



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:37 PM EDT

PDB ID : 5KBY
Title : Crystal structure of dipeptidyl peptidase IV in complex with SYR-472
Authors : Skene, R.J.; Jennings, A.J.
Deposited on : 2016-06-03
Resolution : 2.24 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

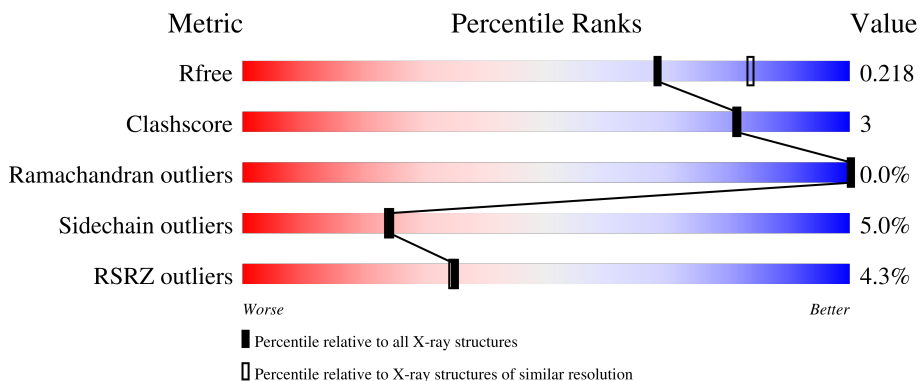
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	 4% 89% 8% ..
1	B	740	 % 89% 9% ..
1	C	740	 7% 87% 9% ..
1	D	740	 4% 87% 10% ..
2	E	2	 50% 50%

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 25867 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
			Total	C	N	O	S			
1	A	725	5936	3813	975	1122	26	0	1	0
1	B	733	6024	3863	1000	1135	26	0	3	0
1	C	717	5882	3784	963	1109	26	0	2	0
1	D	725	5946	3819	980	1121	26	0	1	0

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

Continued on next page...

Continued from previous page...

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			

Continued on next page...

Continued from previous page...

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			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



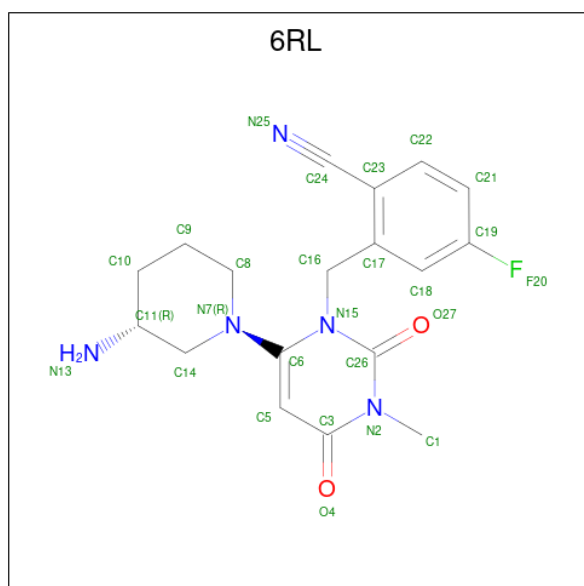
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 2-[[6-[(3 {R})-3-azanylpiperidin-1-yl]-3-methyl-2,4-bis(oxidanylidene)pyrimidin-1-yl]methyl]-4-fluoranyl-benzenecarbonitrile (three-letter code: 6RL) (formula: C₁₈H₂₀FN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	18	1	5	2		
4	B	1	Total	C	F	N	O	0	0
			26	18	1	5	2		
4	C	1	Total	C	F	N	O	0	0
			26	18	1	5	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	D	1	26	18	1	5	2	0	0

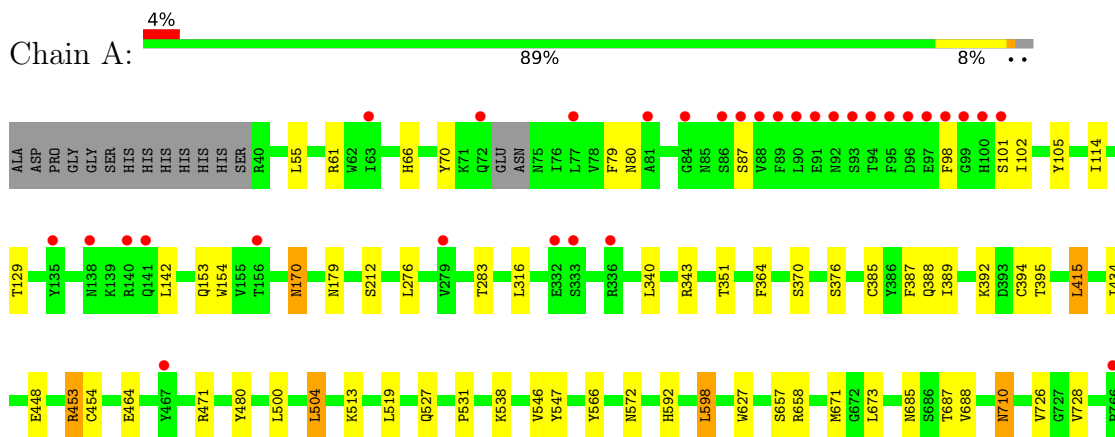
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	422	Total 422	O 422	0	0
5	B	497	Total 497	O 497	0	0
5	C	300	Total 300	O 300	0	0
5	D	378	Total 378	O 378	0	0

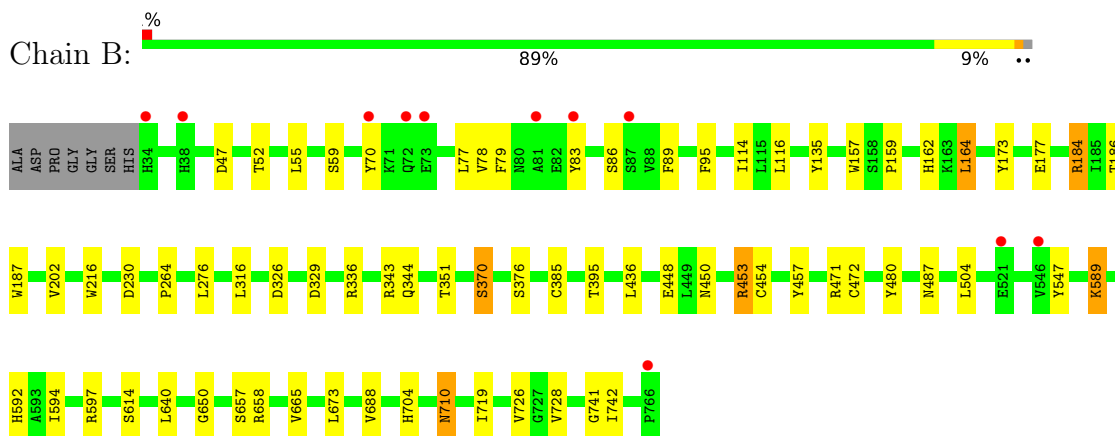
3 Residue-property plots [i](#)

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.

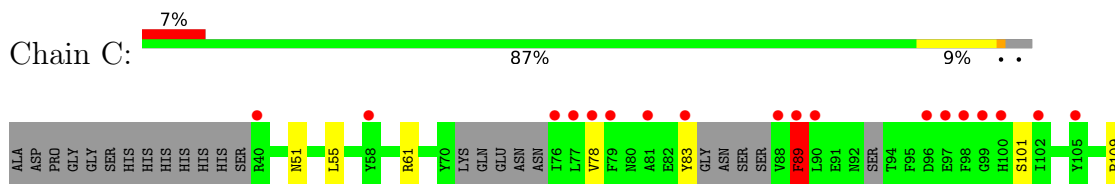
- Molecule 1: Dipeptidyl peptidase 4

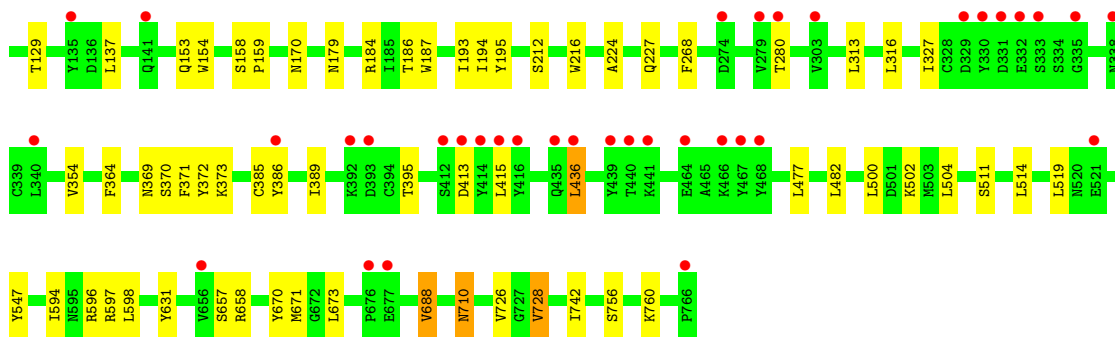


- Molecule 1: Dipeptidyl peptidase 4

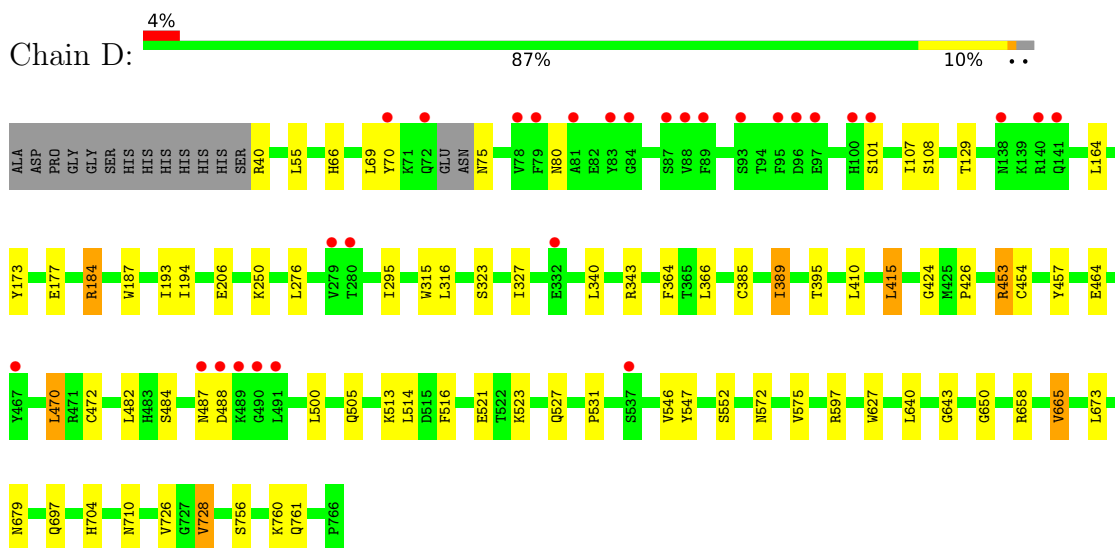


- Molecule 1: Dipeptidyl peptidase 4





- Molecule 1: Dipeptidyl peptidase 4



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

Chain E: 50% 50%

MAG1
MAG2

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

Chain F: 100%

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-glucofuranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucofuranose

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.57Å 122.17Å 143.70Å 90.00° 114.57° 90.00°	Depositor
Resolution (Å)	34.57 – 2.24 34.33 – 2.24	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.57-2.24) 97.8 (34.33-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.174 , 0.215 0.180 , 0.218	Depositor DCC
R_{free} test set	8950 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25867	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 6RL

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	0.42	0/6111	0.62	1/8311 (0.0%)
1	B	0.43	0/6213	0.64	1/8449 (0.0%)
1	C	0.39	0/6059	0.59	0/8239
1	D	0.40	0/6120	0.61	1/8319 (0.0%)
All	All	0.41	0/24503	0.62	3/33318 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	453	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	D	415	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	453	ARG	NE-CZ-NH2	5.09	122.84	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	5936	0	5651	28	0
1	B	6024	0	5725	37	0
1	C	5882	0	5600	27	0
1	D	5946	0	5669	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
2	J	28	0	25	1	0
3	A	42	0	39	1	0
3	B	70	0	65	0	0
3	C	42	0	38	0	0
3	D	56	0	52	0	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
4	C	26	0	0	0	0
4	D	26	0	0	0	0
5	A	422	0	0	1	0
5	B	497	0	0	4	0
5	C	300	0	0	1	0
5	D	378	0	0	1	0
All	All	25867	0	22989	123	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 3.

