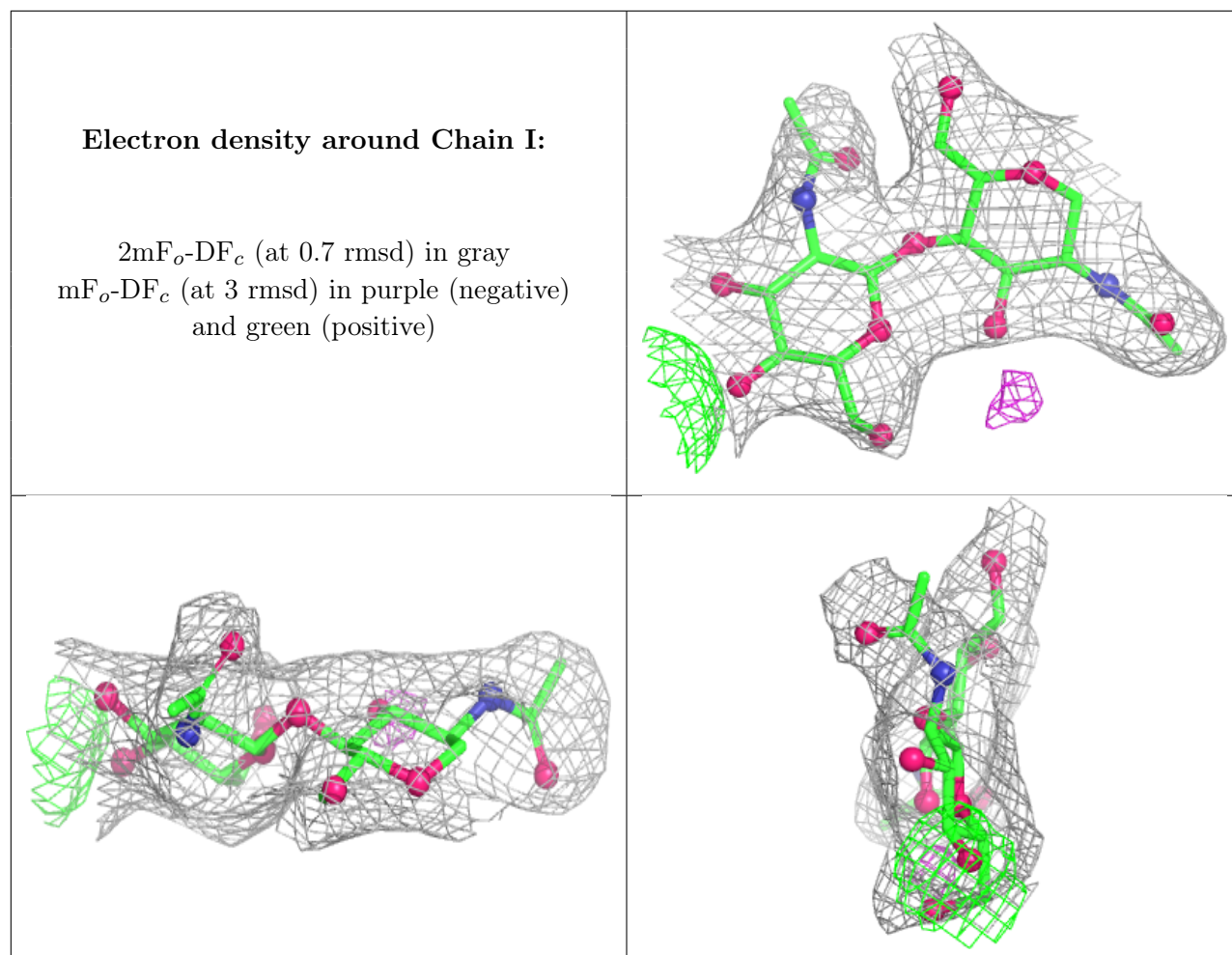
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	801	14/15	0.54	0.15	51,55,58,60	0
4	NAG	A	801	14/15	0.62	0.16	58,62,64,64	0
4	NAG	A	802	14/15	0.63	0.16	73,81,83,84	0
4	NAG	C	802	14/15	0.68	0.15	66,73,77,81	0
4	NAG	A	803	14/15	0.71	0.14	61,68,78,79	0
4	NAG	B	803	14/15	0.73	0.13	51,56,58,59	0
4	NAG	C	801	14/15	0.75	0.16	24,26,26,26	0
4	NAG	B	802	14/15	0.77	0.10	51,55,57,60	0
4	NAG	D	801	14/15	0.77	0.13	34,36,36,37	0
4	NAG	A	808	14/15	0.84	0.11	46,53,56,61	0

