



# Full wwPDB X-ray Structure Validation Report i

Jan 13, 2024 – 07:43 pm GMT

PDB ID : 6RW3  
Title : The molecular basis for sugar import in malaria parasites.  
Authors : Qureshi, A.; Matsuoka, R.; Brock, J.; Drew, D.  
Deposited on : 2019-06-03  
Resolution : 3.65 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](mailto: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 i symbol.

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

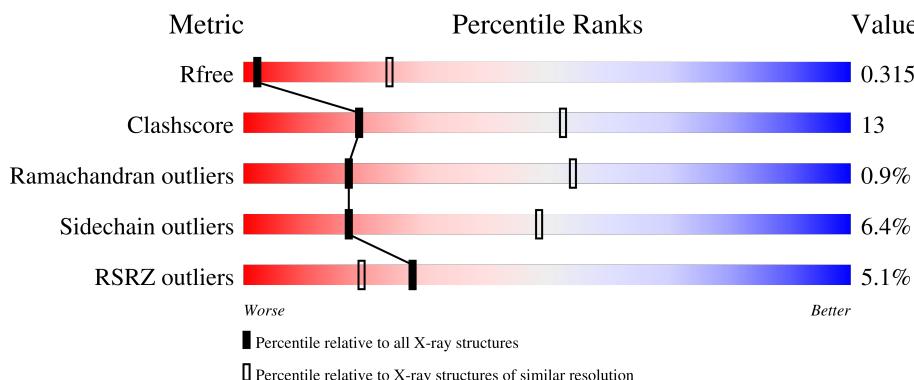
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

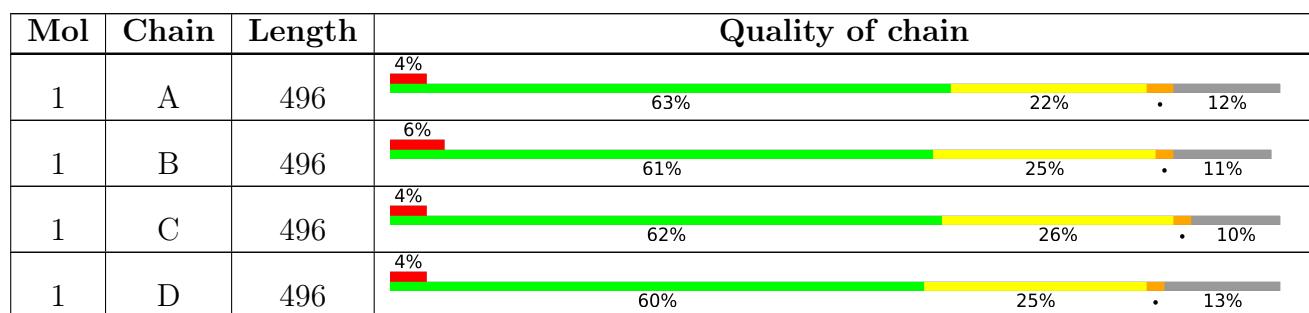
The reported resolution of this entry is 3.65 Å.

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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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  $\geq 3$ , 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.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14004 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 Hexose transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C 3462	N 2325	O 525	S 595	17	0	0
1	B	439	Total	C 3481	N 2339	O 529	S 596	17	0	0
1	C	447	Total	C 3548	N 2378	O 542	S 610	18	0	0
1	D	430	Total	C 3417	N 2302	O 516	S 583	16	0	0

There are 44 discrepancies between the modelled and reference sequences:

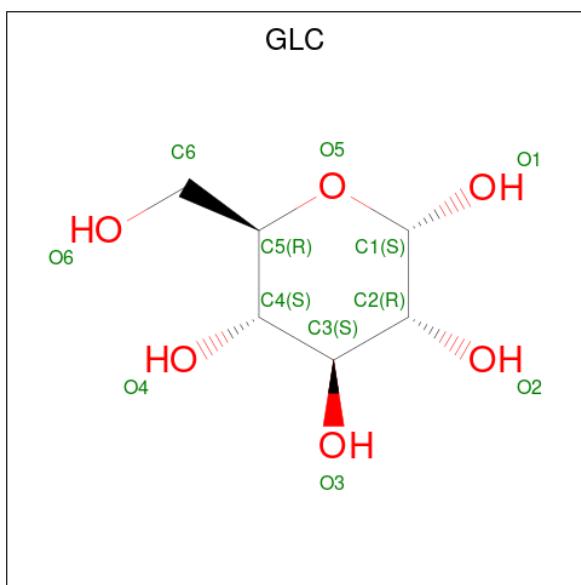
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP O97467
A	16	GLU	-	expression tag	UNP O97467
A	17	LYS	-	expression tag	UNP O97467
A	18	GLU	-	expression tag	UNP O97467
A	19	ASP	-	expression tag	UNP O97467
A	505	GLU	-	expression tag	UNP O97467
A	506	ASN	-	expression tag	UNP O97467
A	507	LEU	-	expression tag	UNP O97467
A	508	TYR	-	expression tag	UNP O97467
A	509	PHE	-	expression tag	UNP O97467
A	510	GLN	-	expression tag	UNP O97467
B	15	MET	-	initiating methionine	UNP O97467
B	16	GLU	-	expression tag	UNP O97467
B	17	LYS	-	expression tag	UNP O97467
B	18	GLU	-	expression tag	UNP O97467
B	19	ASP	-	expression tag	UNP O97467
B	505	GLU	-	expression tag	UNP O97467
B	506	ASN	-	expression tag	UNP O97467
B	507	LEU	-	expression tag	UNP O97467
B	508	TYR	-	expression tag	UNP O97467
B	509	PHE	-	expression tag	UNP O97467

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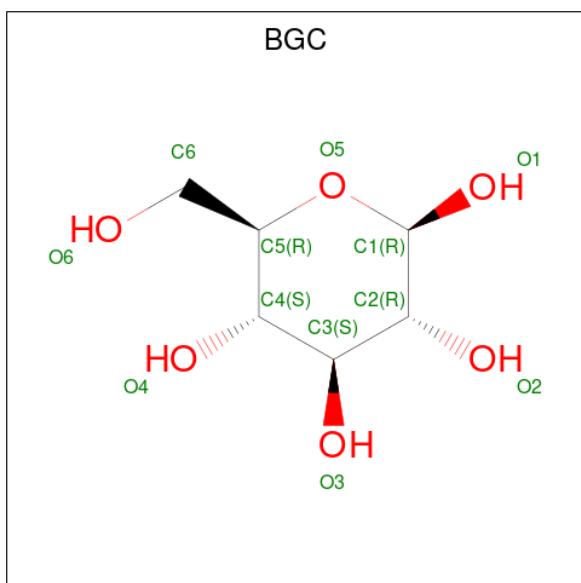
Chain	Residue	Modelled	Actual	Comment	Reference
B	510	GLN	-	expression tag	UNP O97467
C	15	MET	-	initiating methionine	UNP O97467
C	16	GLU	-	expression tag	UNP O97467
C	17	LYS	-	expression tag	UNP O97467
C	18	GLU	-	expression tag	UNP O97467
C	19	ASP	-	expression tag	UNP O97467
C	505	GLU	-	expression tag	UNP O97467
C	506	ASN	-	expression tag	UNP O97467
C	507	LEU	-	expression tag	UNP O97467
C	508	TYR	-	expression tag	UNP O97467
C	509	PHE	-	expression tag	UNP O97467
C	510	GLN	-	expression tag	UNP O97467
D	15	MET	-	initiating methionine	UNP O97467
D	16	GLU	-	expression tag	UNP O97467
D	17	LYS	-	expression tag	UNP O97467
D	18	GLU	-	expression tag	UNP O97467
D	19	ASP	-	expression tag	UNP O97467
D	505	GLU	-	expression tag	UNP O97467
D	506	ASN	-	expression tag	UNP O97467
D	507	LEU	-	expression tag	UNP O97467
D	508	TYR	-	expression tag	UNP O97467
D	509	PHE	-	expression tag	UNP O97467
D	510	GLN	-	expression tag	UNP O97467

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	1
2	B	1	Total C O 12 6 6	0	1
2	C	1	Total C O 12 6 6	0	1
2	D	1	Total C O 12 6 6	0	1

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

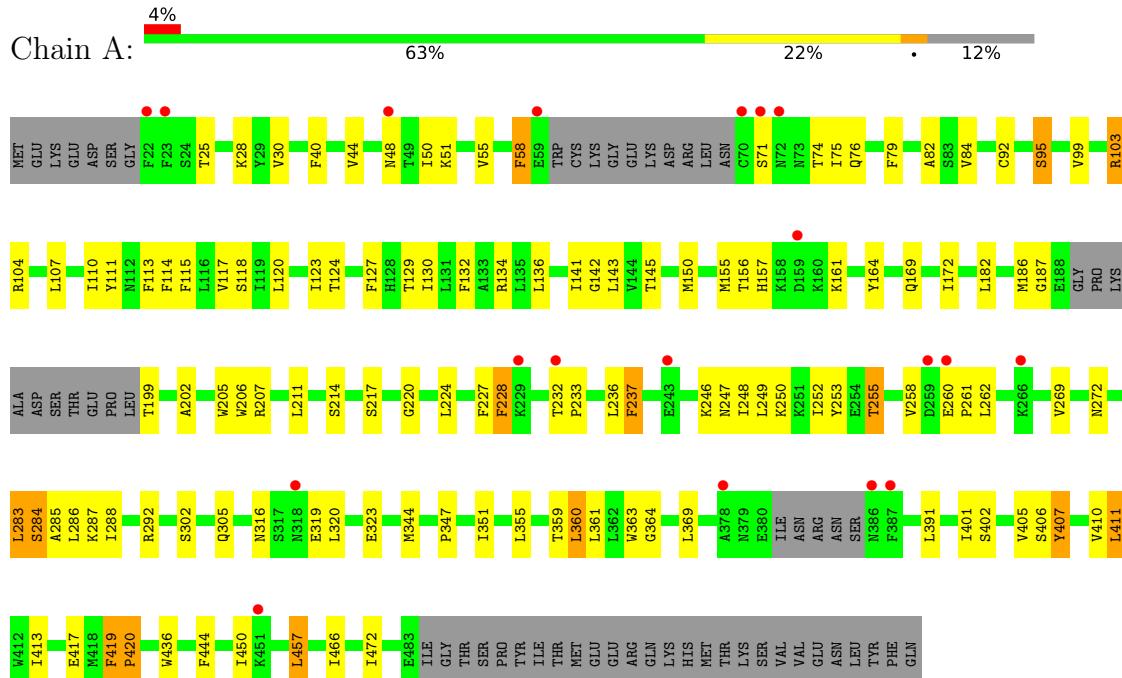


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	1
3	B	1	Total C O 12 6 6	0	1
3	C	1	Total C O 12 6 6	0	1
3	D	1	Total C O 12 6 6	0	1

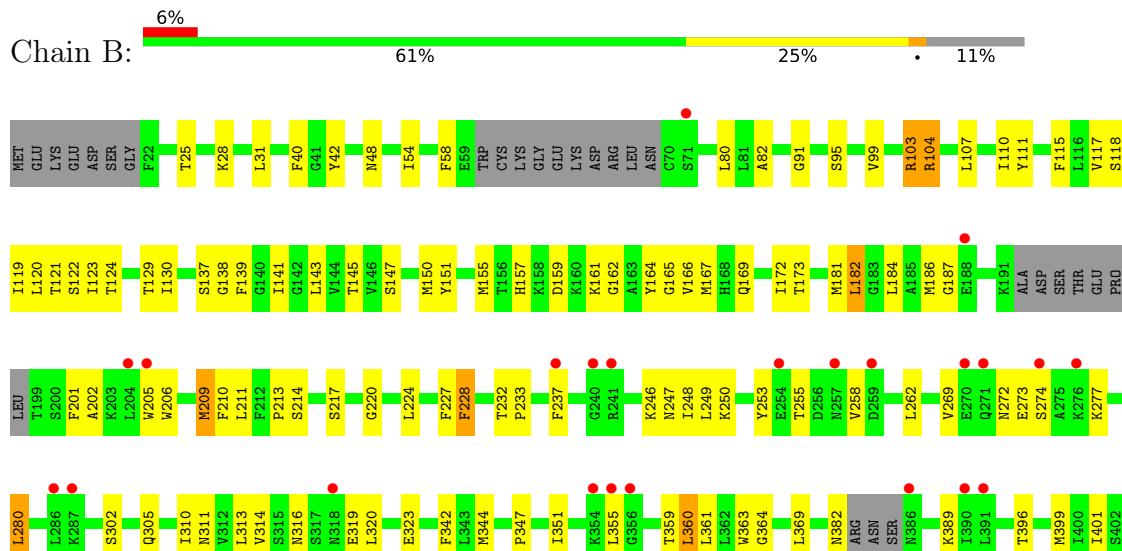
### 3 Residue-property plots

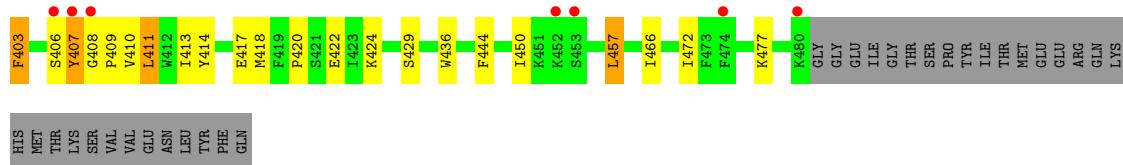
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Hexose transporter 1