All (123) 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:A:153:GLN:HE22	1:A:170:ASN:H	1.30	0.79
1:C:153:GLN:HE22	1:C:170:ASN:H	1.31	0.77
1:C:369:ASN:O	1:C:389:ILE:HG12	1.86	0.75
1:D:552:SER:OG	5:D:1601:HOH:O	2.03	0.75
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.24	0.72
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.70	0.71
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.72	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.29	0.68
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.76	0.67
5:C:1601:HOH:O	2:I:2:NAG:O4	2.15	0.65
1:C:184:ARG:HD3	1:C:186:THR:O	1.96	0.65
1:B:70:TYR:HB3	1:B:79:PHE:CE2	2.32	0.64
1:D:173:TYR:CE1	1:D:184:ARG:HG2	2.34	0.62
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.36	0.61
1:A:212[B]:SER:OG	5:A:1601:HOH:O	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HD3	1:B:186:THR:O	2.05	0.56
1:B:657:SER:HA	1:B:688:VAL:HG13	1.89	0.55
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.71	0.54
1:B:589:LYS:HD3	5:B:947:HOH:O	2.07	0.54
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.73	0.54
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.43	0.53
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.89	0.53
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.90	0.53
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.44	0.52
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.91	0.52
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.49	0.52
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.75	0.51
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.93	0.51
1:D:340:LEU:HB2	1:D:343:ARG:HG3	1.93	0.51
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.92	0.51
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.51	0.51
1:C:78:VAL:CG2	1:C:89:PHE:HB2	2.41	0.51
1:C:194:ILE:HG12	2:I:1:NAG:H82	1.93	0.50
1:D:107:ILE:HG22	1:D:108:SER:O	2.10	0.50
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.93	0.50
1:C:756:SER:O	1:C:760:LYS:HG3	2.11	0.50
1:D:364:PHE:HE2	1:D:389:ILE:HD11	1.77	0.50
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.92	0.50
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.94	0.50
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.93	0.50
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.95	0.49
1:D:69:LEU:C	1:D:70:TYR:CA	2.81	0.49
1:C:657:SER:HA	1:C:688:VAL:HG13	1.94	0.48
1:A:170:ASN:HD22	1:A:170:ASN:N	2.11	0.48
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.49	0.48
1:C:109:PRO:HG2	1:C:158:SER:O	2.15	0.47
1:C:742:ILE:O	1:C:742:ILE:HG22	2.13	0.47
1:D:327:ILE:HD13	1:D:389:ILE:HG13	1.95	0.47
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.49	0.47
1:B:710:ASN:C	1:B:710:ASN:HD22	2.17	0.47
1:D:55:LEU:HD12	1:D:500:LEU:CD2	2.44	0.47
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.45	0.46
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.79	0.46
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.30	0.46
1:D:726:VAL:HG23	1:D:728:VAL:CG1	2.46	0.46
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.47	0.45
1:C:372:TYR:CE1	1:C:386:TYR:CD2	3.05	0.45
1:A:351:THR:OG1	1:A:592:HIS:HD2	2.00	0.45
1:A:154:TRP:CE2	1:A:212[A]:SER:HB3	2.51	0.44
1:D:194:ILE:HG12	2:J:1:NAG:H82	1.98	0.44
1:B:230:ASP:OD1	1:B:264:PRO:HB3	2.17	0.44
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.98	0.44
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.47	0.44
1:D:756:SER:O	1:D:760:LYS:HG3	2.17	0.44
1:B:370:SER:HB2	5:B:927:HOH:O	2.17	0.44
1:D:546:VAL:HG12	1:D:627:TRP:O	2.17	0.44
1:B:70:TYR:HB3	1:B:79:PHE:HE2	1.76	0.44
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.47	0.44
1:B:326:ASP:OD2	1:B:344:GLN:HG2	2.17	0.44
1:B:592:HIS:CE1	5:B:929:HOH:O	2.70	0.44
1:C:364:PHE:CD2	1:C:371:PHE:HB3	2.53	0.44
1:C:710:ASN:C	1:C:710:ASN:HD22	2.20	0.44
1:A:415:LEU:HB3	1:A:434:ILE:HG23	2.00	0.43
1:B:471[A]:ARG:HG3	1:B:480:TYR:CE1	2.53	0.43
1:A:598:LEU:HB2	1:A:671:MET:SD	2.58	0.43
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.43
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.43
1:B:592:HIS:HE1	5:B:929:HOH:O	2.01	0.43
1:B:47:ASP:HA	1:B:52:THR:OG1	2.19	0.43
1:D:516:PHE:CZ	1:D:523:LYS:HE3	2.54	0.43
1:A:657:SER:HA	1:A:688:VAL:HG13	2.01	0.42
1:A:70:TYR:HB3	1:A:79:PHE:HE1	1.82	0.42
1:D:453:ARG:HG3	1:D:454:CYS:SG	2.59	0.42
1:D:484:SER:O	1:D:488:ASP:HA	2.18	0.42
1:A:500:LEU:HG	1:A:504:LEU:HD22	2.02	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:D:173:TYR:CE1	1:D:184:ARG:CG	3.02	0.42
1:A:546:VAL:HG12	1:A:627:TRP:O	2.19	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.54	0.42
1:D:640:LEU:HD11	1:D:650:GLY:HA3	2.02	0.42
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.50	0.42
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.52	0.41
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.02	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.02	0.41
1:D:513:LYS:O	1:D:527:GLN:HA	2.21	0.41
1:B:726:VAL:HG23	1:B:728:VAL:CG1	2.50	0.41
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.50	0.41
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.36	0.41
1:B:79:PHE:CD1	1:B:86:SER:HB3	2.56	0.41
1:B:162:HIS:NE2	1:B:177:GLU:OE1	2.54	0.41
1:A:98:PHE:CD1	1:A:102:ILE:HD11	2.56	0.41
1:A:598:LEU:HD22	1:A:671:MET:CG	2.49	0.41
1:C:598:LEU:HG	1:C:631:TYR:OH	2.21	0.41
1:A:387:PHE:CD1	1:A:394:CYS:HB3	2.56	0.41
1:B:688:VAL:HG22	1:B:719:ILE:HG12	2.03	0.41
1:D:424:GLY:O	1:D:426:PRO:HD3	2.21	0.41
1:A:87:SER:H	3:A:1509:NAG:H81	1.87	0.40
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.56	0.40
1:B:471[A]:ARG:CG	1:B:480:TYR:CE1	3.04	0.40
1:D:315:TRP:O	1:D:323:SER:HB2	2.21	0.40
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.54	0.40
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.56	0.40
1:C:415:LEU:HB2	1:C:436:LEU:HD11	2.02	0.40
1:C:195:TYR:O	1:C:227:GLN:HA	2.21	0.40
1:C:596:ARG:N	1:C:670:TYR:O	2.48	0.40
1:D:457:TYR:CD1	1:D:470:LEU:HG	2.57	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	722/740 (98%)	691 (96%)	31 (4%)	0	100 100
1	B	734/740 (99%)	711 (97%)	23 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	711/740 (96%)	682 (96%)	28 (4%)	1 (0%)	51	58
1	D	720/740 (97%)	691 (96%)	29 (4%)	0	100	100
All	All	2887/2960 (98%)	2775 (96%)	111 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/662 (98%)	620 (95%)	30 (5%)	27	28
1	B	661/662 (100%)	630 (95%)	31 (5%)	26	27
1	C	644/662 (97%)	611 (95%)	33 (5%)	24	23
1	D	650/662 (98%)	613 (94%)	37 (6%)	20	19
All	All	2605/2648 (98%)	2474 (95%)	131 (5%)	24	24

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	66	HIS
1	A	80	ASN
1	A	101	SER
1	A	129	THR
1	A	142	LEU
1	A	170	ASN
1	A	179	ASN
1	A	276	LEU
1	A	283	THR
1	A	316	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	LEU
1	A	370	SER
1	A	376	SER
1	A	385	CYS
1	A	388	GLN
1	A	392	LYS
1	A	395	THR
1	A	415	LEU
1	A	448	GLU
1	A	464	GLU
1	A	504	LEU
1	A	519	LEU
1	A	538	LYS
1	A	547	TYR
1	A	566	TYR
1	A	598	LEU
1	A	673	LEU
1	A	685	ASN
1	A	710	ASN
1	B	55	LEU
1	B	59[A]	SER
1	B	59[B]	SER
1	B	77	LEU
1	B	83	TYR
1	B	164	LEU
1	B	184	ARG
1	B	202	VAL
1	B	276	LEU
1	B	316	LEU
1	B	336	ARG
1	B	370	SER
1	B	376	SER
1	B	385	CYS
1	B	395	THR
1	B	436	LEU
1	B	448	GLU
1	B	450	ASN
1	B	472	CYS
1	B	487	ASN
1	B	504	LEU
1	B	547	TYR
1	B	589	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	704	HIS
1	B	710	ASN
1	C	51	ASN
1	C	61	ARG
1	C	83	TYR
1	C	89	PHE
1	C	101	SER
1	C	129	THR
1	C	137	LEU
1	C	179	ASN
1	C	280	THR
1	C	313	LEU
1	C	316	LEU
1	C	354	VAL
1	C	370	SER
1	C	373	LYS
1	C	385	CYS
1	C	395	THR
1	C	413	ASP
1	C	436	LEU
1	C	477	LEU
1	C	482	LEU
1	C	502	LYS
1	C	504	LEU
1	C	511	SER
1	C	514	LEU
1	C	519	LEU
1	C	547	TYR
1	C	594	ILE
1	C	597	ARG
1	C	658	ARG
1	C	673	LEU
1	C	688	VAL
1	C	710	ASN
1	C	728	VAL
1	D	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	66	HIS
1	D	75	ASN
1	D	80	ASN
1	D	101	SER
1	D	129	THR
1	D	164	LEU
1	D	177	GLU
1	D	184	ARG
1	D	250	LYS
1	D	276	LEU
1	D	295	ILE
1	D	316	LEU
1	D	366	LEU
1	D	385	CYS
1	D	389	ILE
1	D	395	THR
1	D	410	LEU
1	D	415	LEU
1	D	453	ARG
1	D	464	GLU
1	D	470	LEU
1	D	472	CYS
1	D	482	LEU
1	D	487	ASN
1	D	505	GLN
1	D	514	LEU
1	D	521	GLU
1	D	547	TYR
1	D	575	VAL
1	D	658	ARG
1	D	665	VAL
1	D	673	LEU
1	D	704	HIS
1	D	710	ASN
1	D	728	VAL
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	ASN
1	A	455	GLN
1	A	520	ASN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	B	80	ASN
1	B	100	HIS
1	B	169	ASN
1	B	196	ASN
1	B	344	GLN
1	B	592	HIS
1	B	710	ASN
1	B	731	GLN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	506	ASN
1	C	572	ASN
1	C	592	HIS
1	C	710	ASN
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	344	GLN
1	D	520	ASN
1	D	572	ASN
1	D	685	ASN
1	D	697	GLN
1	D	710	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

12 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	0.67	0	17,19,21	1.65	4 (23%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.97	0
2	NAG	F	1	1,2	14,14,15	0.67	0	17,19,21	1.01	1 (5%)
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	1.54	3 (17%)
2	NAG	G	1	1,2	14,14,15	0.48	0	17,19,21	1.05	2 (11%)
2	NAG	G	2	2	14,14,15	0.47	0	17,19,21	1.46	3 (17%)
2	NAG	H	1	1,2	14,14,15	0.59	0	17,19,21	1.24	2 (11%)
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.70	0	17,19,21	1.24	3 (17%)
2	NAG	I	2	2	14,14,15	0.58	0	17,19,21	1.60	4 (23%)
2	NAG	J	1	1,2	14,14,15	0.72	0	17,19,21	1.46	1 (5%)
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	1.40	2 (11%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	O5-C1-C2	-4.22	104.63	111.29
2	I	2	NAG	C8-C7-N2	3.87	122.65	116.10
2	F	2	NAG	C8-C7-N2	3.81	122.55	116.10
2	H	2	NAG	C8-C7-N2	3.64	122.25	116.10
2	J	2	NAG	C8-C7-N2	3.41	121.86	116.10
2	E	1	NAG	C4-C3-C2	-3.39	106.05	111.02
2	G	2	NAG	C4-C3-C2	-3.07	106.52	111.02
2	G	2	NAG	O5-C1-C2	-2.94	106.65	111.29
2	E	1	NAG	C1-O5-C5	2.69	115.83	112.19
2	H	1	NAG	C1-C2-N2	2.63	114.99	110.49
2	I	2	NAG	O7-C7-C8	-2.58	117.27	122.06
2	I	2	NAG	C1-O5-C5	2.50	115.58	112.19
2	J	2	NAG	C2-N2-C7	2.46	126.41	122.90
2	F	2	NAG	C2-N2-C7	2.41	126.33	122.90
2	E	1	NAG	C2-N2-C7	2.40	126.32	122.90
2	G	1	NAG	O5-C1-C2	-2.39	107.52	111.29
2	I	2	NAG	C4-C3-C2	-2.37	107.54	111.02
2	I	1	NAG	O5-C1-C2	-2.35	107.58	111.29
2	G	1	NAG	O4-C4-C3	-2.34	104.95	110.35
2	I	1	NAG	C1-O5-C5	2.29	115.29	112.19
2	I	1	NAG	O4-C4-C3	-2.28	105.08	110.35
2	G	2	NAG	O3-C3-C2	2.27	114.16	109.47
2	F	2	NAG	O7-C7-C8	-2.24	117.89	122.06
2	F	1	NAG	O5-C1-C2	-2.23	107.77	111.29
2	H	1	NAG	C1-O5-C5	2.22	115.20	112.19
2	E	1	NAG	O3-C3-C2	2.19	114.00	109.47
2	H	2	NAG	C2-N2-C7	2.08	125.86	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7

Continued on next page...

Continued from previous page...