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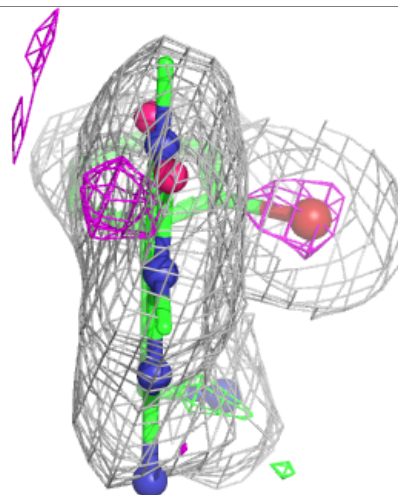
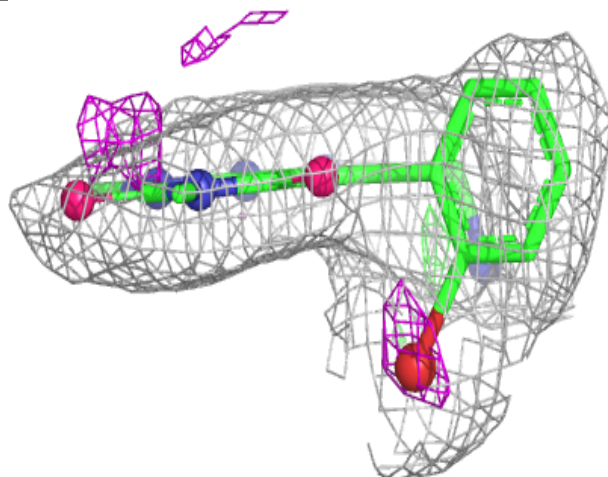
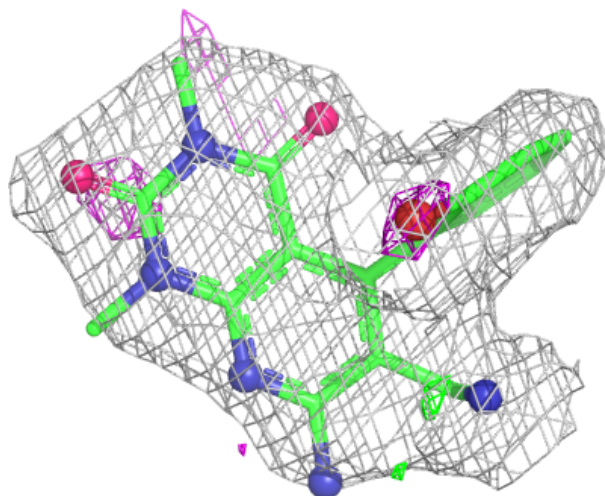
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	806	14/15	0.85	0.10	52,56,57,60	0
4	NAG	D	804	14/15	0.85	0.10	62,66,70,70	0
3	0WG	B	800	24/24	0.95	0.10	26,32,35,46	0
3	0WG	D	800	24/24	0.95	0.10	29,31,35,45	0
3	0WG	C	800	24/24	0.96	0.10	26,31,32,41	0
3	0WG	A	800	24/24	0.97	0.08	25,29,32,39	0

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

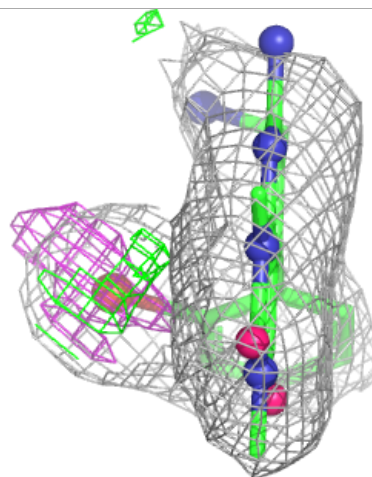
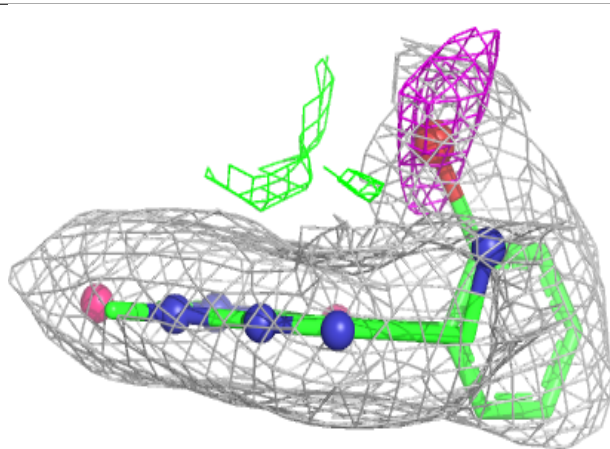
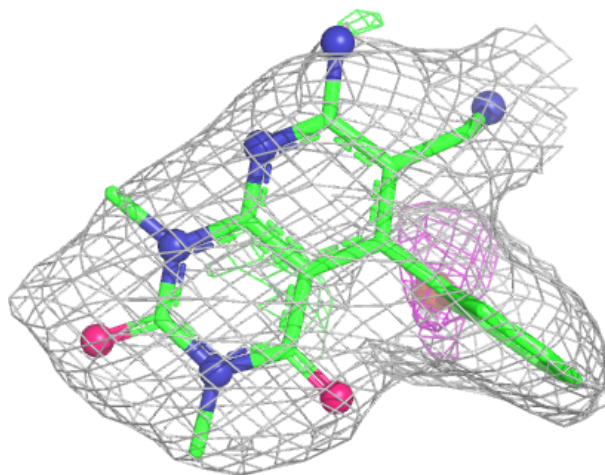
Electron density around 0WG B 800:

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



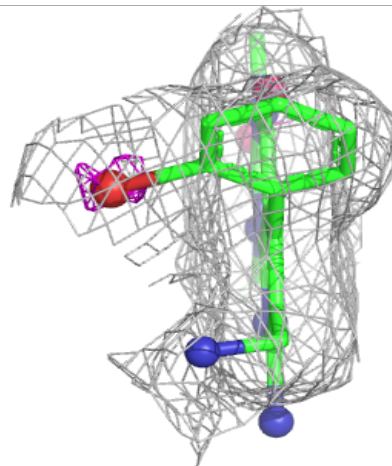
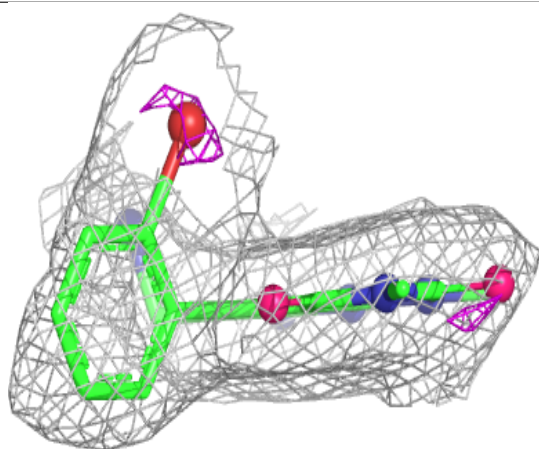
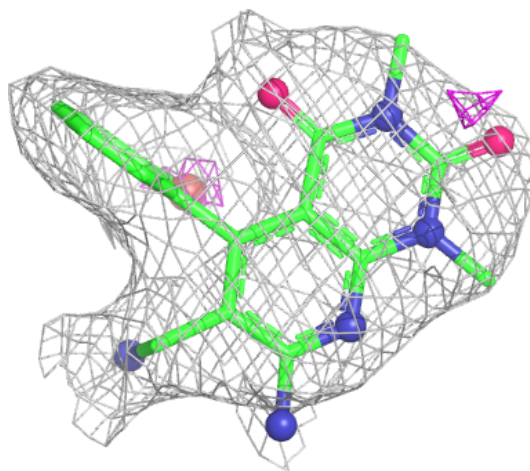
Electron density around 0WG D 800:

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



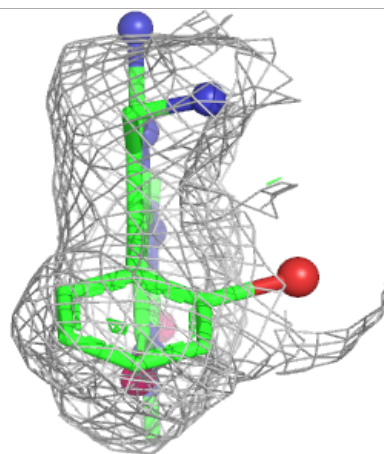
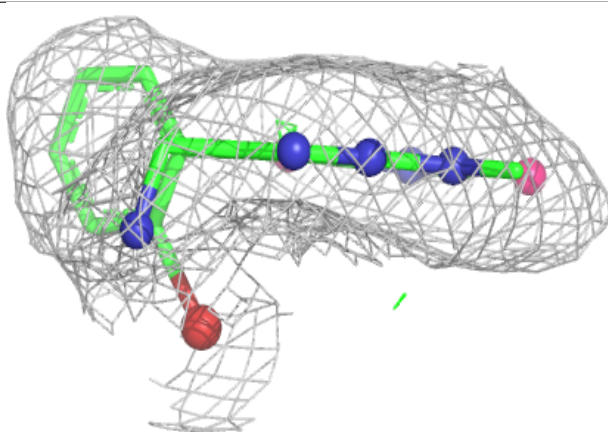
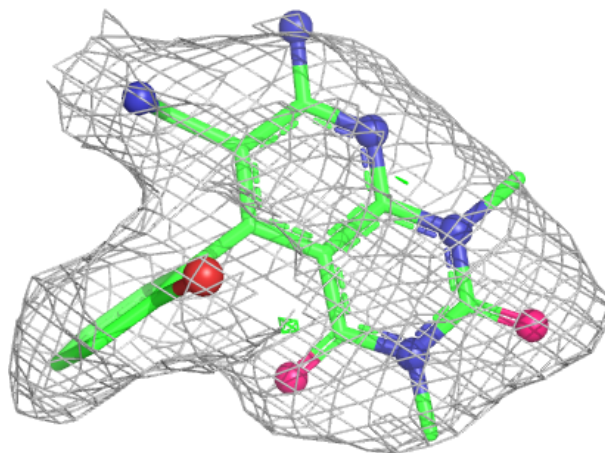
Electron density around 0WG C 800:

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



Electron density around 0WG A 800:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.