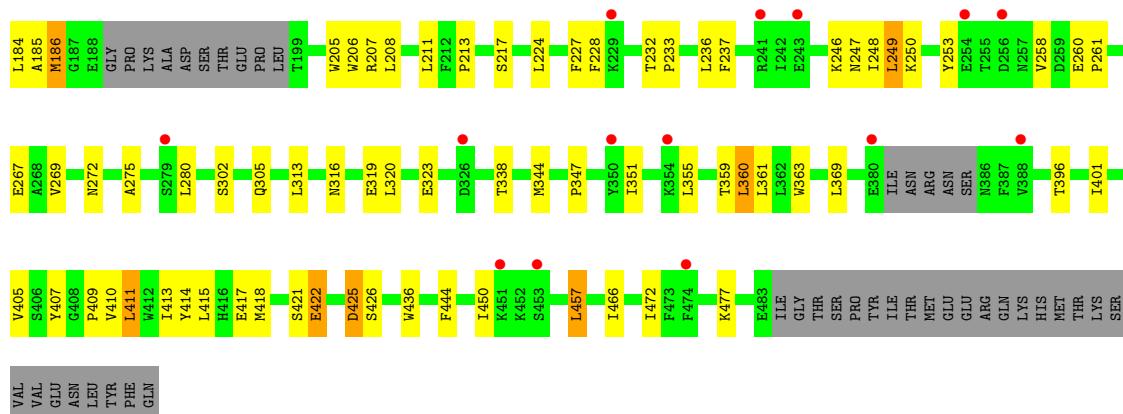


- Molecule 1: Hexose transporter 1

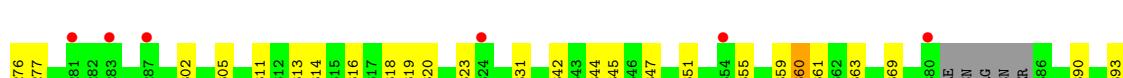
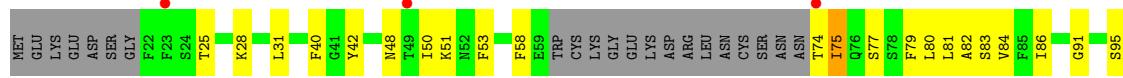




- Molecule 1: Hexose transporter 1



- Molecule 1: Hexose transporter 1



THR  
LYS  
SER  
VAL  
GLU  
ASN  
LEU  
TYR  
PHE  
GLN

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.74 Å    189.45 Å    136.89 Å 90.00°    96.43°    90.00°	Depositor
Resolution (Å)	21.85 – 3.65 21.85 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.85-3.65) 100.0 (21.85-3.65)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.10 (at 3.63 Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
$R$ , $R_{free}$	0.273 , 0.284 0.304 , 0.315	Depositor DCC
$R_{free}$ test set	2114 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	178.2	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 188.1	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.42$ , $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	230.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, BGC

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	0.40	0/3545	0.59	0/4802
1	B	0.39	0/3565	0.57	0/4830
1	C	0.43	0/3634	0.61	0/4922
1	D	0.40	0/3500	0.59	0/4742
All	All	0.41	0/14244	0.59	0/19296

There are no bond length outliers.

There are no bond angle outliers.

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	3462	0	3586	92	0
1	B	3481	0	3614	99	0
1	C	3548	0	3671	93	0
1	D	3417	0	3552	97	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	12	0	0
3	C	12	0	12	0	0
3	D	12	0	12	0	0
All	All	14004	0	14519	372	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 13.