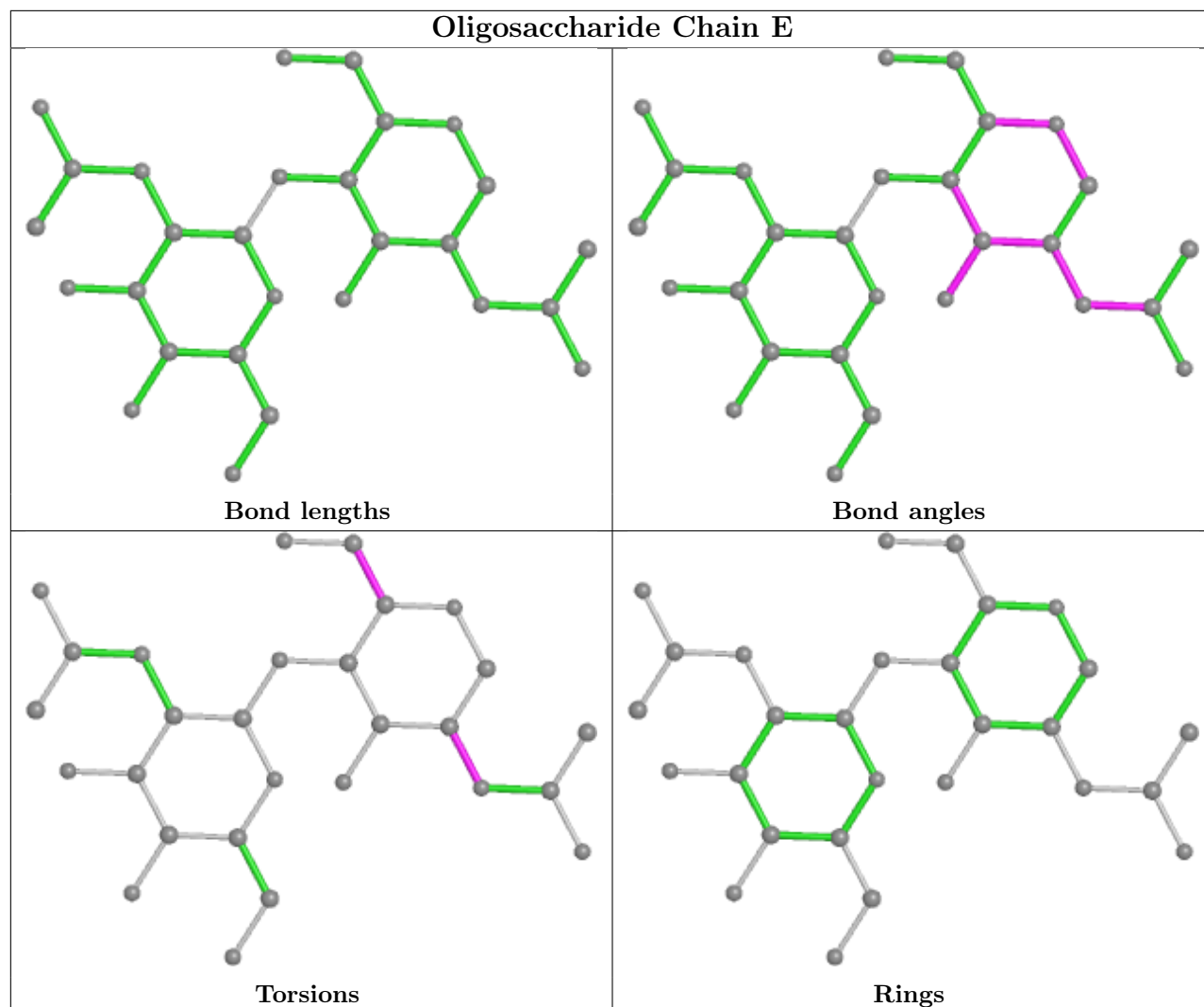
Mol	Chain	Res	Type	Atoms
2	J	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6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

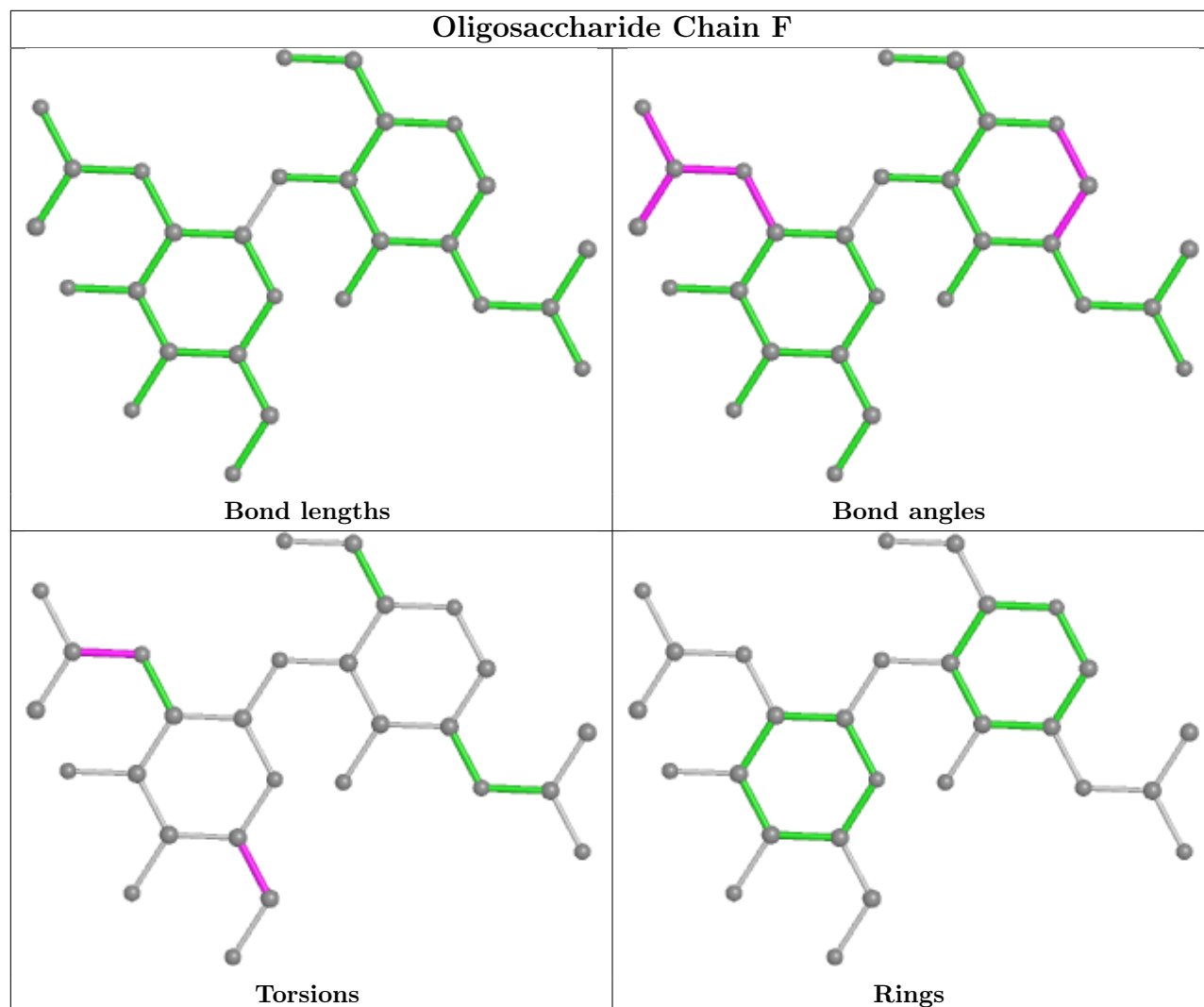
There are no ring outliers.

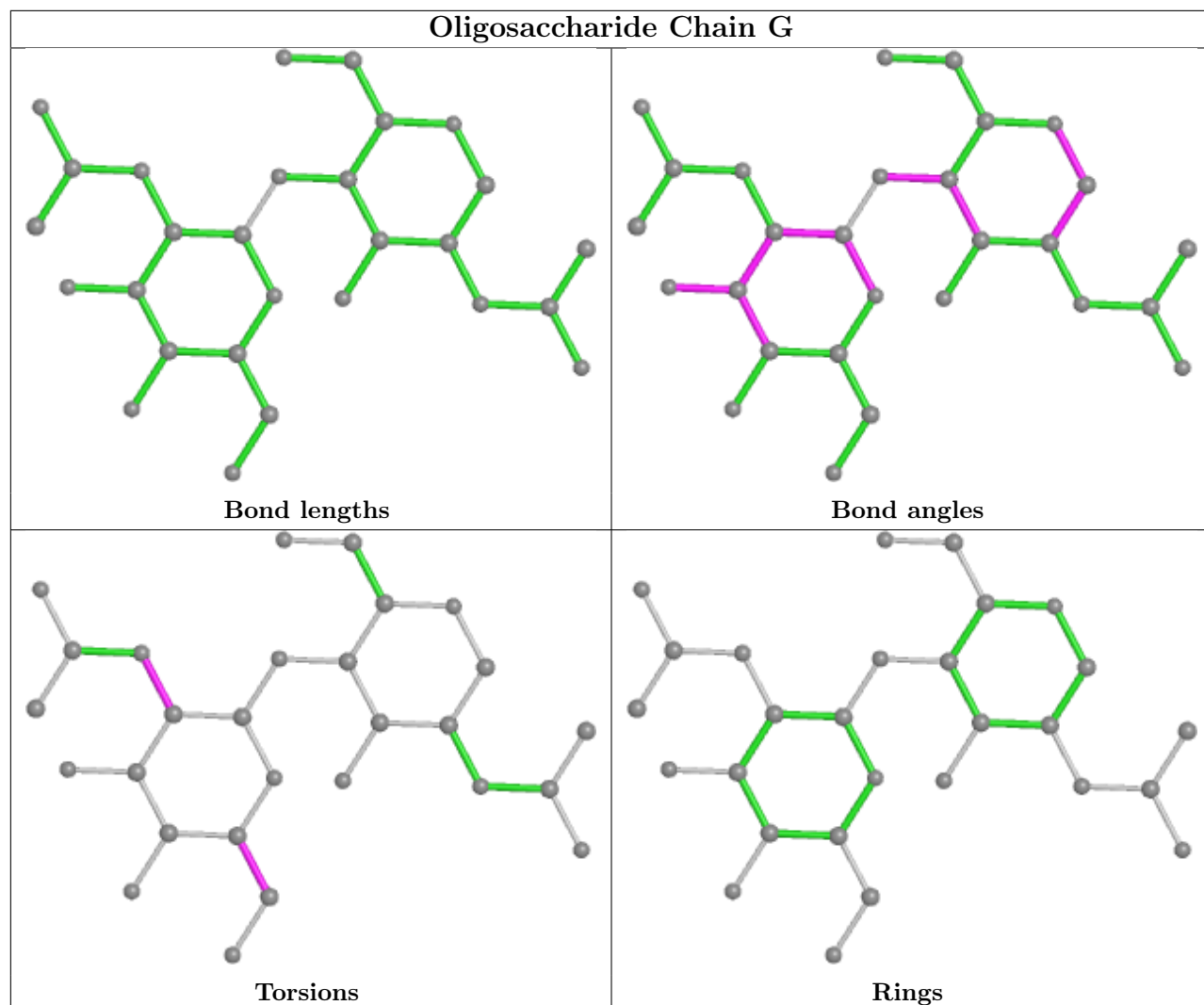
3 monomers are involved in 3 short contacts:

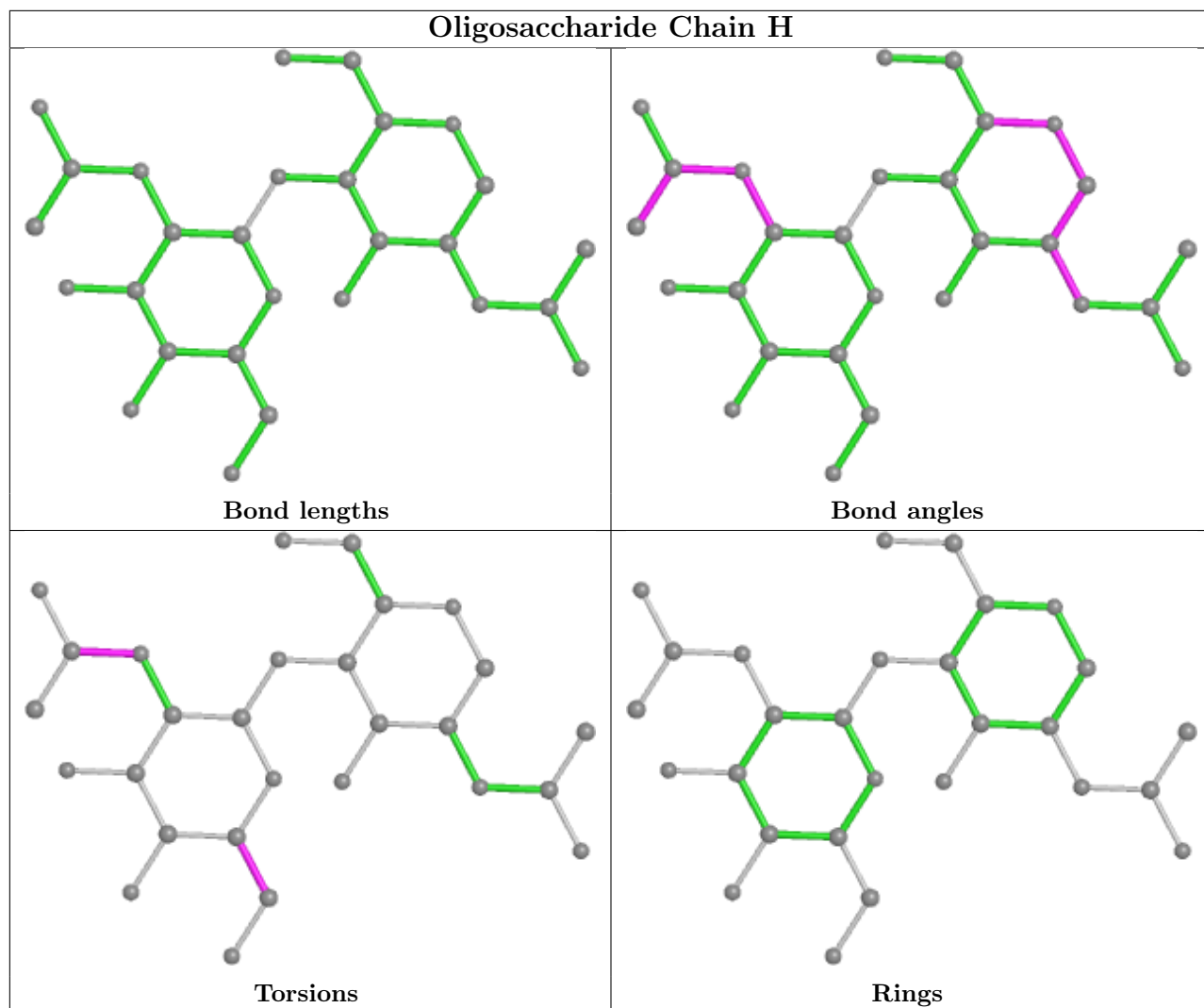
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	1	0
2	I	1	NAG	1	0
2	J	1	NAG	1	0

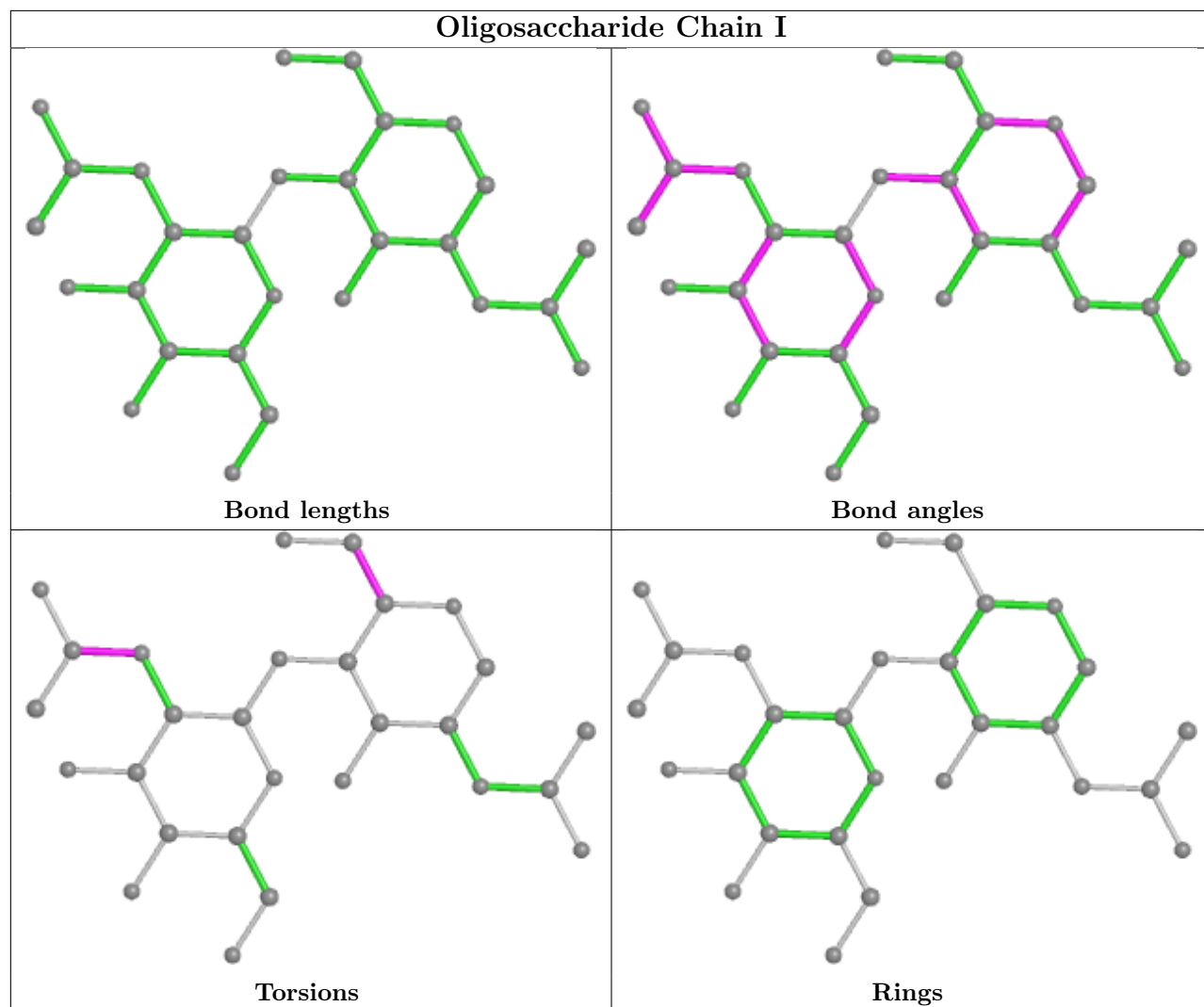
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

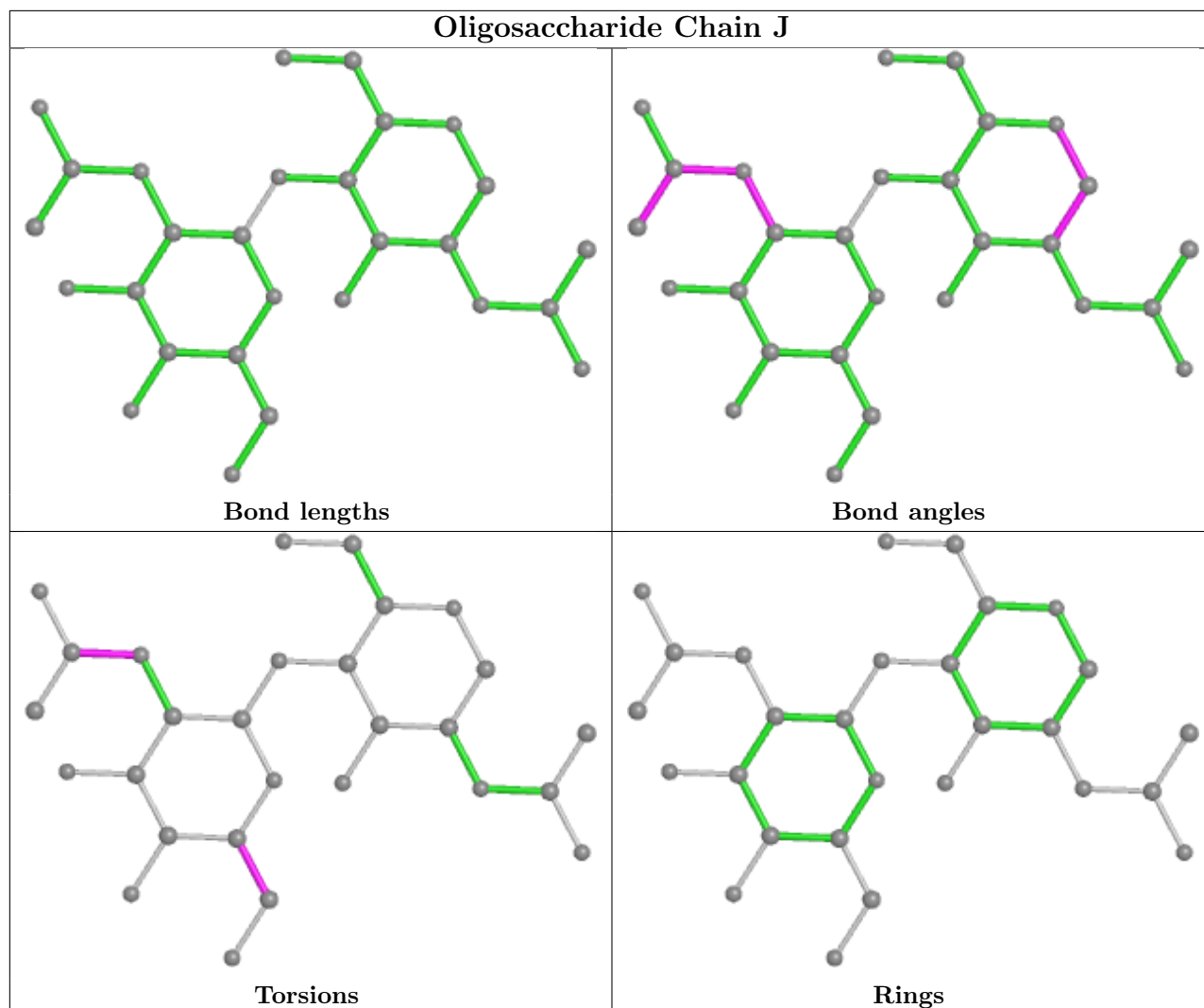












5.6 Ligand geometry [i](#)

19 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	NAG	C	1505	1	14,14,15	0.81	0	17,19,21	1.72	2 (11%)
3	NAG	A	1503	1	14,14,15	0.68	0	17,19,21	2.07	6 (35%)
3	NAG	D	1501	1	14,14,15	0.58	0	17,19,21	1.80	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	806	1	14,14,15	0.54	0	17,19,21	1.36	1 (5%)
3	NAG	A	1508	1	14,14,15	0.48	0	17,19,21	0.92	1 (5%)
3	NAG	A	1509	1	14,14,15	0.60	0	17,19,21	1.15	1 (5%)
4	6RL	B	808	-	28,28,28	0.93	1 (3%)	35,40,40	1.78	9 (25%)
4	6RL	C	1506	-	28,28,28	0.92	1 (3%)	35,40,40	1.80	6 (17%)
3	NAG	B	802	1	14,14,15	0.47	0	17,19,21	2.73	6 (35%)
3	NAG	B	801	1	14,14,15	0.52	0	17,19,21	2.03	4 (23%)
4	6RL	A	1510	-	28,28,28	0.94	0	35,40,40	1.80	9 (25%)
3	NAG	D	1502	1	14,14,15	0.64	0	17,19,21	1.07	1 (5%)
4	6RL	D	1507	-	28,28,28	0.89	1 (3%)	35,40,40	1.86	10 (28%)
3	NAG	B	805	1	14,14,15	0.36	0	17,19,21	1.47	2 (11%)
3	NAG	B	807	1	14,14,15	0.54	0	17,19,21	0.92	0
3	NAG	C	1501	1	14,14,15	0.56	0	17,19,21	1.66	3 (17%)
3	NAG	D	1506	1	14,14,15	0.63	0	17,19,21	1.34	2 (11%)
3	NAG	D	1505	1	14,14,15	0.56	0	17,19,21	0.98	1 (5%)
3	NAG	C	1504	1	14,14,15	0.49	0	17,19,21	1.31	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
3	NAG	C	1505	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1503	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1501	1	-	1/6/23/26	0/1/1/1
3	NAG	B	806	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1508	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1509	1	-	2/6/23/26	0/1/1/1
4	6RL	B	808	-	-	4/10/20/20	0/3/3/3
4	6RL	C	1506	-	-	5/10/20/20	0/3/3/3
3	NAG	B	802	1	-	1/6/23/26	0/1/1/1
3	NAG	B	801	1	-	4/6/23/26	0/1/1/1
4	6RL	A	1510	-	-	3/10/20/20	0/3/3/3
3	NAG	D	1502	1	-	0/6/23/26	0/1/1/1
4	6RL	D	1507	-	-	3/10/20/20	0/3/3/3
3	NAG	B	805	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	807	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1501	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1506	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1505	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1504	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	808	6RL	C26-N15	-2.15	1.35	1.38
4	C	1506	6RL	C3-N2	-2.07	1.36	1.40
4	D	1507	6RL	C3-N2	-2.01	1.36	1.40