All (372) 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:421:SER:HA	1:D:424:LYS:HD2	1.30	1.10
1:A:302:SER:HA	1:A:411:LEU:HD11	1.29	1.06
1:C:302:SER:HA	1:C:411:LEU:HD11	1.40	1.00
1:A:284:SER:HA	1:A:287:LYS:HD2	1.42	0.99
1:D:51:LYS:NZ	1:D:81:LEU:HD11	1.79	0.95
1:B:399:MET:O	1:B:403:PHE:HB2	1.68	0.94
1:C:59:GLU:OE1	1:C:73:ASN:ND2	2.02	0.92
1:C:92:CYS:SG	1:C:436:TRP:CD1	2.63	0.91
1:A:124:THR:HG21	1:A:206:TRP:HH2	1.39	0.88
1:C:92:CYS:SG	1:C:436:TRP:HD1	1.97	0.87
1:B:277:LYS:HD2	1:B:422:GLU:HB2	1.56	0.86
1:C:161:LYS:NZ	1:C:417:GLU:HG3	1.90	0.86
1:B:201:PHE:O	1:B:205:TRP:HD1	1.60	0.84
1:B:310:ILE:HB	1:B:403:PHE:HZ	1.41	0.84
1:D:42:TYR:HE2	1:D:182:LEU:HD12	1.41	0.84
1:D:276:LYS:NZ	1:D:277:LYS:HZ1	1.77	0.83
1:D:103:ARG:HA	1:D:106:SER:OG	1.78	0.82
1:D:276:LYS:NZ	1:D:277:LYS:NZ	2.28	0.82
1:D:51:LYS:HZ1	1:D:81:LEU:HD11	1.41	0.81
1:D:276:LYS:HZ3	1:D:277:LYS:HZ1	1.23	0.81
1:A:258:VAL:CG1	1:A:261:PRO:HD2	2.11	0.79
1:A:199:THR:OG1	1:A:202:ALA:HB2	1.83	0.78
1:B:258:VAL:HG12	1:B:262:LEU:HG	1.64	0.78
1:B:310:ILE:HB	1:B:403:PHE:CZ	2.18	0.78
1:D:51:LYS:NZ	1:D:81:LEU:CD1	2.48	0.77
1:B:124:THR:HG21	1:B:206:TRP:HH2	1.49	0.77
1:C:161:LYS:HZ2	1:C:417:GLU:HG3	1.50	0.76
1:A:258:VAL:HG13	1:A:261:PRO:HD2	1.67	0.75
1:A:199:THR:OG1	1:A:202:ALA:CB	2.35	0.75
1:D:81:LEU:CD2	1:D:134:ARG:HH21	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:NZ	1:B:417:GLU:HG3	2.03	0.74
1:C:103:ARG:NH2	1:C:425:ASP:OD2	2.20	0.74
1:D:421:SER:HA	1:D:424:LYS:CD	2.15	0.73
1:D:95:SER:HB3	1:D:143:LEU:HD12	1.69	0.73
1:B:182:LEU:HB3	1:B:209:MET:CE	2.19	0.73
1:B:145:THR:HG21	1:B:436:TRP:HE1	1.53	0.73
1:C:121:THR:HG23	1:C:133:ALA:HB1	1.70	0.72
1:A:249:LEU:HD23	1:A:252:ILE:HD12	1.72	0.72
1:C:414:TYR:CE2	1:C:418:MET:HG3	2.25	0.72
1:A:258:VAL:HG12	1:A:258:VAL:O	1.89	0.71
1:C:182:LEU:O	1:C:185:ALA:HB3	1.91	0.71
1:B:310:ILE:HG23	1:B:311:ASN:H	1.54	0.71
1:D:178:VAL:O	1:D:182:LEU:HG	1.91	0.71
1:D:184:LEU:HD11	1:D:318:ASN:HD21	1.57	0.69
1:A:246:LYS:HA	1:A:262:LEU:HD11	1.73	0.69
1:C:124:THR:HG21	1:C:206:TRP:HH2	1.57	0.69
1:D:249:LEU:HD23	1:D:252:ILE:HD12	1.73	0.69
1:D:258:VAL:HG13	1:D:261:PRO:HD2	1.76	0.68
1:C:63:GLY:O	1:C:64:GLU:HG3	1.94	0.68
1:A:258:VAL:HG13	1:A:261:PRO:CD	2.24	0.67
1:D:51:LYS:HZ3	1:D:81:LEU:CD1	2.07	0.67
1:C:182:LEU:HD23	1:C:182:LEU:N	2.09	0.67
1:B:186:MET:HE3	1:B:205:TRP:HB3	1.76	0.67
1:D:276:LYS:HZ2	1:D:277:LYS:NZ	1.92	0.66
1:D:42:TYR:CE2	1:D:182:LEU:HD12	2.28	0.66
1:D:184:LEU:HD22	1:D:331:THR:HG22	1.78	0.66
1:C:121:THR:CG2	1:C:133:ALA:HB1	2.25	0.65
1:A:161:LYS:NZ	1:A:417:GLU:HG3	2.11	0.65
1:B:302:SER:HA	1:B:411:LEU:HD11	1.76	0.65
1:C:249:LEU:HB3	1:C:258:VAL:HG21	1.79	0.65
1:D:83:SER:HA	1:D:86:ILE:HG12	1.79	0.64
1:A:50:ILE:HD13	1:A:206:TRP:HB2	1.79	0.64
1:A:224:LEU:HB3	1:A:228:PHE:HB2	1.78	0.64
1:A:255:THR:HG23	1:A:258:VAL:HG22	1.79	0.64
1:B:201:PHE:O	1:B:205:TRP:CD1	2.48	0.63
1:D:81:LEU:HD23	1:D:134:ARG:HH21	1.62	0.63
1:B:224:LEU:HB3	1:B:228:PHE:HB2	1.80	0.63
1:B:310:ILE:HG23	1:B:311:ASN:N	2.13	0.63
1:C:411:LEU:O	1:C:415:LEU:HB2	1.98	0.63
1:D:162:GLY:HA2	1:D:413:ILE:HG21	1.78	0.63
1:B:182:LEU:HB3	1:B:209:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLY:HA2	1:D:139:PHE:CD1	2.34	0.63
1:C:236:LEU:HD23	1:C:269:VAL:HG21	1.81	0.63
1:C:361:LEU:HB3	1:C:472:ILE:HD13	1.81	0.62
1:A:258:VAL:HG12	1:A:261:PRO:HD2	1.82	0.62
1:B:166:VAL:HG13	1:B:409:PRO:HB3	1.81	0.61
1:B:361:LEU:HB3	1:B:472:ILE:HD13	1.81	0.61
1:D:361:LEU:HB3	1:D:472:ILE:HD13	1.82	0.61
1:A:361:LEU:HG	1:A:410:VAL:HG11	1.83	0.61
1:B:311:ASN:HA	1:B:314:VAL:HB	1.83	0.61
1:B:403:PHE:O	1:B:407:TYR:HB2	2.01	0.61
1:B:409:PRO:O	1:B:413:ILE:HG12	2.01	0.61
1:D:302:SER:HA	1:D:411:LEU:HD11	1.83	0.61
1:B:129:THR:HG22	1:B:130:ILE:HD13	1.82	0.60
1:A:361:LEU:HB3	1:A:472:ILE:HD13	1.82	0.60
1:C:161:LYS:HZ1	1:C:417:GLU:HG3	1.65	0.60
1:A:129:THR:HG22	1:A:130:ILE:HD13	1.83	0.60
1:C:129:THR:HG22	1:C:130:ILE:HD13	1.83	0.60
1:C:155:MET:HB3	1:C:232:THR:HG22	1.83	0.60
1:D:155:MET:HB3	1:D:232:THR:HG22	1.83	0.60
1:D:236:LEU:HD23	1:D:269:VAL:HG21	1.82	0.60
1:B:182:LEU:HB3	1:B:209:MET:HE3	1.82	0.59
1:A:155:MET:HB3	1:A:232:THR:HG22	1.83	0.59
1:B:155:MET:HB3	1:B:232:THR:HG22	1.84	0.59
1:C:344:MET:O	1:C:405:VAL:HG22	2.03	0.58
1:B:137:SER:O	1:B:141:ILE:HG23	2.03	0.58
1:C:361:LEU:HG	1:C:410:VAL:HG11	1.84	0.58
1:D:344:MET:O	1:D:405:VAL:HG22	2.03	0.58
1:B:111:TYR:CE2	1:B:220:GLY:HA3	2.39	0.58
1:A:186:MET:HB2	1:A:205:TRP:CD1	2.39	0.57
1:C:33:ALA:HA	1:C:107:LEU:HD21	1.86	0.57
1:D:411:LEU:O	1:D:415:LEU:HB2	2.03	0.57
1:D:260:GLU:HB3	1:D:261:PRO:HD3	1.85	0.57
1:A:344:MET:O	1:A:405:VAL:HG22	2.05	0.57
1:C:120:LEU:HD11	1:D:120:LEU:HD11	1.86	0.56
1:A:246:LYS:HA	1:A:262:LEU:CD1	2.35	0.56
1:D:276:LYS:HZ2	1:D:277:LYS:HZ2	1.52	0.56
1:B:161:LYS:HZ1	1:B:417:GLU:HG3	1.70	0.56
1:C:91:GLY:HA2	1:C:139:PHE:CE1	2.41	0.55
1:D:129:THR:HG22	1:D:130:ILE:HD13	1.88	0.55
1:D:40:PHE:CD1	1:D:141:ILE:HB	2.41	0.55
1:C:110:ILE:HD12	1:C:144:VAL:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG13	1:A:261:PRO:HG2	1.87	0.55
1:C:36:ALA:HB2	1:C:111:TYR:HE1	1.72	0.55
1:C:107:LEU:HD23	1:C:228:PHE:CZ	2.42	0.55
1:C:183:GLY:O	1:C:186:MET:HB2	2.06	0.55
1:D:121:THR:HG23	1:D:133:ALA:HB1	1.89	0.55
1:C:91:GLY:HA2	1:C:139:PHE:CD1	2.42	0.54
1:D:169:GLN:HA	1:D:172:ILE:HD12	1.89	0.54
1:A:236:LEU:HB3	1:A:269:VAL:HG21	1.90	0.54
1:A:284:SER:CA	1:A:287:LYS:HD2	2.27	0.54
1:C:63:GLY:O	1:C:64:GLU:CG	2.55	0.54
1:D:111:TYR:HB3	1:D:221:ILE:HG13	1.89	0.54
1:D:82:ALA:HB2	1:D:444:PHE:HZ	1.73	0.54
1:A:103:ARG:H	1:A:103:ARG:HD2	1.72	0.53
1:D:40:PHE:HD1	1:D:141:ILE:HB	1.73	0.53
1:D:249:LEU:HD13	1:D:261:PRO:HB2	1.91	0.53
1:D:355:LEU:HB3	1:D:359:THR:HB	1.91	0.53
1:C:166:VAL:HG22	1:C:409:PRO:HB2	1.89	0.53
1:C:355:LEU:HB3	1:C:359:THR:HB	1.90	0.53
1:A:199:THR:OG1	1:A:202:ALA:HB3	2.08	0.53
1:A:249:LEU:HD13	1:A:261:PRO:HB2	1.90	0.53
1:D:106:SER:O	1:D:110:ILE:HG12	2.09	0.53
1:A:75:ILE:HG22	1:A:79:PHE:CE2	2.43	0.53
1:C:42:TYR:CE1	1:C:46:VAL:HG21	2.44	0.53
1:C:305:GLN:HB2	1:C:411:LEU:HD13	1.91	0.53
1:D:81:LEU:CD2	1:D:134:ARG:NH2	2.72	0.53
1:B:103:ARG:H	1:B:103:ARG:HD2	1.74	0.53
1:B:111:TYR:HE2	1:B:220:GLY:HA3	1.73	0.52
1:C:99:VAL:HG21	1:C:150:MET:SD	2.49	0.52
1:D:82:ALA:HB2	1:D:444:PHE:CZ	2.43	0.52
1:A:157:HIS:HB2	1:A:253:TYR:CZ	2.45	0.52
1:B:117:VAL:HG11	1:B:137:SER:HB3	1.90	0.52
1:B:361:LEU:HG	1:B:410:VAL:HG11	1.90	0.52
1:C:351:ILE:HG13	1:C:360:LEU:HD11	1.91	0.52
1:D:157:HIS:HB2	1:D:253:TYR:CZ	2.44	0.52
1:A:401:ILE:O	1:A:405:VAL:HG23	2.09	0.52
1:B:181:MET:HA	1:B:184:LEU:HD23	1.92	0.52
1:C:414:TYR:CZ	1:C:418:MET:HG3	2.45	0.52
1:B:121:THR:HG21	1:B:210:PHE:CD1	2.45	0.52
1:C:103:ARG:H	1:C:103:ARG:HD2	1.75	0.52
1:C:157:HIS:HB2	1:C:253:TYR:CZ	2.45	0.52
1:B:157:HIS:HB2	1:B:253:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:PHE:O	1:D:119:ILE:HG12	2.10	0.51
1:A:355:LEU:HB3	1:A:359:THR:HB	1.91	0.51
1:C:272:ASN:HA	1:C:422:GLU:HB2	1.93	0.51
1:C:63:GLY:C	1:C:64:GLU:HG3	2.30	0.51
1:D:421:SER:CA	1:D:424:LYS:HD2	2.22	0.51
1:A:419:PHE:N	1:A:420:PRO:HD3	2.26	0.51
1:D:95:SER:CB	1:D:143:LEU:HD12	2.40	0.51
1:B:40:PHE:CD1	1:B:141:ILE:HB	2.46	0.51
1:C:81:LEU:O	1:C:84:VAL:HG12	2.11	0.51
1:A:30:VAL:HG21	1:A:164:TYR:HD1	1.76	0.51
1:B:115:PHE:O	1:B:119:ILE:HG12	2.11	0.51
1:A:124:THR:HG21	1:A:206:TRP:CH2	2.31	0.51
1:B:54:ILE:HG12	1:B:206:TRP:CZ3	2.45	0.50
1:B:258:VAL:CG1	1:B:262:LEU:HG	2.38	0.50
1:B:355:LEU:HB3	1:B:359:THR:HB	1.92	0.50
1:B:351:ILE:HG13	1:B:360:LEU:HD11	1.92	0.50
1:C:36:ALA:HB2	1:C:111:TYR:CE1	2.46	0.50
1:C:82:ALA:HB2	1:C:444:PHE:CZ	2.46	0.50
1:C:122:SER:O	1:C:207:ARG:HD2	2.12	0.50
1:D:84:VAL:HG21	1:D:134:ARG:CZ	2.41	0.50
1:A:351:ILE:HG13	1:A:360:LEU:HD11	1.92	0.50
1:A:104:ARG:HA	1:A:228:PHE:CE1	2.47	0.50
1:A:255:THR:HG23	1:A:258:VAL:CG2	2.40	0.50
1:C:123:ILE:HD12	1:D:129:THR:HA	1.92	0.50
1:A:258:VAL:HG13	1:A:261:PRO:CG	2.41	0.50
1:B:99:VAL:HG21	1:B:150:MET:SD	2.52	0.50
1:B:310:ILE:HD13	1:B:403:PHE:CE2	2.47	0.50
1:B:82:ALA:HB2	1:B:444:PHE:HZ	1.78	0.49
1:D:107:LEU:HD21	1:D:148:VAL:HG22	1.94	0.49
1:A:58:PHE:CE1	1:A:127:PHE:HB2	2.47	0.49
1:C:165:GLY:HA3	1:C:413:ILE:CG2	2.42	0.49
1:C:316:ASN:HB3	1:C:320:LEU:HG	1.95	0.49
1:D:51:LYS:HZ3	1:D:81:LEU:HD12	1.77	0.49
1:D:305:GLN:HG3	1:D:407:TYR:CD1	2.47	0.49
1:B:277:LYS:HE3	1:B:280:LEU:HD22	1.93	0.49
1:C:72:ASN:HA	1:C:75:ILE:HB	1.94	0.49
1:A:360:LEU:HD22	1:A:406:SER:HA	1.93	0.49
1:C:108:LEU:HD13	1:C:228:PHE:HD2	1.76	0.49
1:A:224:LEU:HD23	1:A:227:PHE:HB2	1.95	0.49
1:B:305:GLN:HG2	1:B:407:TYR:CE1	2.48	0.49
1:A:120:LEU:HD11	1:B:120:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:HD23	1:C:227:PHE:HB2	1.93	0.49
1:D:313:LEU:HD21	1:D:396:THR:HG22	1.93	0.49
1:A:316:ASN:HB3	1:A:320:LEU:HG	1.95	0.49
1:A:110:ILE:HD11	1:A:143:LEU:HB3	1.94	0.48
1:D:351:ILE:HG13	1:D:360:LEU:HD11	1.94	0.48
1:C:369:LEU:HD21	1:C:466:ILE:HG12	1.95	0.48
1:D:84:VAL:HG22	1:D:134:ARG:HB3	1.94	0.48
1:A:40:PHE:CD2	1:A:172:ILE:HG12	2.49	0.48
1:B:82:ALA:HB2	1:B:444:PHE:CZ	2.49	0.48
1:C:233:PRO:HG3	1:C:248:ILE:HB	1.96	0.48
1:A:51:LYS:O	1:A:55:VAL:HG23	2.13	0.48
1:A:129:THR:HA	1:B:123:ILE:HD12	1.96	0.48
1:A:249:LEU:HD23	1:A:252:ILE:CD1	2.43	0.48
1:B:316:ASN:HB3	1:B:320:LEU:HG	1.94	0.48
1:B:119:ILE:O	1:B:122:SER:HB3	2.12	0.48
1:B:121:THR:CG2	1:B:210:PHE:CD1	2.97	0.48
1:C:40:PHE:O	1:C:44:VAL:HG23	2.13	0.48
1:B:224:LEU:HD23	1:B:227:PHE:HB2	1.94	0.48
1:B:344:MET:O	1:B:347:PRO:HD2	2.14	0.48
1:A:113:PHE:O	1:A:117:VAL:HG23	2.13	0.48
1:A:233:PRO:HG3	1:A:248:ILE:HB	1.96	0.48
1:B:369:LEU:HD21	1:B:466:ILE:HG12	1.96	0.48
1:C:224:LEU:O	1:C:228:PHE:HB2	2.14	0.48
1:C:313:LEU:HD21	1:C:396:THR:HG22	1.95	0.48
1:D:316:ASN:HB3	1:D:320:LEU:HG	1.94	0.48
1:D:51:LYS:HZ1	1:D:81:LEU:CD1	2.14	0.47
1:D:233:PRO:HG3	1:D:248:ILE:HB	1.95	0.47
1:A:305:GLN:HG3	1:A:407:TYR:CD1	2.48	0.47
1:B:269:VAL:O	1:B:273:GLU:HG2	2.14	0.47
1:C:344:MET:O	1:C:347:PRO:HD2	2.13	0.47
1:A:161:LYS:HZ2	1:A:417:GLU:HG3	1.78	0.47
1:A:369:LEU:HD21	1:A:466:ILE:HG12	1.96	0.47
1:B:104:ARG:HA	1:B:228:PHE:CE1	2.50	0.47
1:B:138:GLY:HA2	1:B:141:ILE:HG12	1.96	0.47
1:B:117:VAL:CG1	1:B:137:SER:HB3	2.45	0.47
1:B:202:ALA:O	1:B:206:TRP:HD1	1.97	0.47
1:C:95:SER:OG	1:C:146:VAL:HG21	2.15	0.47
1:D:369:LEU:HD21	1:D:466:ILE:HG12	1.96	0.47
1:A:344:MET:O	1:A:347:PRO:HD2	2.14	0.47
1:D:138:GLY:HA2	1:D:141:ILE:HG12	1.96	0.47
1:C:42:TYR:CD1	1:C:213:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ALA:HB2	1:C:444:PHE:HZ	1.79	0.46
1:B:233:PRO:HG3	1:B:248:ILE:HB	1.96	0.46
1:C:35:ILE:HB	1:C:111:TYR:OH	2.15	0.46
1:C:169:GLN:HA	1:C:172:ILE:HD12	1.95	0.46
1:C:157:HIS:HB2	1:C:253:TYR:CE2	2.50	0.46
1:B:364:GLY:HA3	1:B:406:SER:OG	2.15	0.46
1:D:344:MET:O	1:D:347:PRO:HD2	2.15	0.46
1:A:118:SER:HB2	1:A:214:SER:HB3	1.97	0.46
1:B:169:GLN:HA	1:B:172:ILE:HD12	1.98	0.46
1:A:84:VAL:HG22	1:A:134:ARG:O	2.16	0.46
1:A:82:ALA:HB2	1:A:444:PHE:CZ	2.51	0.46
1:A:286:LEU:HA	1:A:292:ARG:HG3	1.97	0.46
1:B:165:GLY:HA3	1:B:413:ILE:CG2	2.46	0.46
1:A:107:LEU:HB2	1:A:228:PHE:HE2	1.81	0.45
1:B:91:GLY:HA2	1:B:139:PHE:CD1	2.51	0.45
1:D:53:PHE:HZ	1:D:187:GLY:HA2	1.81	0.45
1:D:311:ASN:HA	1:D:314:VAL:HB	1.98	0.45
1:B:273:GLU:HA	1:B:277:LYS:HB3	1.99	0.45
1:C:421:SER:O	1:C:422:GLU:HB3	2.15	0.45
1:A:169:GLN:HA	1:A:172:ILE:HD12	1.98	0.45
1:C:224:LEU:HB3	1:C:228:PHE:CD2	2.52	0.45
1:C:275:ALA:HB1	1:C:280:LEU:HD12	1.99	0.45
1:A:145:THR:HG21	1:A:436:TRP:HE1	1.81	0.45
1:A:157:HIS:HB2	1:A:253:TYR:CE2	2.52	0.45
1:C:246:LYS:HG2	1:C:250:LYS:HE3	1.98	0.45
1:A:113:PHE:CZ	1:A:136:LEU:HB3	2.52	0.45
1:B:143:LEU:O	1:B:147:SER:HB2	2.17	0.45
1:A:305:GLN:HB2	1:A:411:LEU:HD13	1.98	0.44
1:B:124:THR:HG21	1:B:206:TRP:CH2	2.39	0.44
1:B:450:ILE:HG13	1:B:457:LEU:HD13	2.00	0.44
1:C:95:SER:HB3	1:C:143:LEU:HA	1.99	0.44
1:C:145:THR:HG21	1:C:436:TRP:HE1	1.82	0.44
1:B:107:LEU:HD12	1:B:151:TYR:CD2	2.52	0.44
1:B:161:LYS:HZ2	1:B:417:GLU:HG3	1.77	0.44
1:C:224:LEU:HD13	1:C:228:PHE:CE2	2.52	0.44
1:D:450:ILE:HG13	1:D:457:LEU:HD13	2.00	0.44
1:B:247:ASN:HA	1:B:250:LYS:HB2	1.99	0.44
1:C:165:GLY:HA3	1:C:413:ILE:HG22	1.99	0.44
1:C:186:MET:CE	1:C:205:TRP:HB3	2.48	0.44
1:D:249:LEU:HD23	1:D:252:ILE:CD1	2.44	0.44
1:B:182:LEU:O	1:B:186:MET:SD	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:HD21	1:B:396:THR:HG22	1.98	0.44
1:D:146:VAL:HG21	1:D:429:SER:HA	1.99	0.44
1:C:247:ASN:HA	1:C:250:LYS:HB2	2.00	0.44
1:C:418:MET:HE3	1:C:477:LYS:HD2	2.00	0.44
1:D:50:ILE:HD13	1:D:206:TRP:CD1	2.53	0.44
1:A:247:ASN:HA	1:A:250:LYS:HB2	2.00	0.44
1:B:157:HIS:HB2	1:B:253:TYR:CE2	2.53	0.44
1:B:202:ALA:O	1:B:206:TRP:CD1	2.71	0.44
1:A:58:PHE:HZ	1:A:76:GLN:HG3	1.83	0.44
1:B:40:PHE:HD1	1:B:141:ILE:HB	1.82	0.44
1:C:450:ILE:HG13	1:C:457:LEU:HD13	2.00	0.44
1:C:88:ALA:O	1:C:92:CYS:SG	2.73	0.43
1:B:408:GLY:N	1:B:409:PRO:CD	2.81	0.43
1:D:111:TYR:HB3	1:D:221:ILE:CG1	2.48	0.43
1:D:247:ASN:HA	1:D:250:LYS:HB2	2.00	0.43
1:D:157:HIS:HB2	1:D:253:TYR:OH	2.18	0.43
1:A:99:VAL:HG21	1:A:150:MET:SD	2.58	0.43
1:B:42:TYR:CD1	1:B:213:PRO:HG3	2.53	0.43
1:B:173:THR:HB	1:B:342:PHE:HA	2.00	0.43
1:D:51:LYS:CE	1:D:81:LEU:HD11	2.47	0.43
1:D:121:THR:CG2	1:D:133:ALA:HB1	2.47	0.43
1:D:246:LYS:HG2	1:D:250:LYS:HE3	2.00	0.43
1:A:246:LYS:HG2	1:A:250:LYS:HE3	1.99	0.43
1:A:260:GLU:HB2	1:A:261:PRO:HD3	2.00	0.43
1:C:120:LEU:HD13	1:D:132:PHE:CE2	2.53	0.43
1:C:177:PHE:CZ	1:C:181:MET:SD	3.11	0.43
1:C:180:VAL:HG21	1:C:338:THR:HG21	2.01	0.43
1:D:124:THR:HG21	1:D:206:TRP:HZ2	1.82	0.43
1:D:173:THR:HB	1:D:342:PHE:HA	2.00	0.43
1:A:156:THR:HG21	1:A:164:TYR:CB	2.49	0.43
1:A:255:THR:O	1:A:258:VAL:HG23	2.19	0.43
1:A:402:SER:O	1:A:406:SER:HB3	2.18	0.43
1:B:118:SER:HB2	1:B:214:SER:HB3	2.01	0.43
1:A:364:GLY:HA3	1:A:406:SER:OG	2.18	0.43
1:B:418:MET:HE1	1:B:477:LYS:HE3	2.00	0.43
1:D:75:ILE:HG13	1:D:77:SER:H	1.82	0.43
1:D:103:ARG:H	1:D:103:ARG:HD2	1.84	0.43
1:D:157:HIS:HB2	1:D:253:TYR:CE2	2.54	0.43
1:A:157:HIS:HB2	1:A:253:TYR:OH	2.19	0.43
1:A:249:LEU:HD12	1:A:262:LEU:CD2	2.49	0.43
1:D:80:LEU:HB2	1:D:127:PHE:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:HA	1:B:228:PHE:CZ	2.53	0.42
1:D:91:GLY:HA2	1:D:139:PHE:HD1	1.82	0.42
1:D:145:THR:HG21	1:D:436:TRP:HE1	1.83	0.42
1:D:161:LYS:NZ	1:D:417:GLU:HG3	2.34	0.42
1:A:450:ILE:HG13	1:A:457:LEU:HD13	2.01	0.42
1:B:157:HIS:HB2	1:B:253:TYR:OH	2.19	0.42
1:A:132:PHE:CE2	1:B:120:LEU:HB2	2.54	0.42
1:B:25:THR:HA	1:B:28:LYS:HB2	2.01	0.42
1:D:99:VAL:HG21	1:D:150:MET:SD	2.59	0.42
1:D:313:LEU:HD21	1:D:396:THR:CG2	2.49	0.42
1:B:246:LYS:HG2	1:B:250:LYS:HE3	2.00	0.42
1:C:25:THR:HA	1:C:28:LYS:HB2	2.02	0.42
1:D:180:VAL:HG13	1:D:184:LEU:HD12	2.00	0.42
1:A:142:GLY:O	1:A:145:THR:OG1	2.38	0.42
1:A:124:THR:HB	1:A:207:ARG:NH1	2.34	0.42
1:D:74:THR:HG23	1:D:451:LYS:NZ	2.35	0.42
1:A:82:ALA:HB2	1:A:444:PHE:HZ	1.85	0.42
1:C:129:THR:HA	1:D:123:ILE:HD12	2.01	0.42
1:B:414:TYR:CE2	1:B:418:MET:HG3	2.55	0.42
1:C:42:TYR:HD1	1:C:213:PRO:HG3	1.85	0.42
1:B:414:TYR:CZ	1:B:418:MET:SD	3.13	0.41
1:C:344:MET:HG3	1:C:401:ILE:HA	2.01	0.41
1:A:40:PHE:O	1:A:44:VAL:HG23	2.21	0.41
1:A:123:ILE:HD12	1:B:129:THR:HA	2.02	0.41
1:A:284:SER:O	1:A:288:ILE:HG12	2.20	0.41
1:B:344:MET:HG3	1:B:401:ILE:HA	2.02	0.41
1:C:40:PHE:CD1	1:C:141:ILE:HG23	2.54	0.41
1:B:165:GLY:HA3	1:B:413:ILE:HG21	2.02	0.41
1:D:206:TRP:CD1	1:D:206:TRP:C	2.94	0.41
1:A:283:LEU:C	1:A:285:ALA:H	2.23	0.41
1:C:40:PHE:CE1	1:C:141:ILE:HG23	2.55	0.41
1:C:74:THR:O	1:C:77:SER:HB3	2.19	0.41
1:C:91:GLY:CA	1:C:139:PHE:CD1	3.03	0.41
1:B:162:GLY:HA2	1:B:413:ILE:HD13	2.03	0.41
1:D:345:THR:HG23	1:D:409:PRO:HG3	2.02	0.41
1:A:237:PHE:HB3	1:A:269:VAL:HG22	2.01	0.41
1:D:237:PHE:HB3	1:D:269:VAL:HB	2.03	0.41
1:D:25:THR:HA	1:D:28:LYS:HB2	2.02	0.41
1:B:107:LEU:HD21	1:B:147:SER:HB3	2.03	0.41
1:A:40:PHE:HD2	1:A:172:ILE:HG12	1.85	0.41
1:A:92:CYS:SG	1:A:145:THR:OG1	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:CG2	1:B:143:LEU:HB3	2.51	0.41
1:B:382:ASN:C	1:B:389:LYS:HE2	2.41	0.41
1:C:260:GLU:HB2	1:C:261:PRO:HD3	2.02	0.41
1:A:111:TYR:CE2	1:A:220:GLY:HA3	2.55	0.41
1:C:120:LEU:HB2	1:D:132:PHE:CE2	2.56	0.41
1:D:390:ILE:HA	1:D:393:ILE:HD12	2.02	0.40
1:C:40:PHE:HD1	1:C:141:ILE:HG12	1.86	0.40
1:B:150:MET:HG3	1:B:424:LYS:NZ	2.37	0.40
1:D:406:SER:O	1:D:409:PRO:HD2	2.21	0.40
1:A:344:MET:HG3	1:A:401:ILE:HA	2.03	0.40
1:B:164:TYR:O	1:B:167:MET:HB2	2.21	0.40
1:C:53:PHE:CZ	1:C:186:MET:SD	3.15	0.40
1:A:25:THR:HA	1:A:28:LYS:HB2	2.03	0.40
1:B:305:GLN:HG2	1:B:407:TYR:CZ	2.56	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	429/496 (86%)	395 (92%)	27 (6%)	7 (2%)	9 43
1	B	431/496 (87%)	396 (92%)	31 (7%)	4 (1%)	17 54
1	C	441/496 (89%)	406 (92%)	32 (7%)	3 (1%)	22 59
1	D	422/496 (85%)	390 (92%)	30 (7%)	2 (0%)	29 66
All	All	1723/1984 (87%)	1587 (92%)	120 (7%)	16 (1%)	17 54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	ILE