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	NAG	C1-O5-C5	8.43	123.62	112.19
3	B	801	NAG	C1-O5-C5	5.78	120.03	112.19
3	C	1505	NAG	C4-C3-C2	5.65	119.30	111.02
3	D	1501	NAG	C1-O5-C5	5.59	119.77	112.19
4	D	1507	6RL	C5-C3-N2	5.15	120.79	115.40
3	A	1503	NAG	C1-C2-N2	4.97	118.98	110.49
4	D	1507	6RL	C3-N2-C26	-4.85	120.00	124.56
4	B	808	6RL	C5-C3-N2	4.82	120.44	115.40
4	C	1506	6RL	C3-N2-C26	-4.81	120.04	124.56
4	C	1506	6RL	C5-C3-N2	4.77	120.39	115.40
4	A	1510	6RL	C5-C3-N2	4.59	120.20	115.40
4	A	1510	6RL	C3-N2-C26	-4.52	120.31	124.56
3	C	1501	NAG	C1-O5-C5	4.40	118.15	112.19
3	B	806	NAG	C1-O5-C5	4.26	117.96	112.19
3	C	1504	NAG	C1-O5-C5	4.20	117.88	112.19
3	B	802	NAG	C4-C3-C2	-3.95	105.23	111.02
3	B	805	NAG	C1-O5-C5	3.88	117.45	112.19
4	B	808	6RL	C3-N2-C26	-3.82	120.97	124.56
3	B	801	NAG	C8-C7-N2	3.45	121.94	116.10
3	C	1501	NAG	C8-C7-N2	3.33	121.74	116.10
3	D	1506	NAG	C1-O5-C5	3.31	116.67	112.19
3	B	802	NAG	C1-C2-N2	3.30	116.13	110.49
3	A	1509	NAG	C1-O5-C5	3.27	116.62	112.19
4	A	1510	6RL	C17-C23-C24	3.17	123.18	120.14
4	C	1506	6RL	N15-C26-N2	3.16	121.23	116.74
3	B	805	NAG	O5-C5-C6	3.02	111.93	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1503	NAG	O5-C1-C2	-2.96	106.61	111.29
4	B	808	6RL	C16-C17-C23	2.93	125.13	120.93
4	B	808	6RL	C10-C9-C8	-2.93	106.75	110.85
3	D	1506	NAG	C4-C3-C2	2.86	115.21	111.02
3	B	801	NAG	O7-C7-C8	-2.84	116.78	122.06
4	A	1510	6RL	N15-C26-N2	2.83	120.75	116.74
4	D	1507	6RL	C16-N15-C26	2.82	121.04	116.97
4	D	1507	6RL	N15-C26-N2	2.79	120.69	116.74
3	B	802	NAG	O5-C5-C4	2.71	117.42	110.83
3	D	1501	NAG	C4-C3-C2	-2.57	107.25	111.02
3	B	802	NAG	O5-C1-C2	-2.57	107.23	111.29
4	D	1507	6RL	C16-C17-C18	-2.55	115.84	120.38
4	B	808	6RL	C16-C17-C18	-2.52	115.89	120.38
3	B	801	NAG	C4-C3-C2	-2.43	107.46	111.02
3	A	1508	NAG	C1-O5-C5	2.42	115.47	112.19
3	C	1504	NAG	O5-C5-C6	2.41	110.99	107.20
4	B	808	6RL	O4-C3-C5	-2.41	119.55	125.72
4	A	1510	6RL	O27-C26-N15	-2.38	118.69	121.99
4	B	808	6RL	C8-N7-C6	-2.36	110.16	117.55
4	D	1507	6RL	C10-C11-C14	-2.35	107.63	110.65
3	C	1505	NAG	C3-C4-C5	2.32	114.38	110.24
4	A	1510	6RL	C1-N2-C26	2.26	121.28	117.31
4	B	808	6RL	N15-C26-N2	2.26	119.95	116.74
4	C	1506	6RL	C21-C19-C18	-2.24	120.38	123.29
4	C	1506	6RL	C17-C23-C24	2.21	122.26	120.14
4	B	808	6RL	O27-C26-N15	-2.20	118.93	121.99
4	C	1506	6RL	C16-N15-C26	2.17	120.10	116.97
4	A	1510	6RL	C9-C10-C11	-2.17	109.13	111.87
4	A	1510	6RL	C10-C9-C8	-2.15	107.84	110.85
3	C	1501	NAG	O7-C7-C8	-2.15	118.07	122.06
3	A	1503	NAG	O3-C3-C4	-2.14	105.39	110.35
3	D	1505	NAG	C4-C3-C2	2.12	114.13	111.02
3	B	802	NAG	C3-C4-C5	2.12	114.03	110.24
3	D	1502	NAG	O7-C7-C8	-2.12	118.12	122.06
4	A	1510	6RL	O4-C3-C5	-2.12	120.30	125.72
4	D	1507	6RL	C16-C17-C23	2.11	123.95	120.93
3	A	1503	NAG	O6-C6-C5	-2.08	104.15	111.29
4	D	1507	6RL	C18-C17-C23	2.07	120.21	117.80
3	A	1503	NAG	O7-C7-C8	-2.06	118.22	122.06
3	A	1503	NAG	C3-C4-C5	-2.06	106.57	110.24
4	D	1507	6RL	O4-C3-C5	-2.01	120.58	125.72
4	D	1507	6RL	O27-C26-N2	-2.00	118.52	121.34

There are no chirality outliers.

All (34) torsion outliers are listed below:

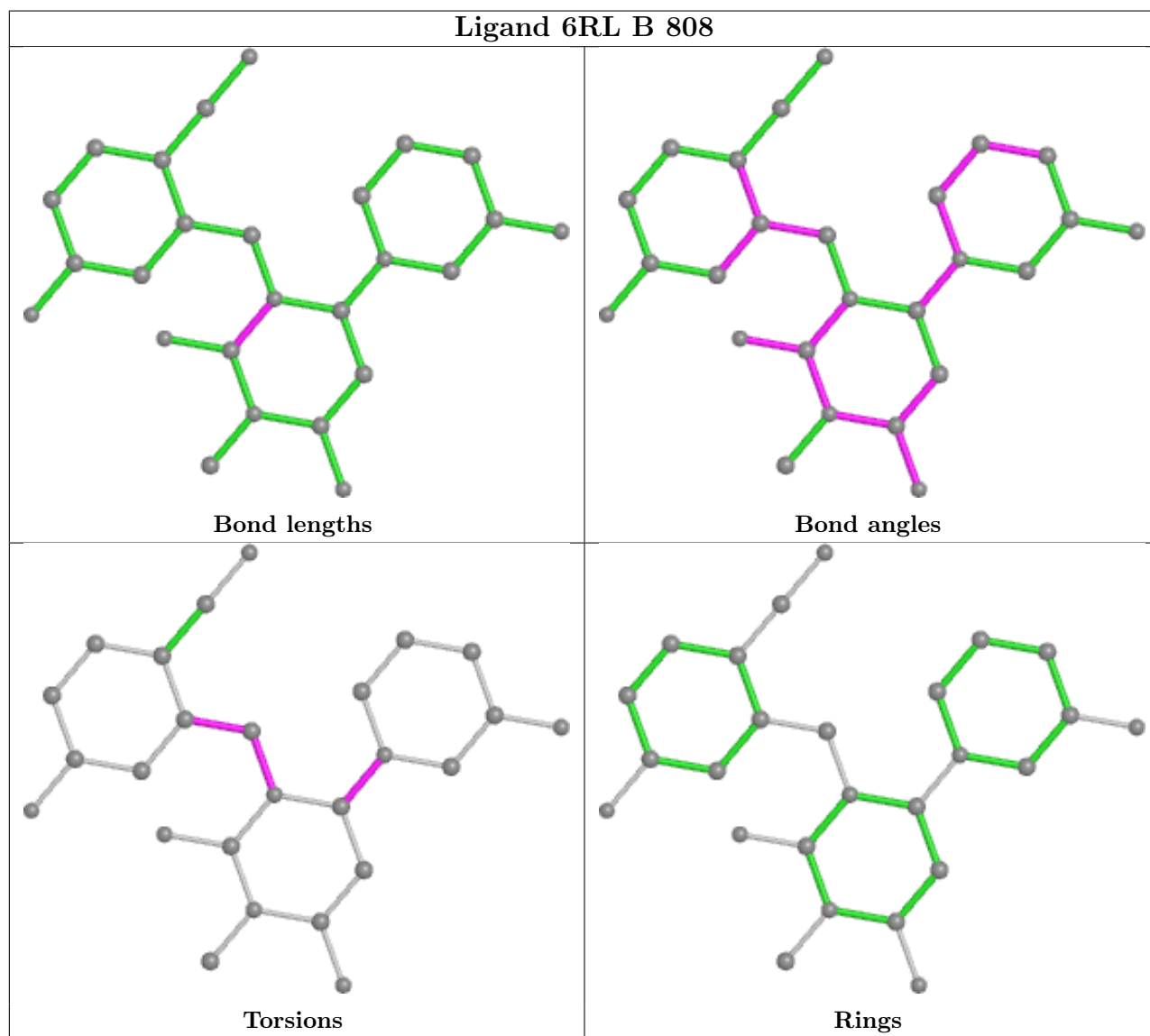
Mol	Chain	Res	Type	Atoms
3	A	1509	NAG	C4-C5-C6-O6
3	C	1505	NAG	C1-C2-N2-C7
3	C	1504	NAG	O5-C5-C6-O6
3	A	1509	NAG	O5-C5-C6-O6
3	B	801	NAG	O5-C5-C6-O6
3	C	1504	NAG	C4-C5-C6-O6
3	B	805	NAG	C4-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
3	B	801	NAG	C8-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	C	1501	NAG	C8-C7-N2-C2
3	C	1501	NAG	O7-C7-N2-C2
3	B	805	NAG	O5-C5-C6-O6
4	D	1507	6RL	C17-C16-N15-C26
4	D	1507	6RL	C17-C16-N15-C6
3	C	1501	NAG	C4-C5-C6-O6
4	A	1510	6RL	C17-C16-N15-C6
4	C	1506	6RL	C17-C16-N15-C6
4	C	1506	6RL	C17-C16-N15-C26
3	B	802	NAG	C3-C2-N2-C7
4	B	808	6RL	C17-C16-N15-C6
4	A	1510	6RL	C17-C16-N15-C26
4	C	1506	6RL	N15-C16-C17-C23
4	B	808	6RL	C17-C16-N15-C26
3	C	1505	NAG	C3-C2-N2-C7
3	D	1501	NAG	C3-C2-N2-C7
4	B	808	6RL	C5-C6-N7-C8
4	C	1506	6RL	C5-C6-N7-C8
4	C	1506	6RL	C5-C6-N7-C14
4	D	1507	6RL	C5-C6-N7-C8
4	B	808	6RL	N15-C16-C17-C23
3	C	1501	NAG	O5-C5-C6-O6
3	B	806	NAG	C4-C5-C6-O6
4	A	1510	6RL	N15-C16-C17-C23

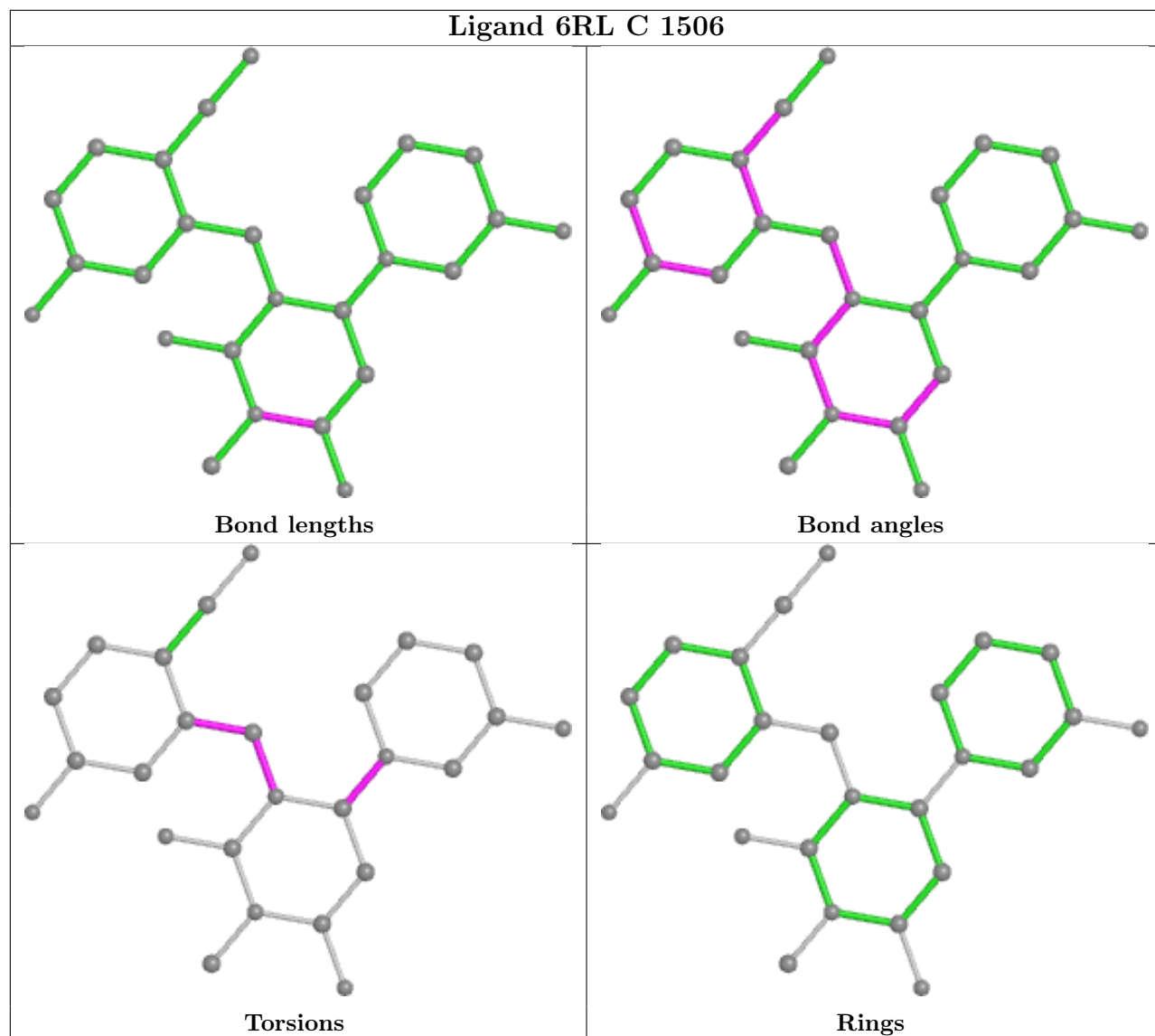
There are no ring outliers.