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Mol	Chain	Res	Type
1	A	187	GLY
1	B	187	GLY
1	B	407	TYR
1	C	422	GLU
1	A	71	SER
1	A	95	SER
1	A	283	LEU
1	A	58	PHE
1	A	284	SER
1	B	403	PHE
1	B	420	PRO
1	C	65	LYS
1	A	420	PRO
1	C	110	ILE
1	D	423	ILE

### 5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	387/441 (88%)	363 (94%)	24 (6%)	18 50
1	B	390/441 (88%)	364 (93%)	26 (7%)	16 48
1	C	396/441 (90%)	368 (93%)	28 (7%)	14 45
1	D	382/441 (87%)	361 (94%)	21 (6%)	21 53
All	All	1555/1764 (88%)	1456 (94%)	99 (6%)	17 49

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	74	THR
1	A	95	SER
1	A	103	ARG
1	A	114	PHE
1	A	115	PHE

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Mol	Chain	Res	Type
1	A	141	ILE
1	A	182	LEU
1	A	211	LEU
1	A	217	SER
1	A	228	PHE
1	A	237	PHE
1	A	255	THR
1	A	272	ASN
1	A	319	GLU
1	A	323	GLU
1	A	360	LEU
1	A	363	TRP
1	A	391	LEU
1	A	407	TYR
1	A	411	LEU
1	A	413	ILE
1	A	419	PHE
1	A	457	LEU
1	B	31	LEU
1	B	48	ASN
1	B	58	PHE
1	B	80	LEU
1	B	95	SER
1	B	103	ARG
1	B	104	ARG
1	B	159	ASP
1	B	182	LEU
1	B	209	MET
1	B	211	LEU
1	B	217	SER
1	B	228	PHE
1	B	237	PHE
1	B	249	LEU
1	B	255	THR
1	B	272	ASN
1	B	274	SER
1	B	280	LEU
1	B	319	GLU
1	B	323	GLU
1	B	360	LEU
1	B	363	TRP
1	B	411	LEU

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Mol	Chain	Res	Type
1	B	429	SER
1	B	457	LEU
1	C	31	LEU
1	C	48	ASN
1	C	54	ILE
1	C	58	PHE
1	C	59	GLU
1	C	68	LEU
1	C	79	PHE
1	C	97	TYR
1	C	103	ARG
1	C	114	PHE
1	C	182	LEU
1	C	184	LEU
1	C	186	MET
1	C	208	LEU
1	C	211	LEU
1	C	217	SER
1	C	237	PHE
1	C	249	LEU
1	C	267	GLU
1	C	319	GLU
1	C	323	GLU
1	C	360	LEU
1	C	363	TRP
1	C	407	TYR
1	C	411	LEU
1	C	425	ASP
1	C	426	SER
1	C	457	LEU
1	D	31	LEU
1	D	48	ASN
1	D	58	PHE
1	D	79	PHE
1	D	97	TYR
1	D	103	ARG
1	D	104	ARG
1	D	107	LEU
1	D	114	PHE
1	D	206	TRP
1	D	210	PHE
1	D	211	LEU

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Mol	Chain	Res	Type
1	D	237	PHE
1	D	255	THR
1	D	267	GLU
1	D	319	GLU
1	D	323	GLU
1	D	360	LEU
1	D	363	TRP
1	D	407	TYR
1	D	457	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	B	76	GLN
1	B	272	ASN
1	C	43	GLN
1	C	73	ASN
1	D	169	GLN
1	D	271	GLN
1	D	318	ASN
1	D	416	HIS

### 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 [\(i\)](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

8 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	BGC	B	602[B]	-	12,12,12	0.21	0	17,17,17	0.22	0
2	GLC	A	601[A]	-	12,12,12	0.31	0	17,17,17	0.50	0
3	BGC	C	602[B]	-	12,12,12	0.21	0	17,17,17	0.26	0
3	BGC	A	602[B]	-	12,12,12	0.22	0	17,17,17	0.24	0
2	GLC	D	601[A]	-	12,12,12	0.29	0	17,17,17	0.47	0
2	GLC	C	601[A]	-	12,12,12	0.23	0	17,17,17	0.50	0
2	GLC	B	601[A]	-	12,12,12	0.30	0	17,17,17	0.47	0
3	BGC	D	602[B]	-	12,12,12	0.22	0	17,17,17	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	B	602[B]	-	-	0/2/22/22	0/1/1/1
2	GLC	A	601[A]	-	-	0/2/22/22	0/1/1/1
3	BGC	C	602[B]	-	-	0/2/22/22	0/1/1/1
3	BGC	A	602[B]	-	-	0/2/22/22	0/1/1/1
2	GLC	D	601[A]	-	-	0/2/22/22	0/1/1/1
2	GLC	C	601[A]	-	-	0/2/22/22	0/1/1/1
2	GLC	B	601[A]	-	-	0/2/22/22	0/1/1/1
3	BGC	D	602[B]	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

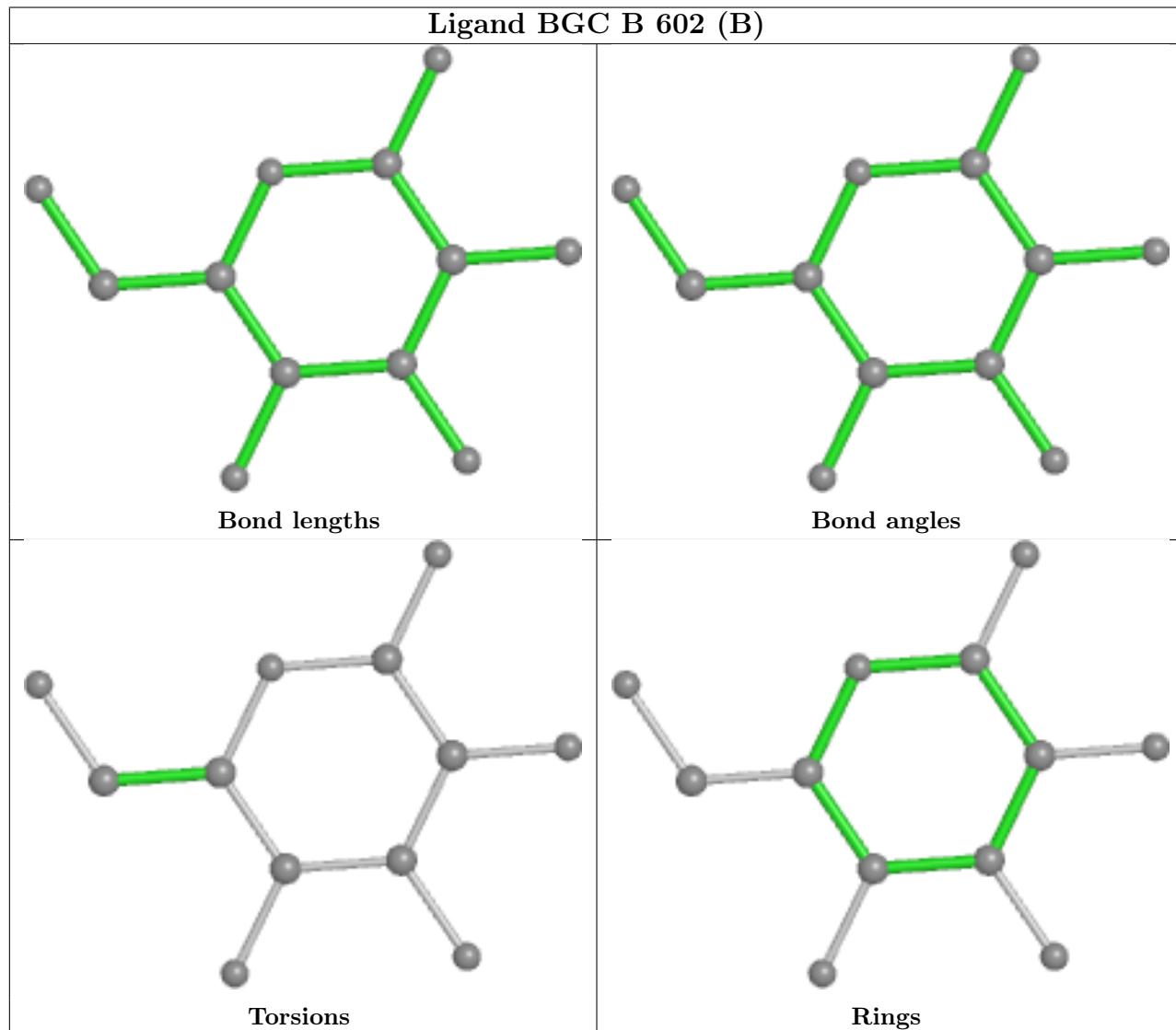
There are no torsion outliers.