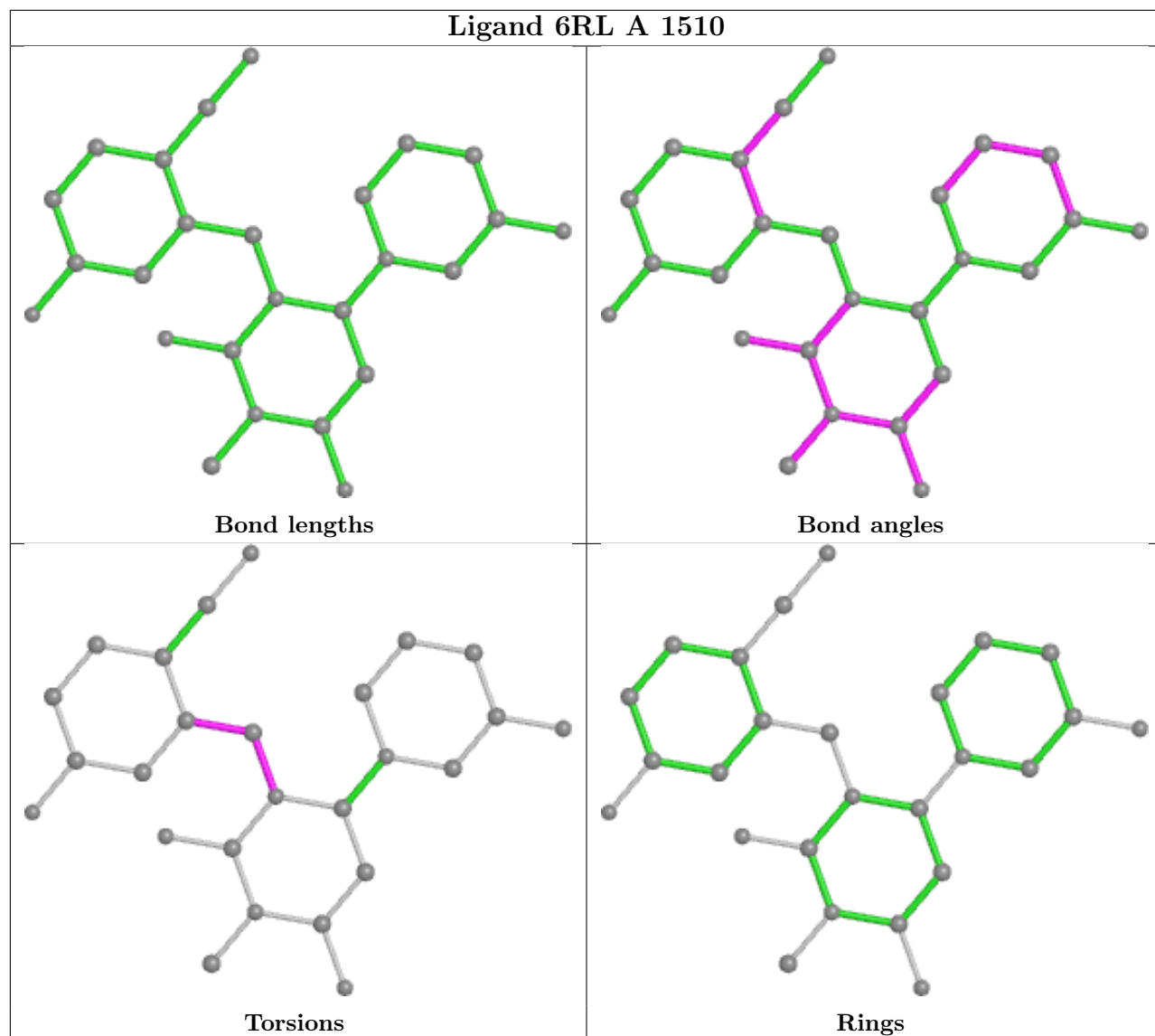
1 monomer is involved in 1 short contact:

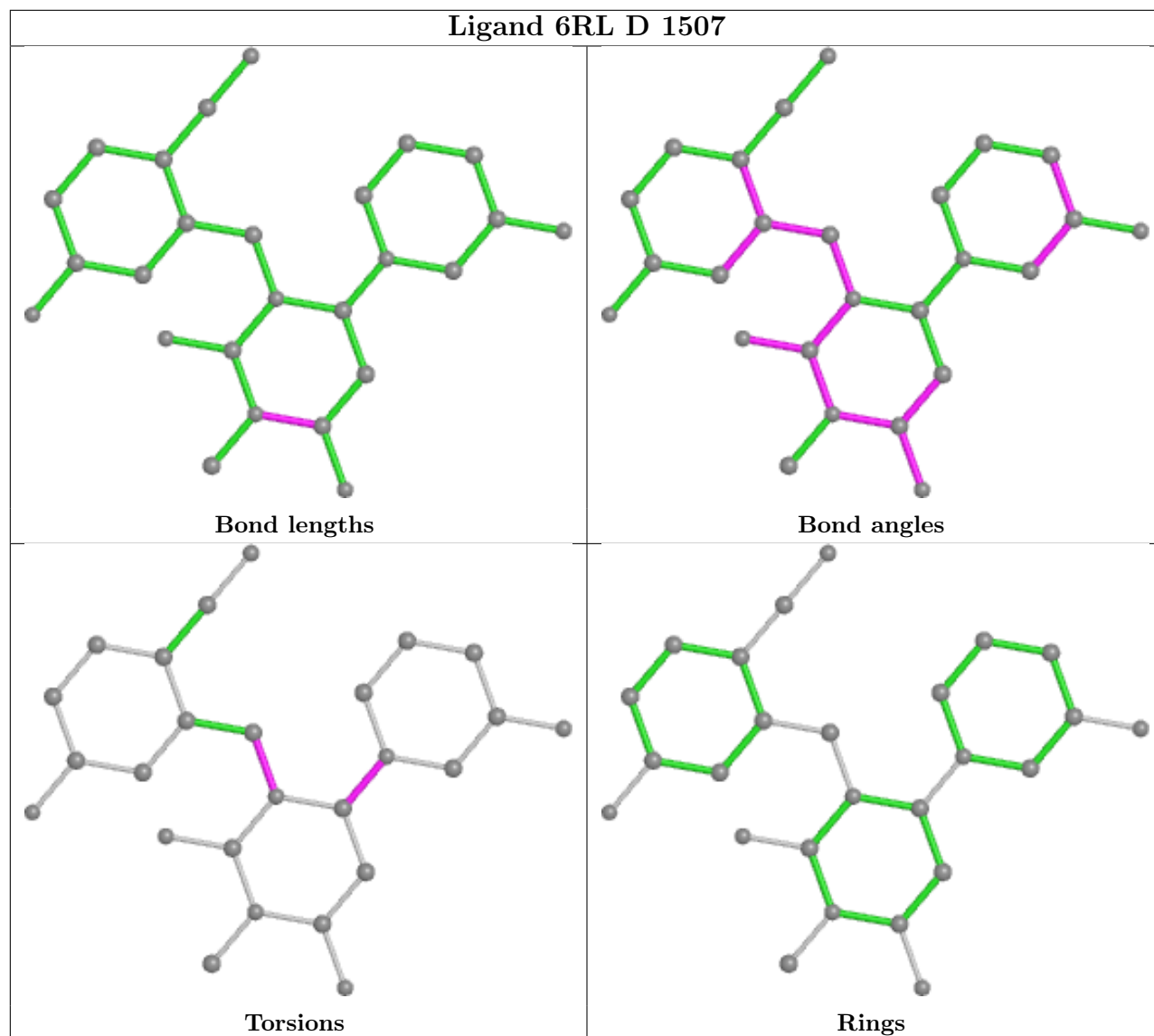
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1509	NAG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	725/740 (97%)	0.03	32 (4%) 34 34	23, 43, 88, 137	0
1	B	733/740 (99%)	-0.23	11 (1%) 73 74	23, 42, 74, 108	0
1	C	717/740 (96%)	0.20	54 (7%) 14 13	24, 55, 102, 135	0
1	D	725/740 (97%)	0.04	29 (4%) 38 38	22, 48, 94, 124	0
All	All	2900/2960 (97%)	0.01	126 (4%) 35 34	22, 46, 92, 137	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	GLU	7.4
1	D	81	ALA	6.3
1	C	77	LEU	6.0
1	A	81	ALA	5.9
1	C	335	GLY	5.6
1	A	96	ASP	5.5
1	A	86	SER	5.5
1	D	84	GLY	5.2
1	D	89	PHE	5.1
1	A	88	VAL	4.9
1	D	83	TYR	4.8
1	A	89	PHE	4.8
1	C	439	TYR	4.6
1	C	89	PHE	4.6
1	D	487	ASN	4.5
1	A	97	GLU	4.5
1	D	279	VAL	4.4
1	A	98	PHE	4.4
1	D	70	TYR	4.4
1	C	392	LYS	4.4
1	B	83	TYR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	76	ILE	4.3
1	C	330	TYR	4.3
1	C	88	VAL	4.2
1	C	96	ASP	4.2
1	C	99	GLY	4.1
1	B	87	SER	4.1
1	A	93	SER	4.1
1	D	87	SER	4.1
1	A	279	VAL	4.0
1	A	90	LEU	4.0
1	C	766	PRO	4.0
1	B	70	TYR	3.9
1	C	81	ALA	3.9
1	C	100	HIS	3.8
1	A	99	GLY	3.8
1	A	87	SER	3.7
1	C	412	SER	3.7
1	A	72	GLN	3.7
1	D	490	GLY	3.6
1	C	78	VAL	3.6
1	A	140	ARG	3.5
1	C	333	SER	3.5
1	A	95	PHE	3.5
1	D	93	SER	3.4
1	D	78	VAL	3.4
1	B	73	GLU	3.3
1	C	98	PHE	3.3
1	C	464	GLU	3.3
1	A	332	GLU	3.3
1	C	332	GLU	3.3
1	D	489	LYS	3.2
1	D	79	PHE	3.1
1	D	537	SER	3.1
1	C	331	ASP	3.1
1	A	138	ASN	3.1
1	B	521	GLU	3.1
1	D	96	ASP	3.1
1	C	415	LEU	3.1
1	C	414	TYR	3.0
1	A	92	ASN	3.0
1	D	141	GLN	3.0
1	C	83	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	34	HIS	2.9
1	D	280	THR	2.9
1	D	95	PHE	2.8
1	D	140	ARG	2.8
1	A	77	LEU	2.8
1	A	766	PRO	2.8
1	D	491	LEU	2.8
1	C	105	TYR	2.8
1	A	467	TYR	2.7
1	B	766	PRO	2.7
1	C	274	ASP	2.7
1	C	40	ARG	2.6
1	C	413	ASP	2.6
1	B	72	GLN	2.6
1	C	79	PHE	2.5
1	A	135	TYR	2.5
1	A	91	GLU	2.5
1	C	656	VAL	2.5
1	C	441	LYS	2.5
1	C	90	LEU	2.5
1	A	333	SER	2.4
1	C	338	ASN	2.4
1	A	141	GLN	2.4
1	D	100	HIS	2.4
1	C	521	GLU	2.4
1	D	72	GLN	2.4
1	D	332	GLU	2.4
1	C	677	GLU	2.4
1	A	100	HIS	2.3
1	C	279	VAL	2.3
1	C	676	PRO	2.3
1	A	101	SER	2.3
1	D	97	GLU	2.3
1	C	468	TYR	2.3
1	C	280	THR	2.2
1	C	102	ILE	2.2
1	C	436	LEU	2.2
1	C	467	TYR	2.2
1	D	488	ASP	2.2
1	A	156	THR	2.2
1	B	81	ALA	2.2
1	C	135	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	393	ASP	2.2
1	C	466	LYS	2.1
1	A	63	ILE	2.1
1	C	58	TYR	2.1
1	C	435	GLN	2.1
1	C	303	VAL	2.1
1	A	84	GLY	2.1
1	B	38	HIS	2.1
1	C	386	TYR	2.1
1	C	416	TYR	2.1
1	A	336	ARG	2.1
1	B	546	VAL	2.1
1	D	88	VAL	2.1
1	D	101	SER	2.1
1	A	94	THR	2.0
1	C	440	THR	2.0
1	D	138	ASN	2.0
1	D	467	TYR	2.0
1	C	340	LEU	2.0
1	C	141	GLN	2.0
1	C	329	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

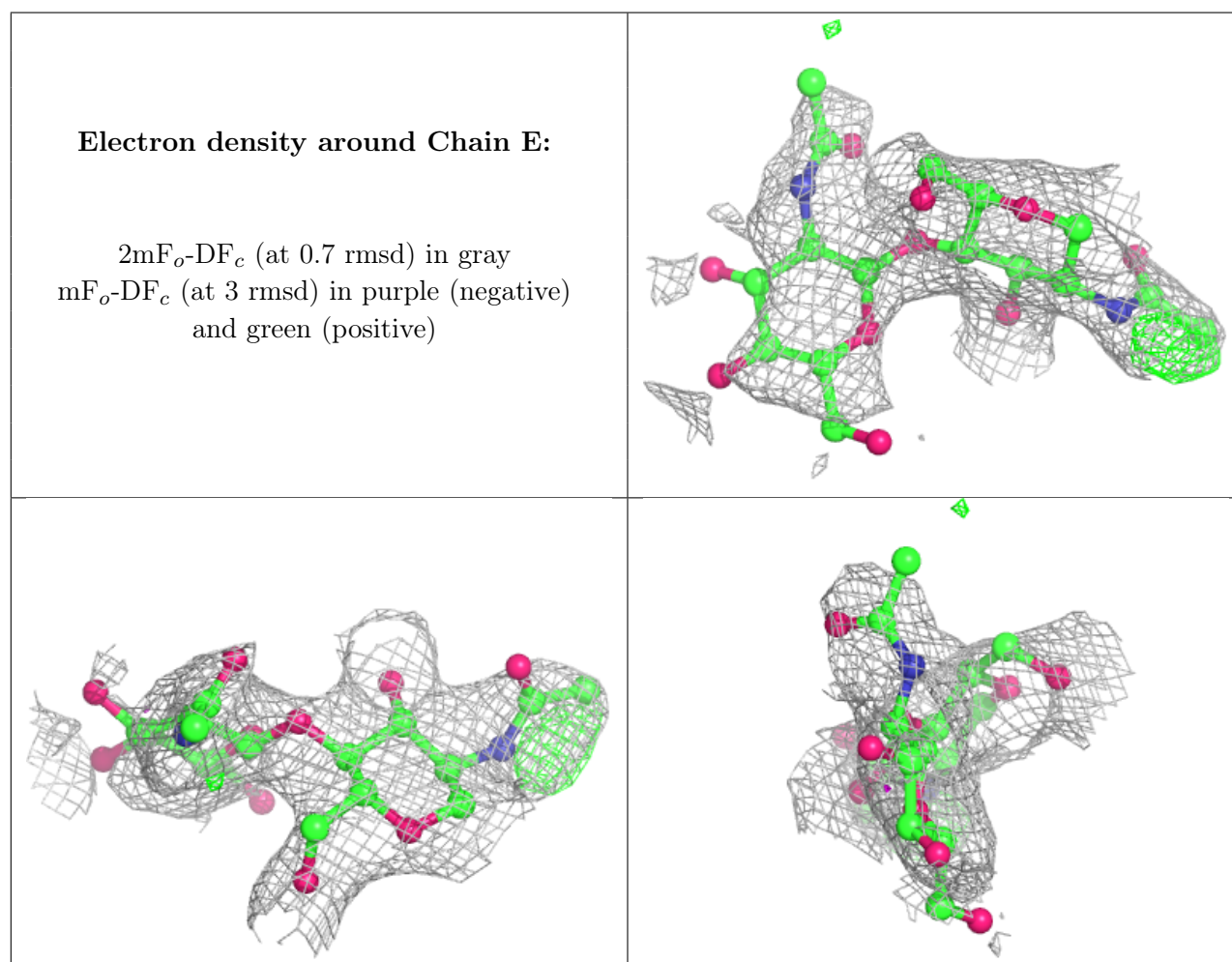
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	1	14/15	0.65	0.31	75,86,99,114	0
2	NAG	E	2	14/15	0.73	0.47	101,120,128,132	0
2	NAG	H	2	14/15	0.77	0.25	62,85,99,105	0
2	NAG	J	2	14/15	0.82	0.36	60,93,108,112	0
2	NAG	G	2	14/15	0.86	0.23	88,93,99,102	0
2	NAG	F	2	14/15	0.87	0.28	59,69,73,75	0
2	NAG	G	1	14/15	0.89	0.16	60,80,91,92	0

Continued on next page...