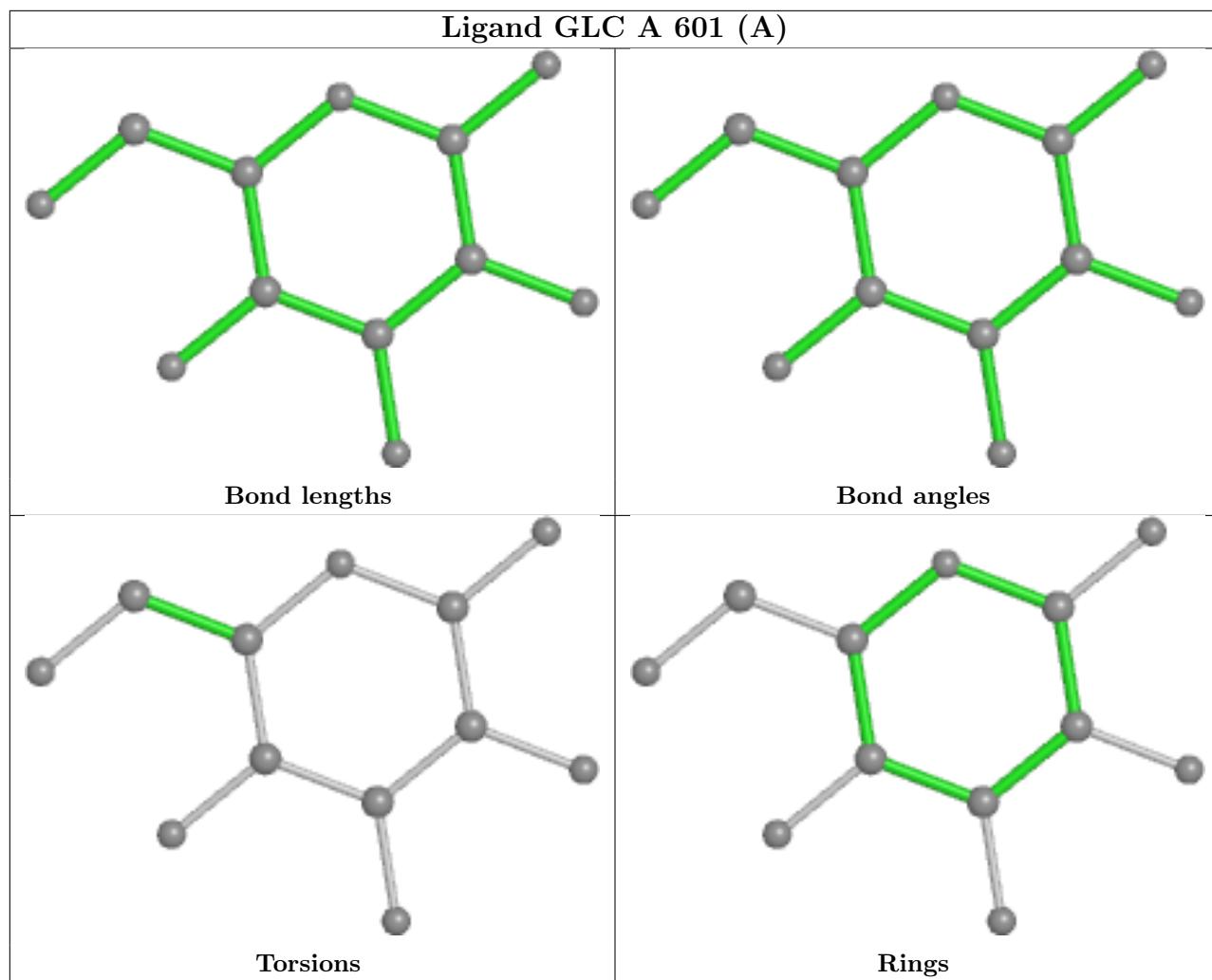
There are no ring outliers.

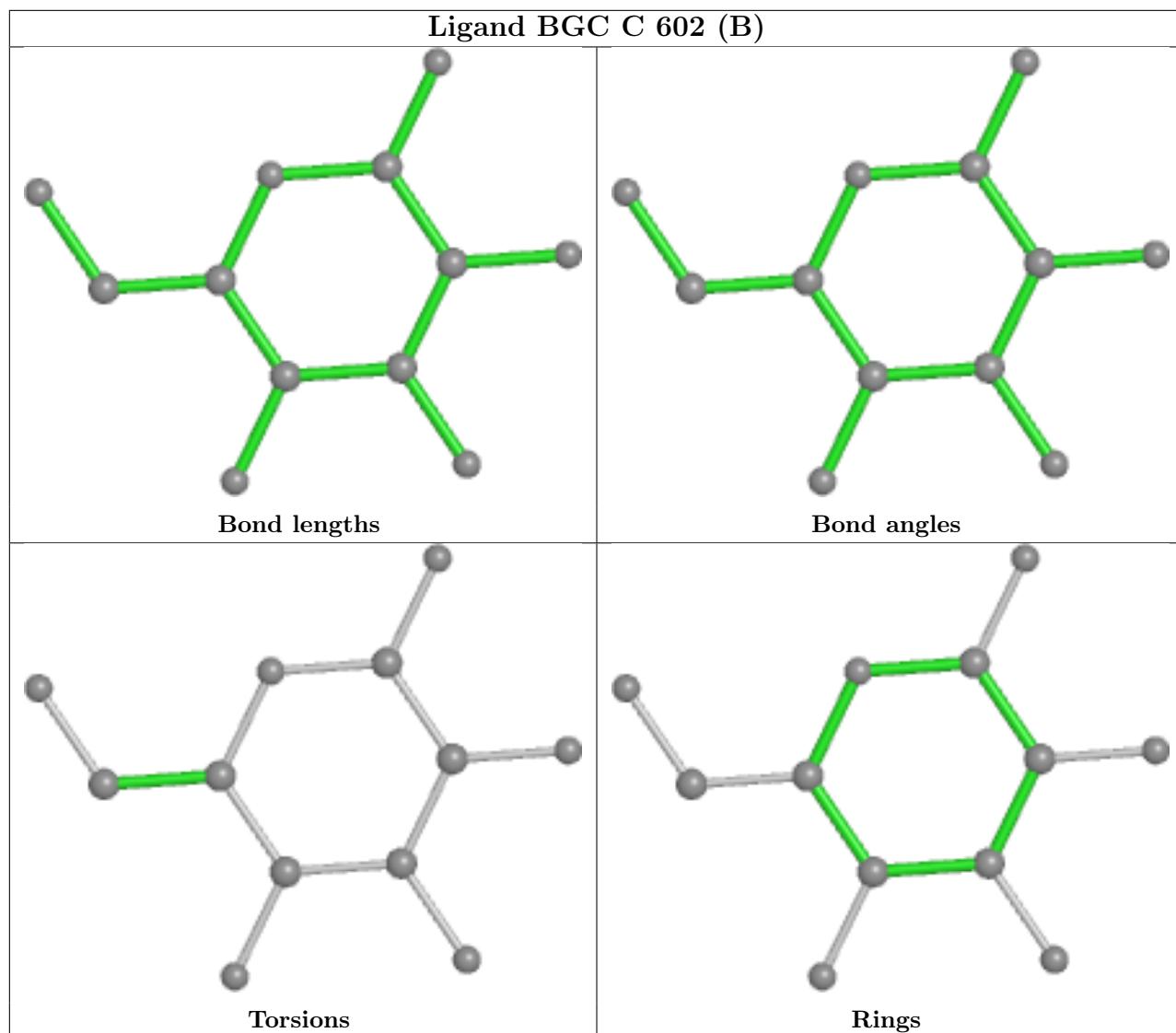
No monomer is involved in short contacts.

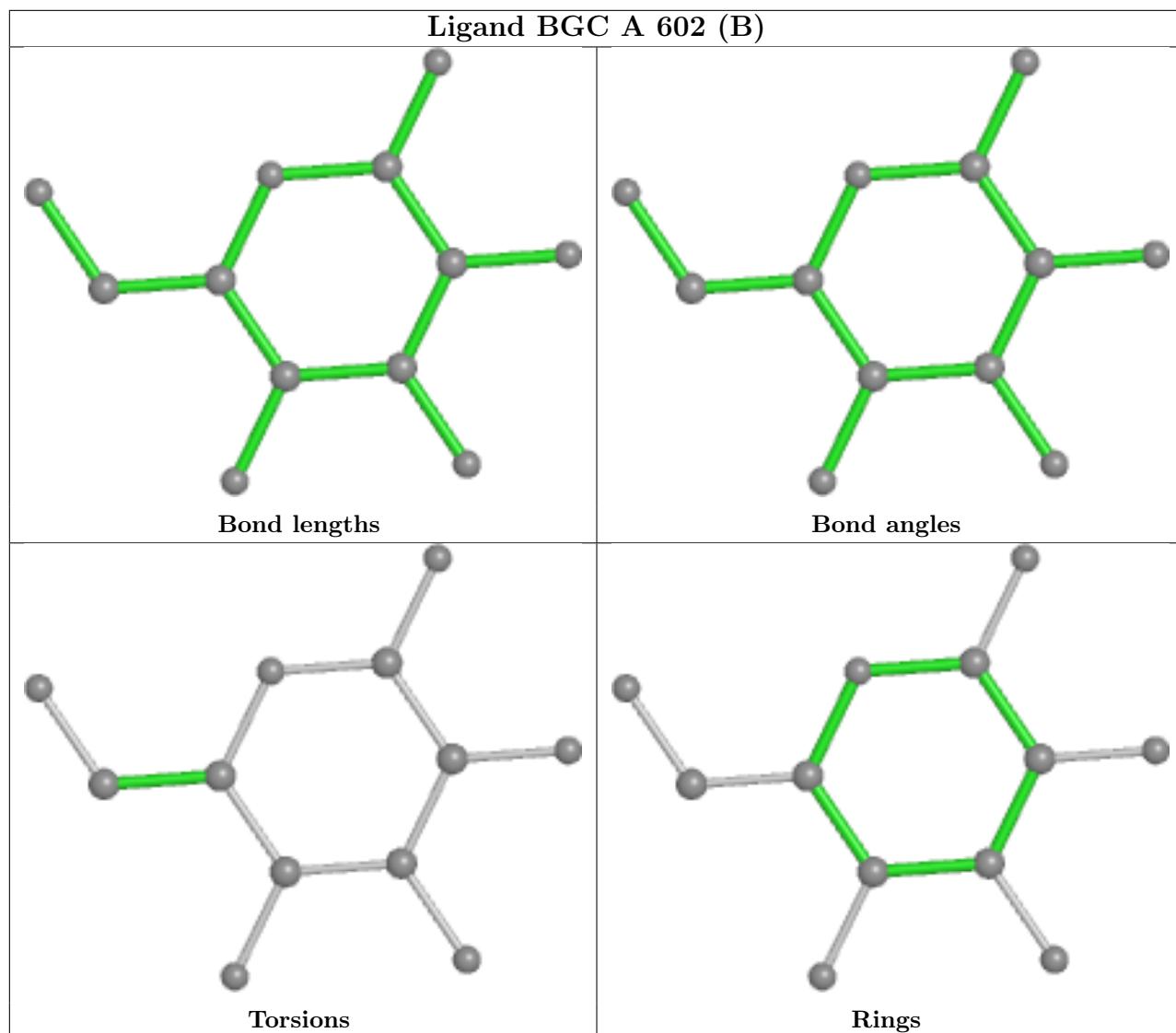
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