Continued from previous page...

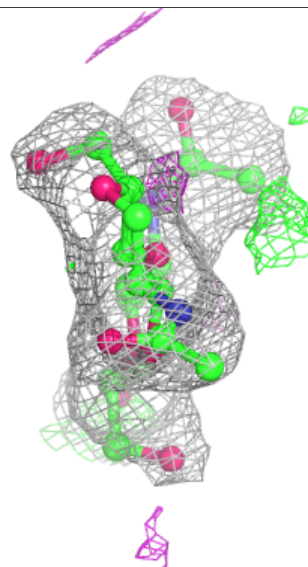
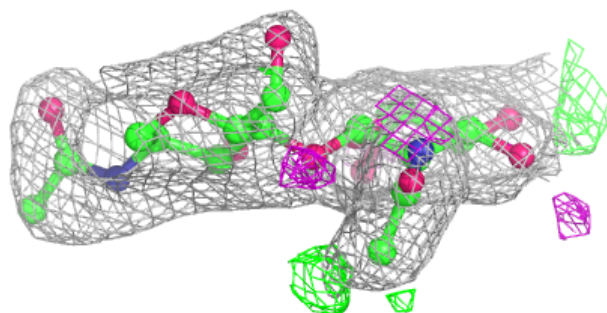
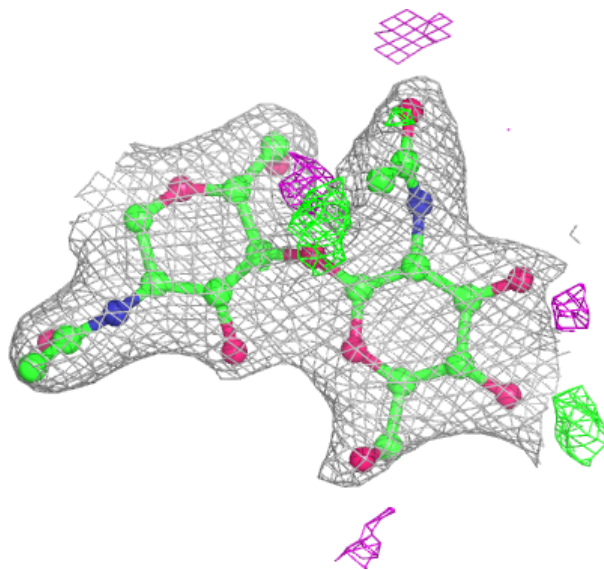
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	I	2	14/15	0.92	0.17	50,58,67,69	0
2	NAG	J	1	14/15	0.94	0.12	47,54,68,71	0
2	NAG	H	1	14/15	0.95	0.11	44,54,63,74	0
2	NAG	I	1	14/15	0.96	0.08	37,47,54,58	0
2	NAG	F	1	14/15	0.96	0.19	40,46,58,60	0

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.



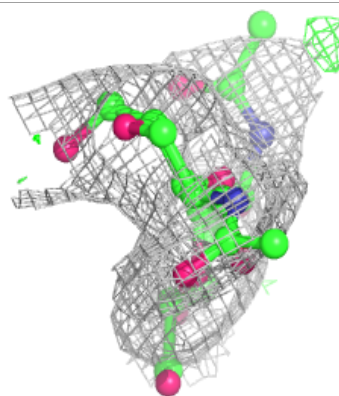
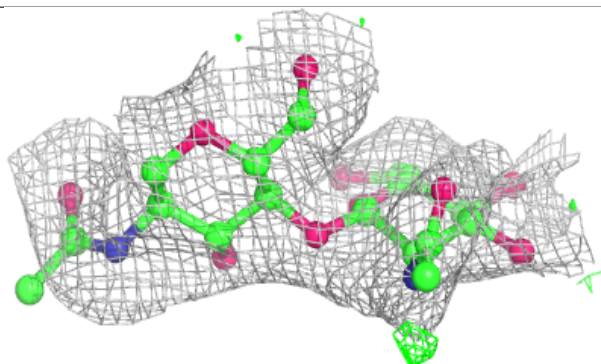
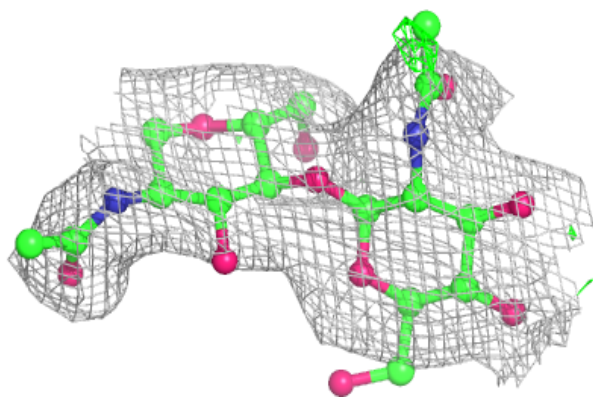
Electron density around Chain F:

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

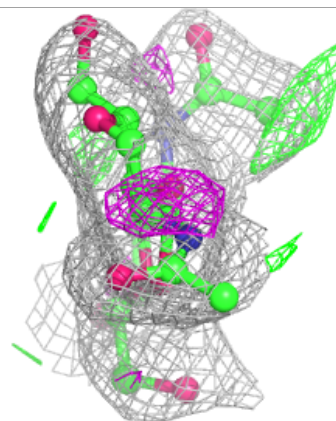
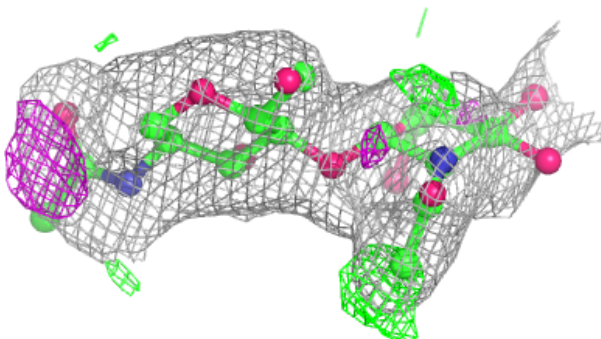
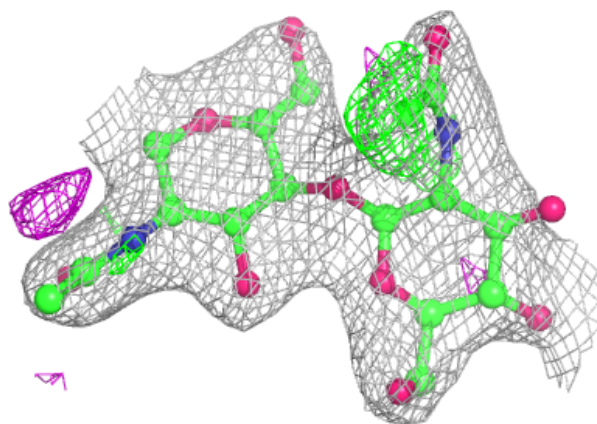


Electron density around Chain G:

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

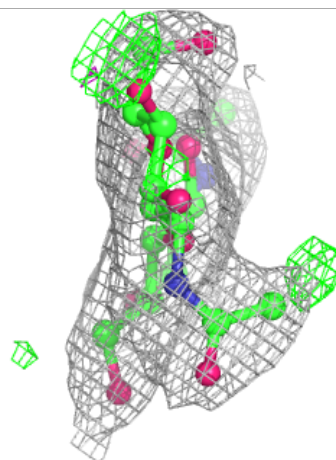
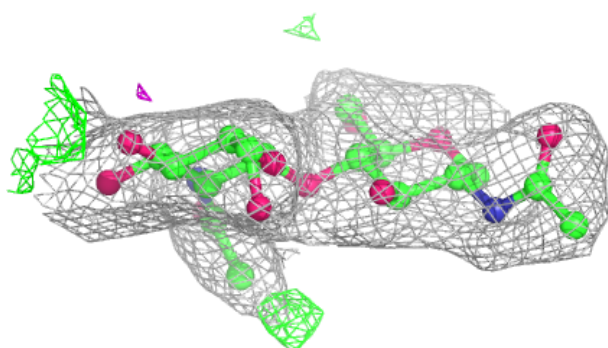
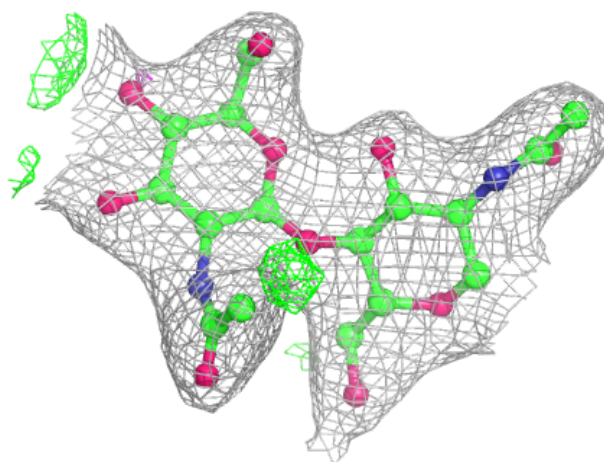
**Electron density around Chain H:**

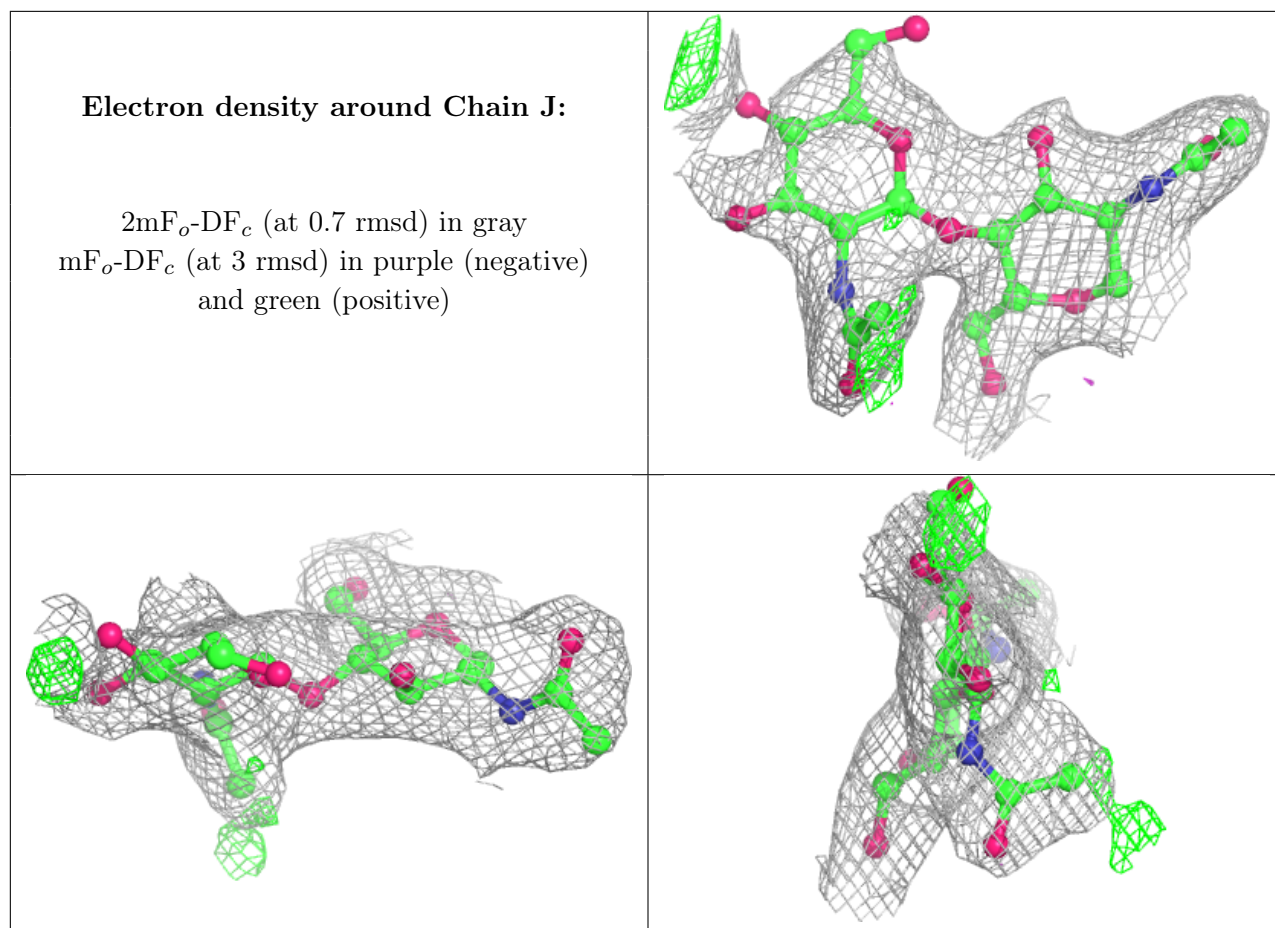
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





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
3	NAG	A	1509	14/15	0.66	0.23	99,115,122,124	0
3	NAG	C	1505	14/15	0.68	0.32	76,87,98,106	0
3	NAG	C	1501	14/15	0.71	0.17	64,74,83,85	0
3	NAG	B	801	14/15	0.73	0.19	69,85,94,94	0
3	NAG	D	1505	14/15	0.74	0.19	74,84,91,96	0
3	NAG	B	806	14/15	0.79	0.35	67,76,80,82	0
3	NAG	A	1503	14/15	0.79	0.38	35,40,50,51	0
3	NAG	B	805	14/15	0.81	0.16	64,71,78,79	0
3	NAG	C	1504	14/15	0.81	0.15	61,83,107,108	0
3	NAG	D	1501	14/15	0.82	0.24	66,77,88,89	0
3	NAG	B	802	14/15	0.86	0.22	56,63,67,71	0
3	NAG	B	807	14/15	0.88	0.28	54,65,72,75	0

Continued on next page...