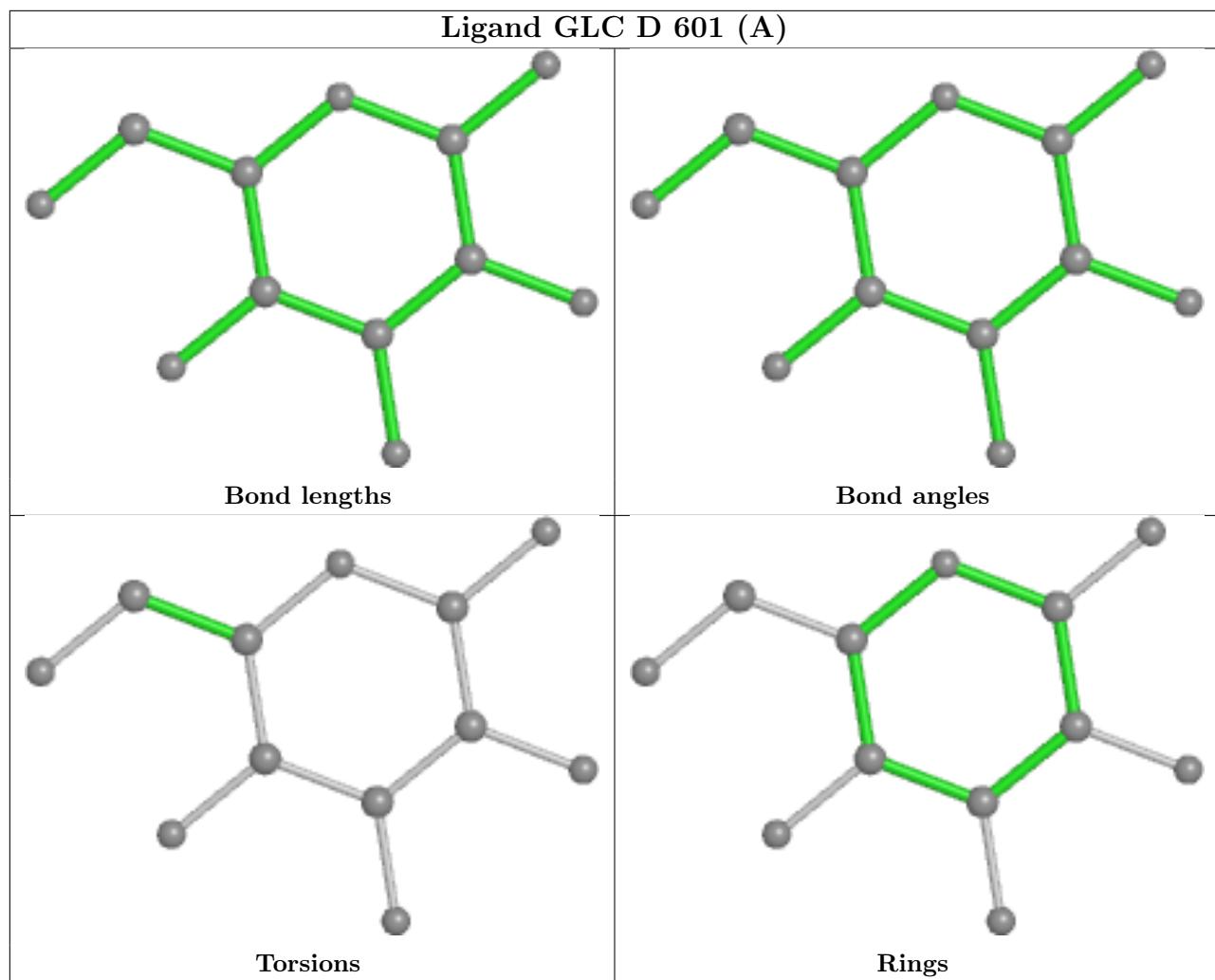
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

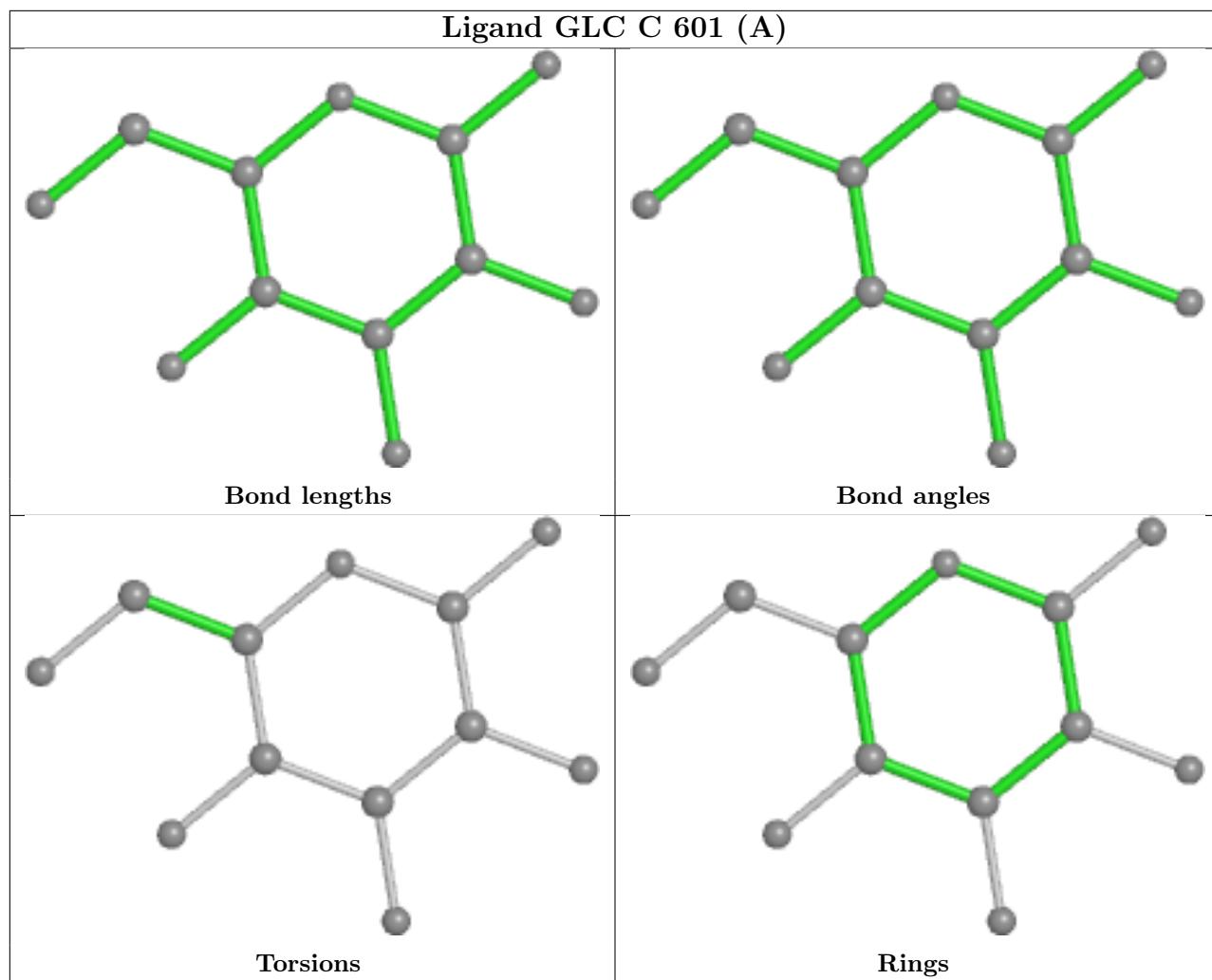


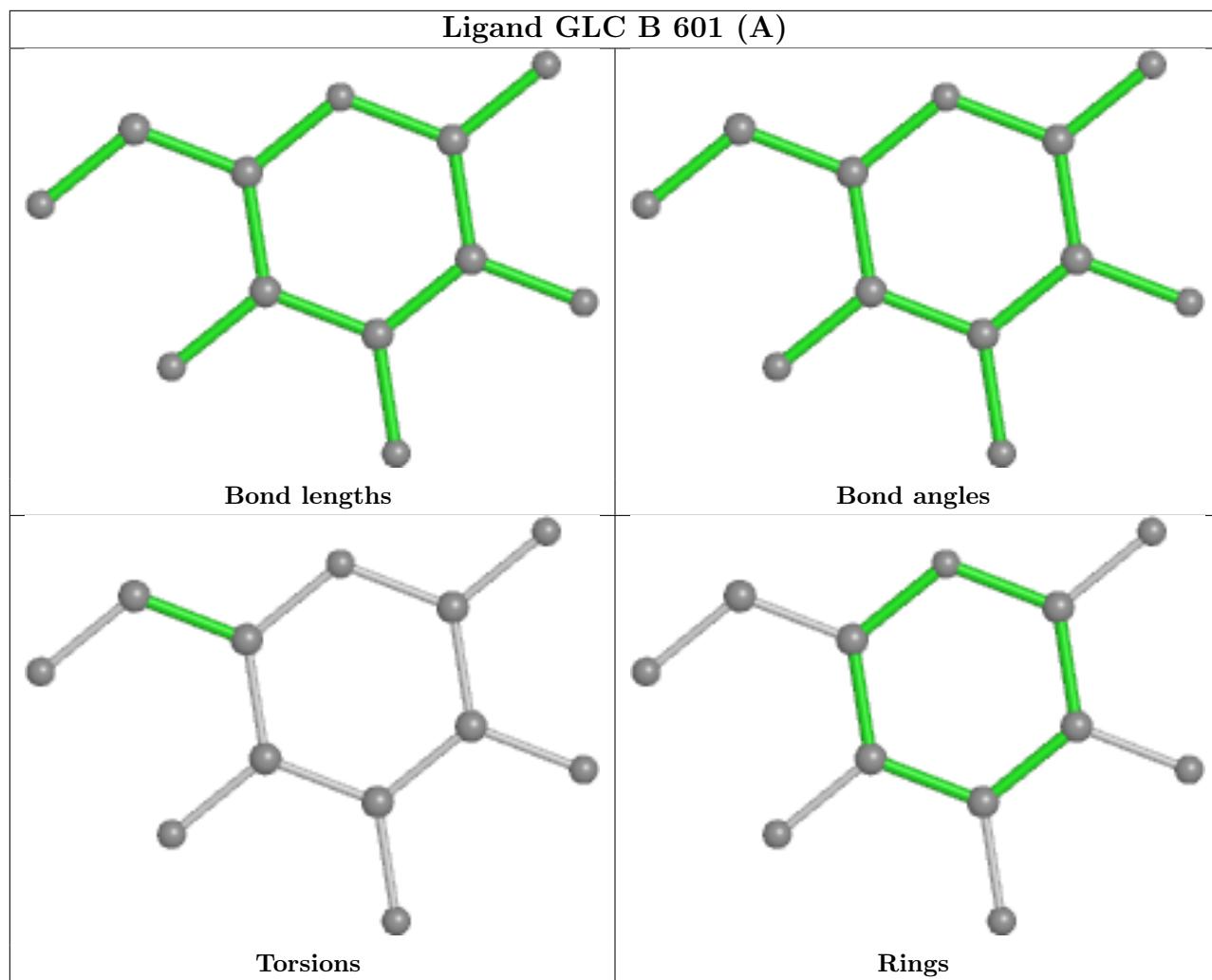


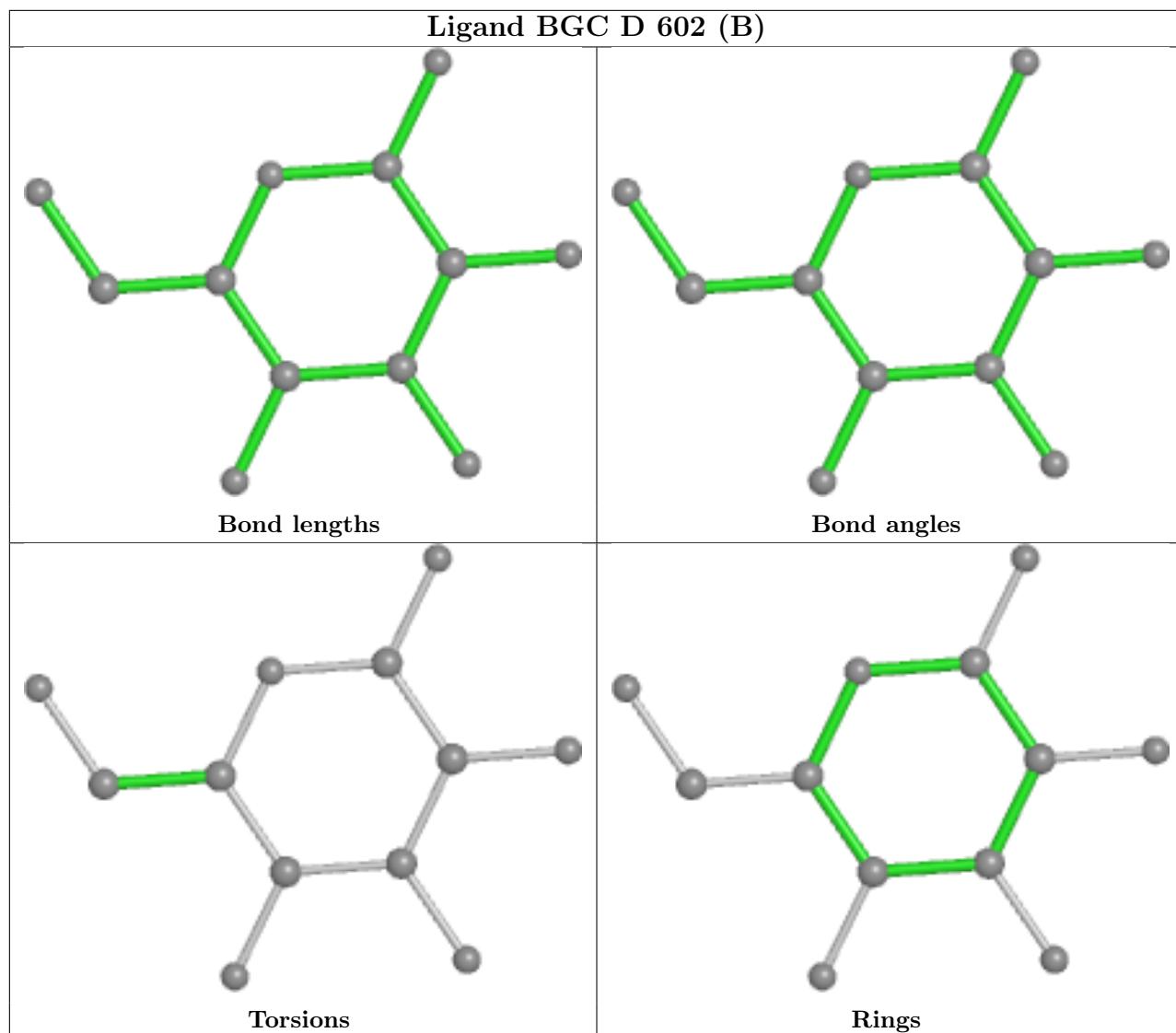












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/496 (88%)	0.04	19 (4%) 35 24	159, 239, 263, 277	0
1	B	439/496 (88%)	0.06	30 (6%) 17 11	155, 246, 270, 278	0
1	C	447/496 (90%)	-0.05	19 (4%) 35 24	126, 225, 255, 264	0
1	D	430/496 (86%)	0.14	22 (5%) 28 19	165, 240, 272, 277	0
All	All	1753/1984 (88%)	0.04	90 (5%) 28 19	126, 237, 267, 278	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	GLN	6.3
1	B	274	SER	5.8
1	D	259	ASP	5.3
1	D	260	GLU	4.4
1	B	205	TRP	4.2
1	C	474	PHE	4.1
1	A	22	PHE	4.1
1	A	451	LYS	4.1
1	B	406	SER	4.0
1	B	408	GLY	4.0
1	D	74	THR	4.0
1	B	287	LYS	3.9
1	B	259	ASP	3.8
1	D	380	GLU	3.8
1	A	229	LYS	3.8
1	C	451	LYS	3.6
1	D	354	LYS	3.5
1	B	188	GLU	3.4
1	C	66	ASP	3.4
1	A	59	GLU	3.3
1	A	378	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASN	3.3
1	D	200	SER	3.2
1	C	326	ASP	3.2
1	C	65	LYS	3.2
1	B	407	TYR	3.1
1	D	256	ASP	3.1
1	A	260	GLU	3.1
1	C	279	SER	3.1
1	D	453	SER	3.1
1	B	391	LEU	3.0
1	D	406	SER	3.0
1	B	386	ASN	3.0
1	A	259	ASP	3.0
1	A	71	SER	2.9
1	C	388	VAL	2.9
1	A	243	GLU	2.8
1	B	453	SER	2.8
1	D	324	PHE	2.8
1	B	354	LYS	2.8
1	C	380	GLU	2.8
1	A	159	ASP	2.8
1	B	390	ILE	2.8
1	C	243	GLU	2.7
1	C	453	SER	2.7
1	B	276	LYS	2.7
1	A	318	ASN	2.6
1	B	241	ARG	2.6
1	C	23	PHE	2.6
1	A	232	THR	2.6
1	B	71	SER	2.6
1	A	386	ASN	2.5
1	D	281	SER	2.5
1	B	254	GLU	2.5
1	B	240	GLY	2.5
1	C	241	ARG	2.5
1	A	72	ASN	2.4
1	C	354	LYS	2.4
1	D	23	PHE	2.4
1	C	229	LYS	2.4
1	D	287	LYS	2.4
1	C	254	GLU	2.4
1	D	157	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	257	ASN	2.4
1	B	286	LEU	2.3
1	D	199	THR	2.3
1	A	70	CYS	2.3
1	B	355	LEU	2.3
1	D	159	ASP	2.3
1	A	23	PHE	2.3
1	D	250	LYS	2.2
1	C	64	GLU	2.2
1	B	356	GLY	2.2
1	A	387	PHE	2.2
1	C	256	ASP	2.2
1	B	452	LYS	2.2
1	B	474	PHE	2.2
1	B	237	PHE	2.2
1	B	270	GLU	2.2
1	D	449	ILE	2.1
1	A	266	LYS	2.1
1	B	480	LYS	2.1
1	D	101	PHE	2.1
1	C	73	ASN	2.1
1	D	283	LEU	2.1
1	B	204	LEU	2.0
1	C	350	TYR	2.0
1	D	255	THR	2.0
1	D	49	THR	2.0
1	B	318	ASN	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 [\(i\)](#)

There are no monosaccharides in this entry.

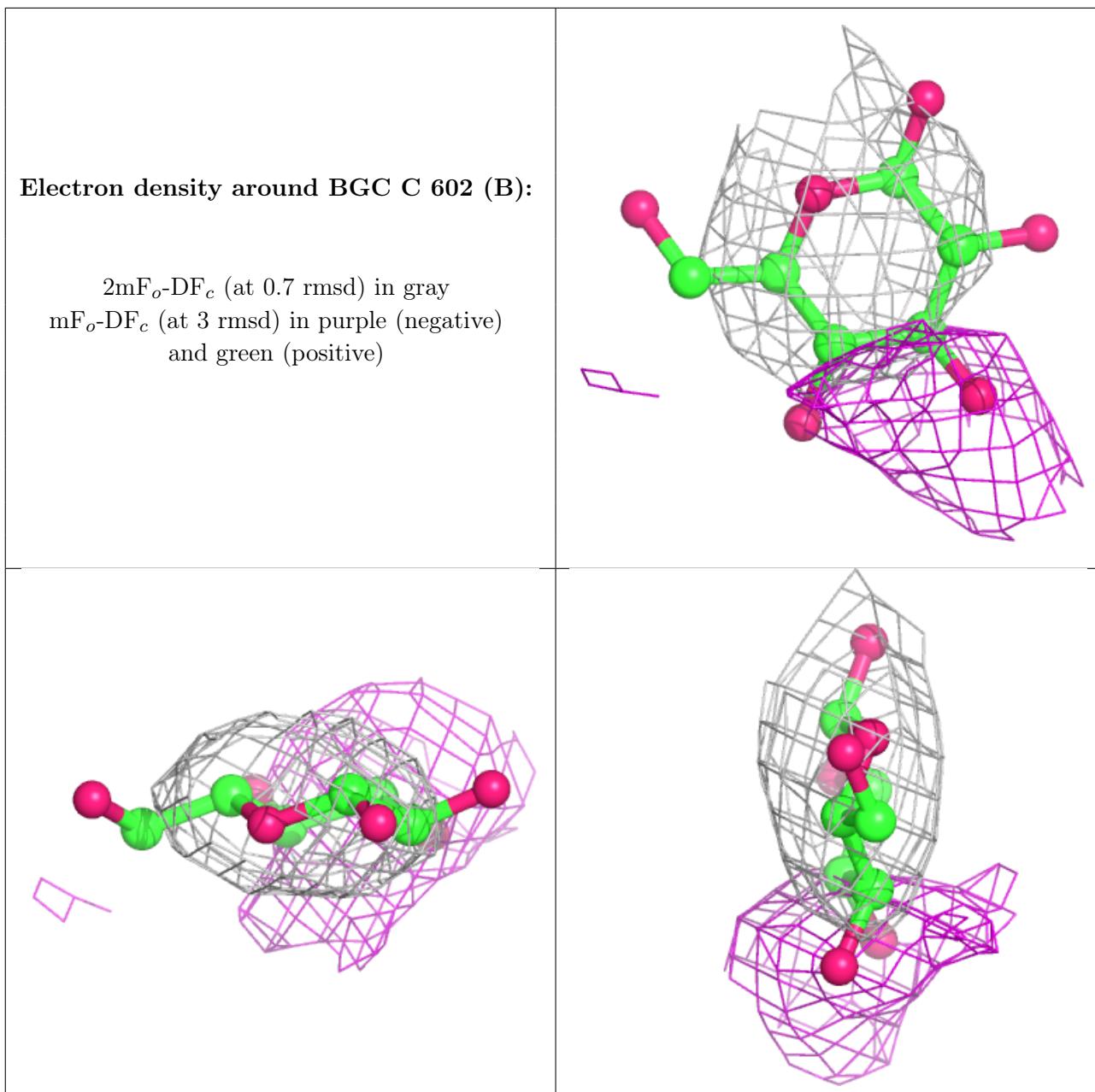
## 6.4 Ligands [\(i\)](#)

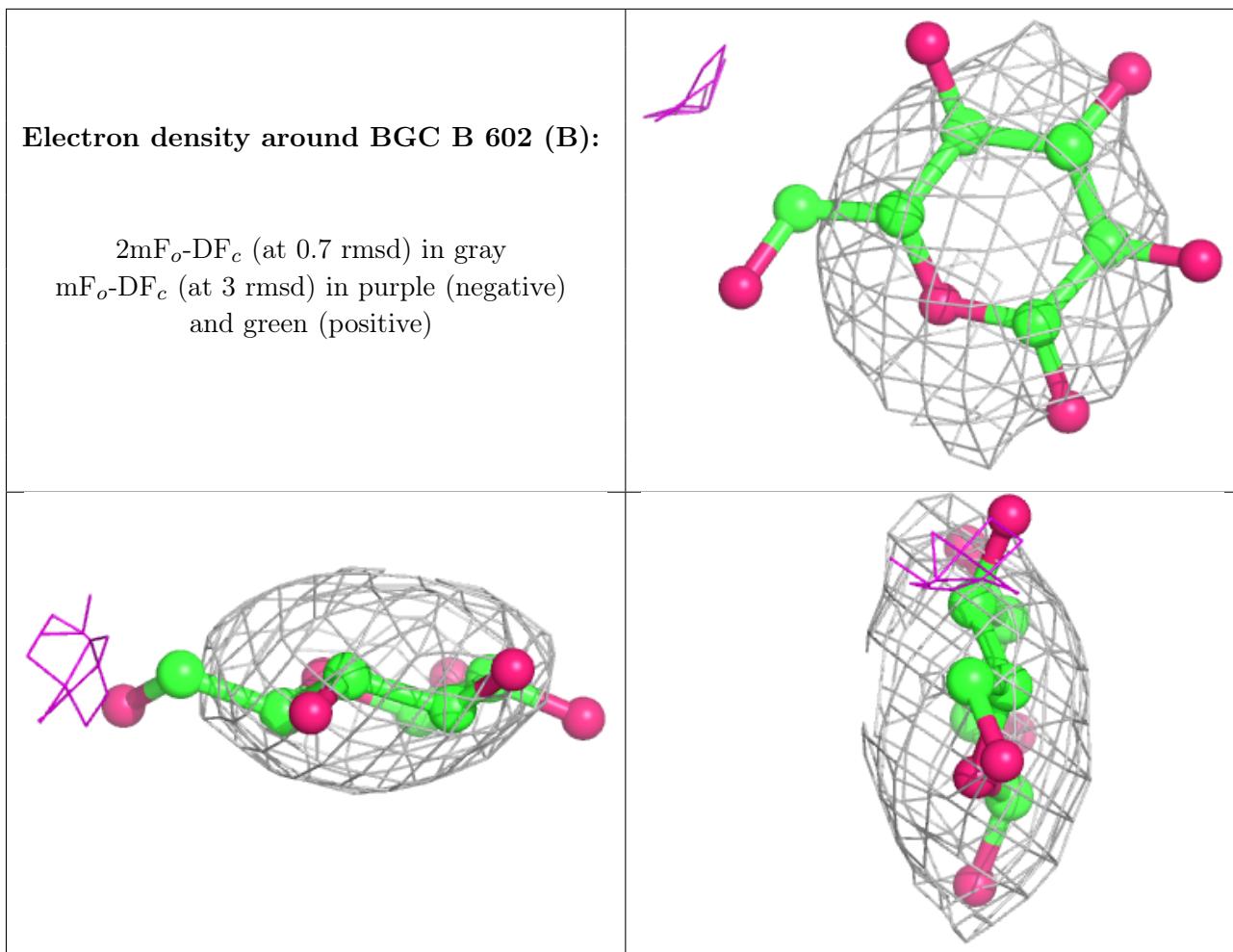
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

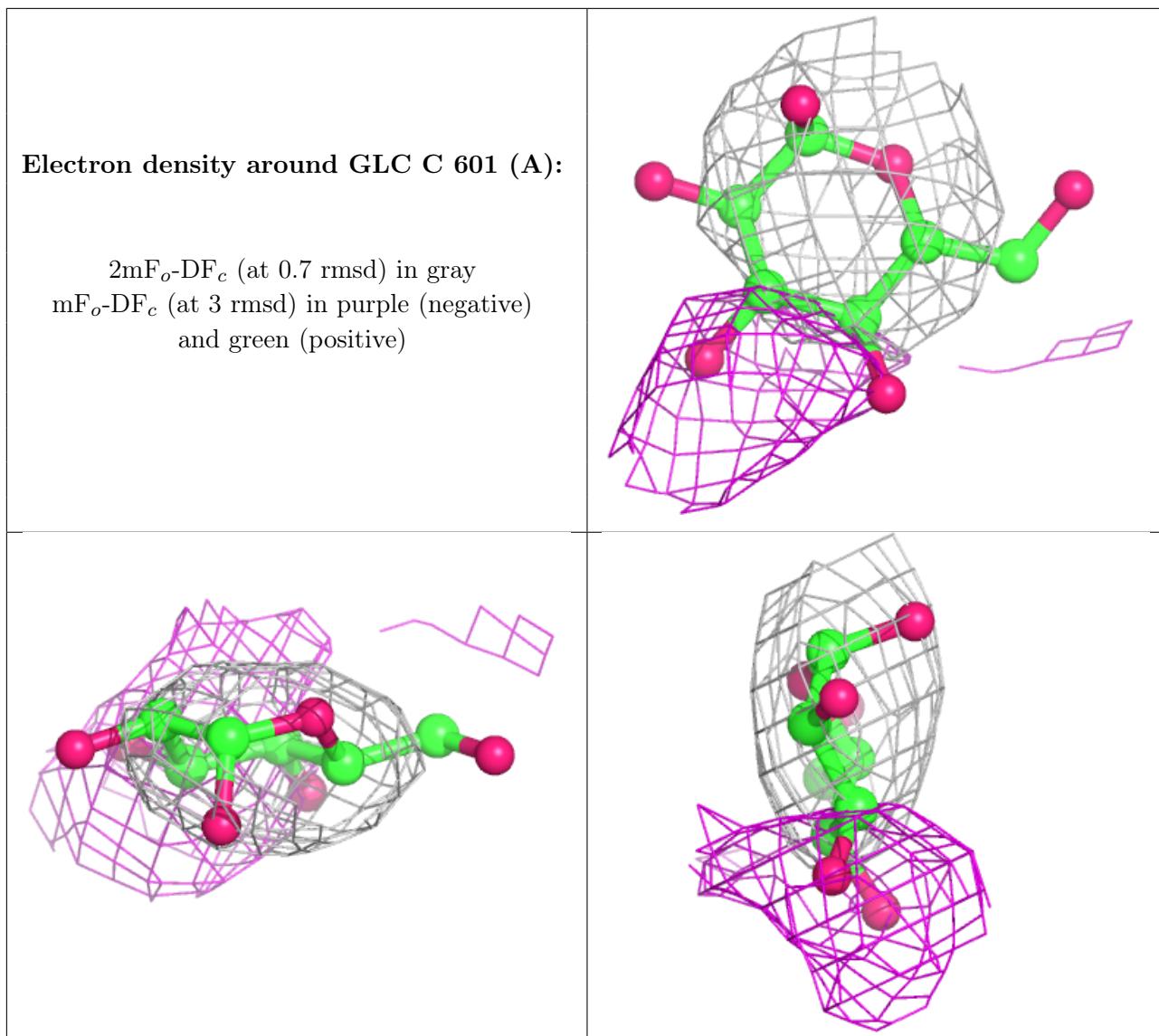
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