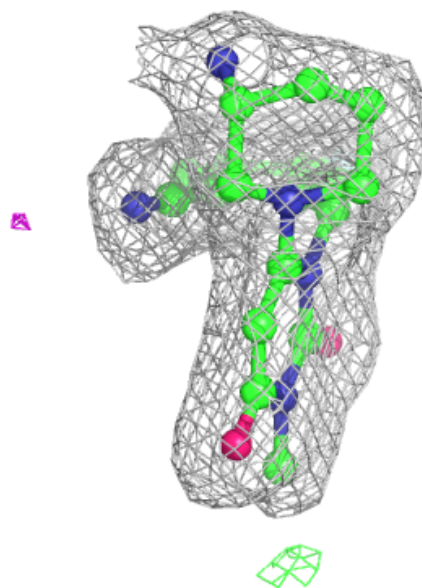
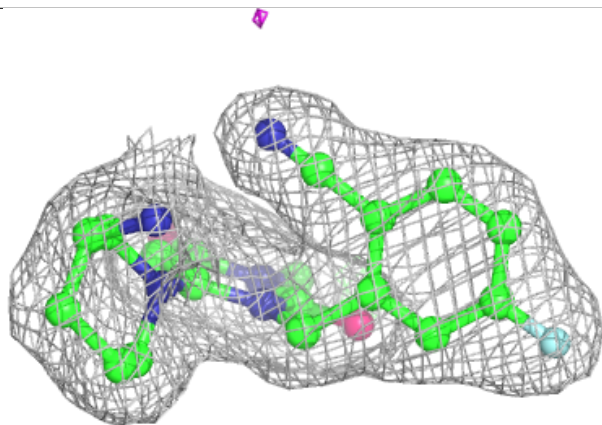
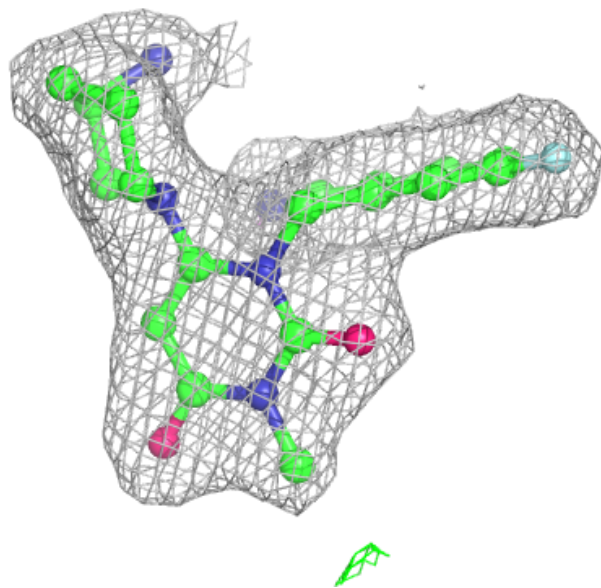
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	1502	14/15	0.89	0.31	60,68,81,85	0
3	NAG	D	1506	14/15	0.89	0.23	64,79,86,87	0
3	NAG	A	1508	14/15	0.90	0.20	59,69,73,79	0
4	6RL	A	1510	26/26	0.97	0.15	24,27,30,33	0
4	6RL	D	1507	26/26	0.97	0.12	22,28,32,37	0
4	6RL	C	1506	26/26	0.98	0.14	26,30,34,36	0
4	6RL	B	808	26/26	0.98	0.14	19,26,31,33	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.

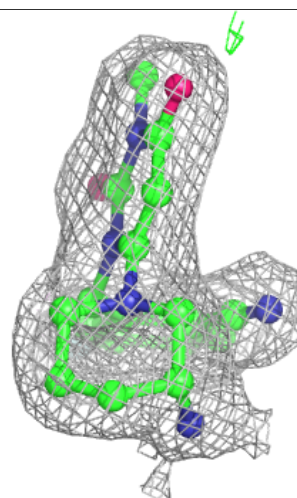
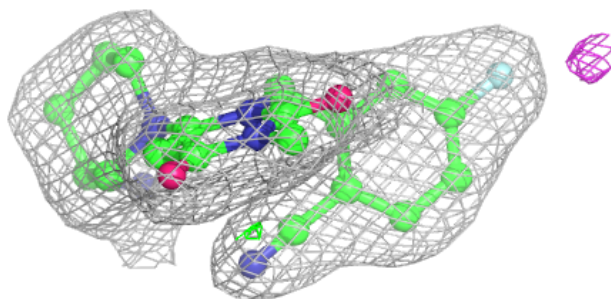
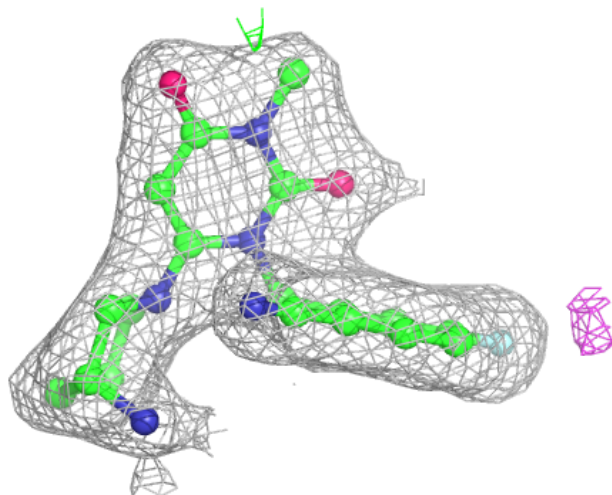
Electron density around 6RL A 1510:

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



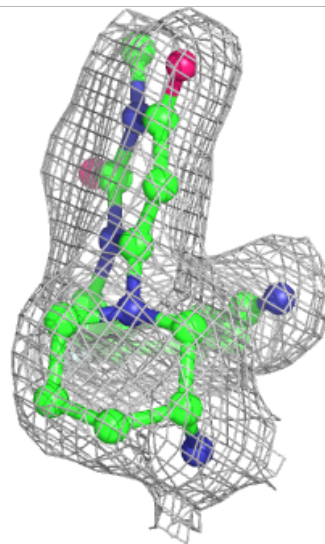
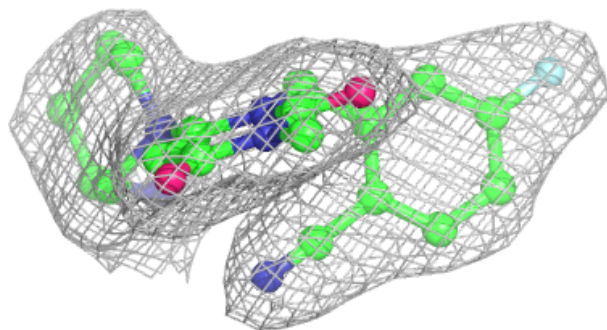
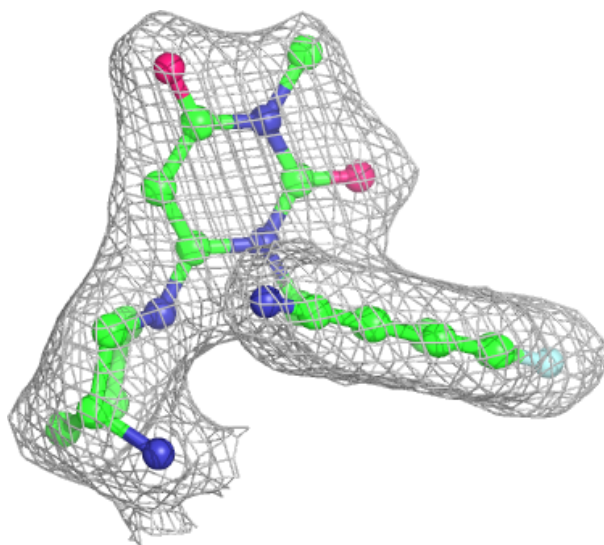
Electron density around 6RL D 1507:

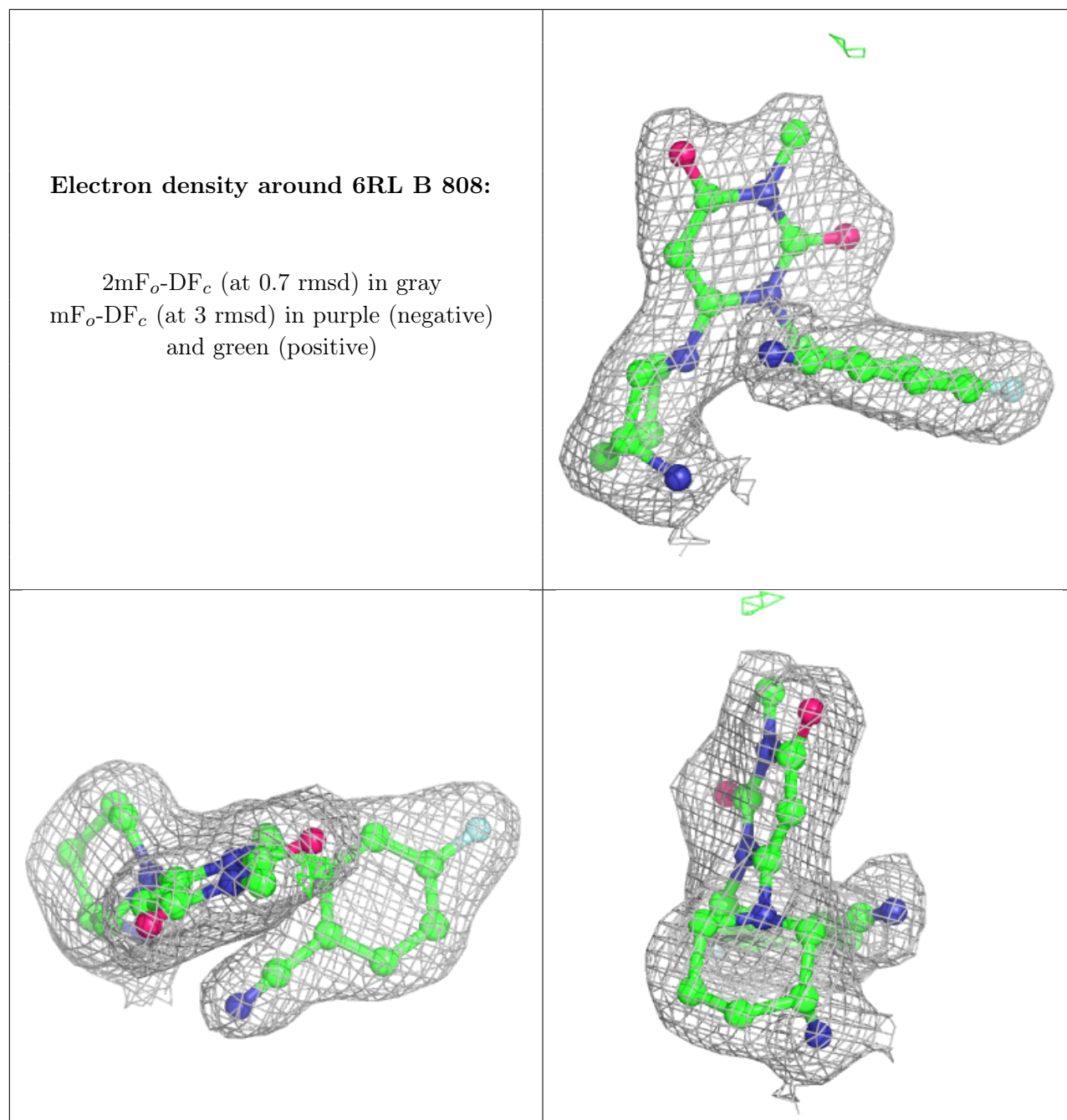
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6RL C 1506:

$2mF_o-DF_c$ (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.