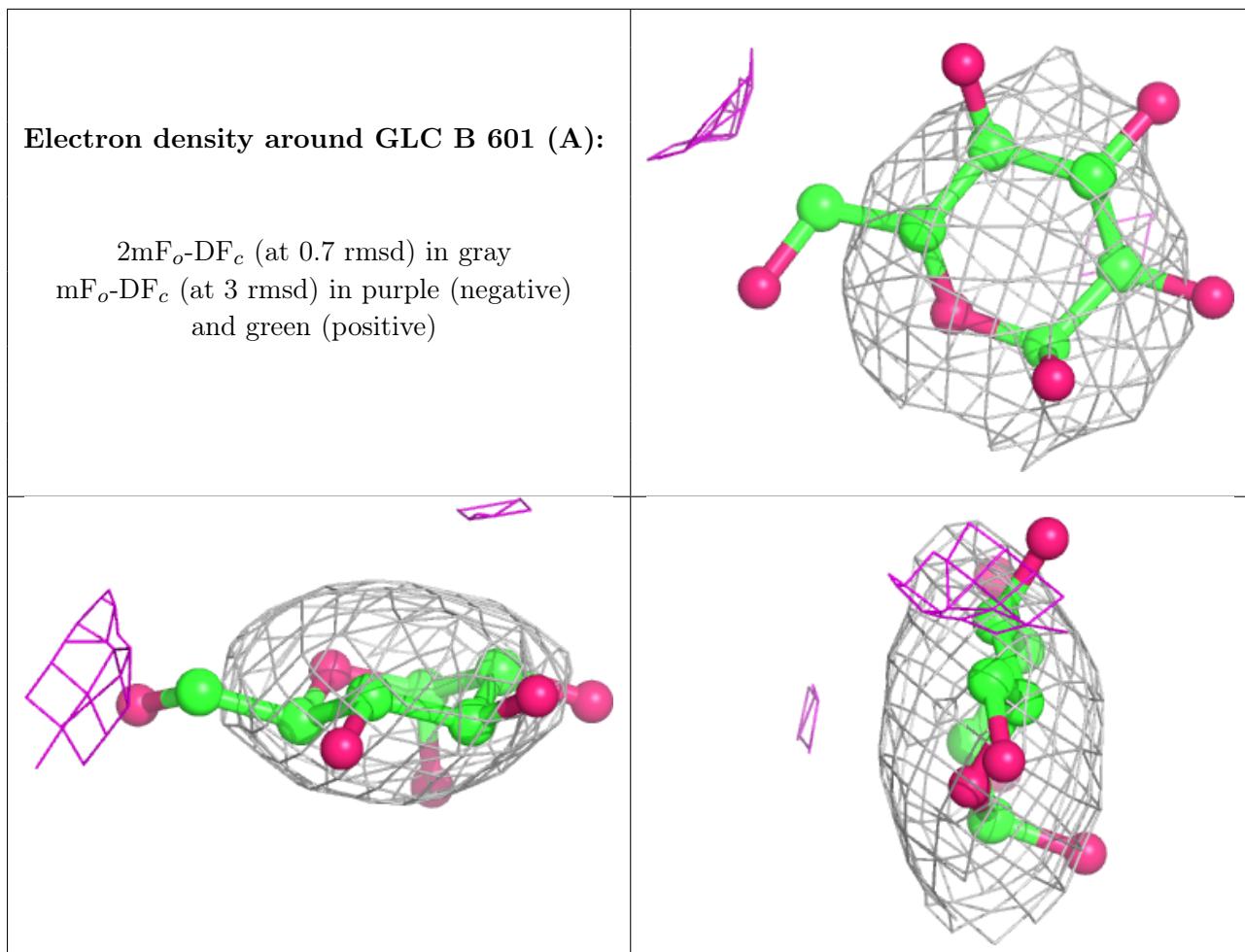
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BGC	C	602[B]	12/12	0.91	0.38	219,219,219,219	12
3	BGC	B	602[B]	12/12	0.92	0.28	227,227,227,227	12
2	GLC	C	601[A]	12/12	0.92	0.37	169,170,170,170	12
2	GLC	B	601[A]	12/12	0.93	0.27	164,165,165,165	12
3	BGC	A	602[B]	12/12	0.94	0.31	215,216,216,216	12
2	GLC	A	601[A]	12/12	0.95	0.29	161,162,162,163	12
3	BGC	D	602[B]	12/12	0.96	0.23	203,203,203,203	12
2	GLC	D	601[A]	12/12	0.97	0.23	204,204,205,205	12

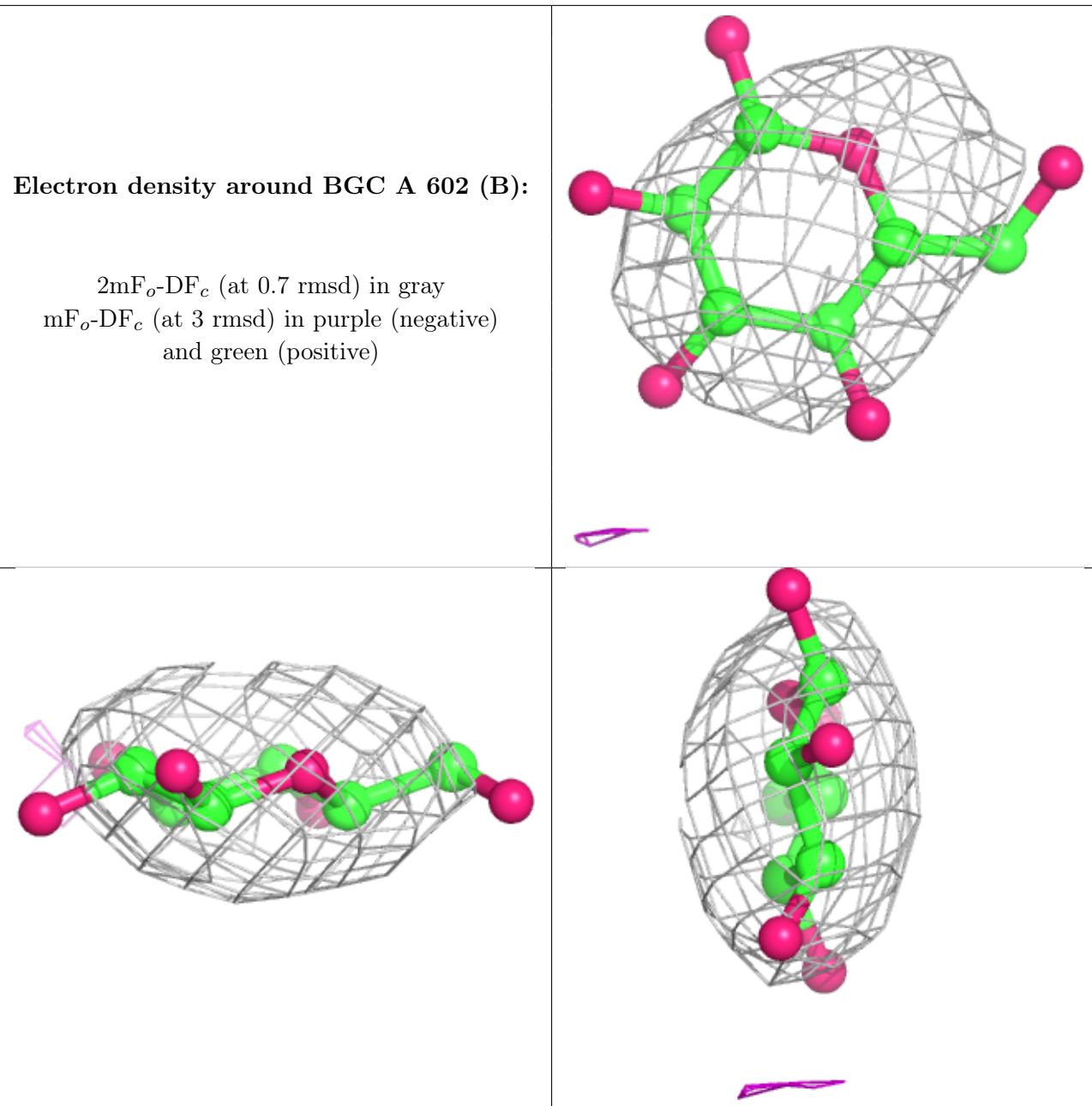
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

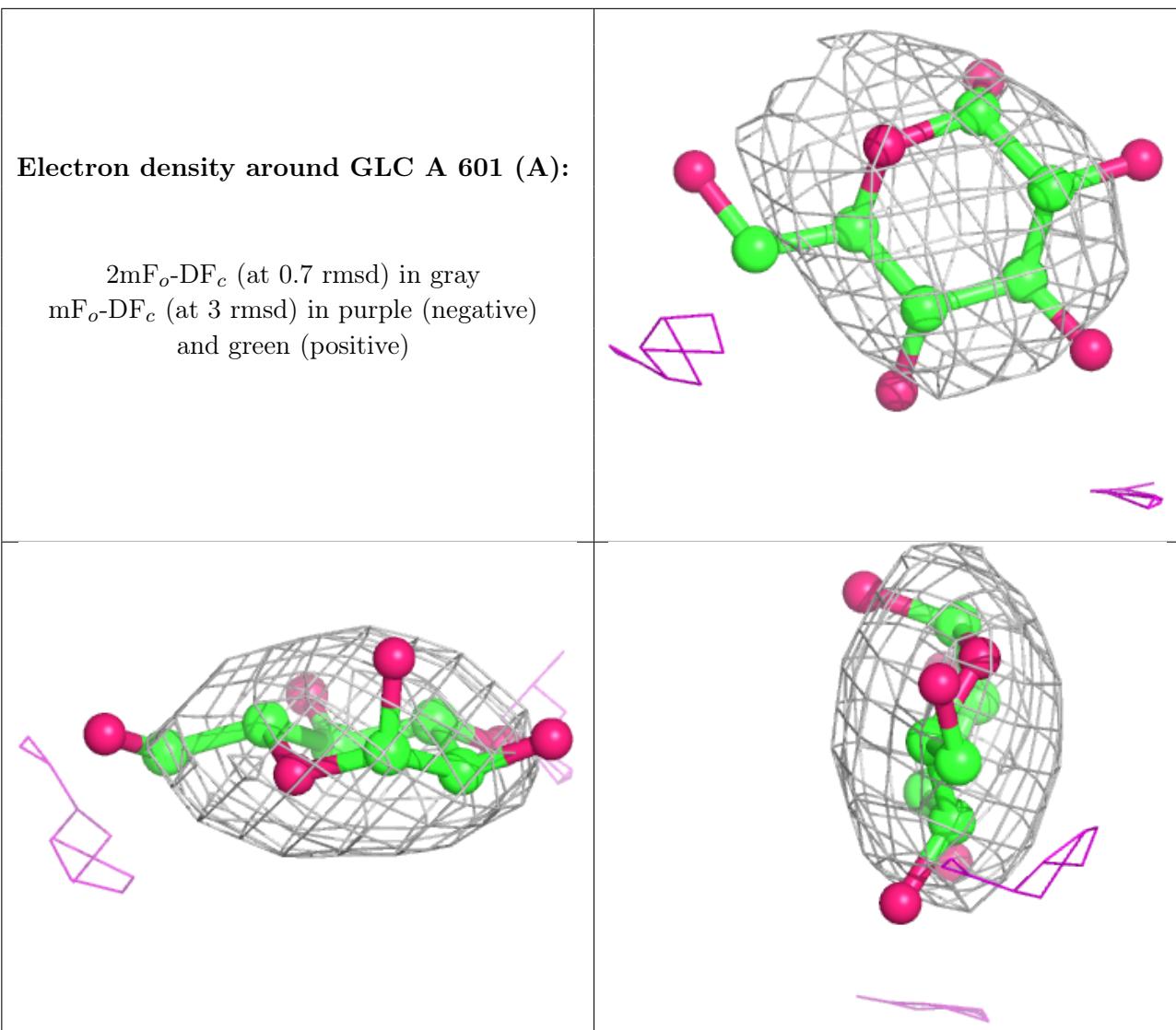


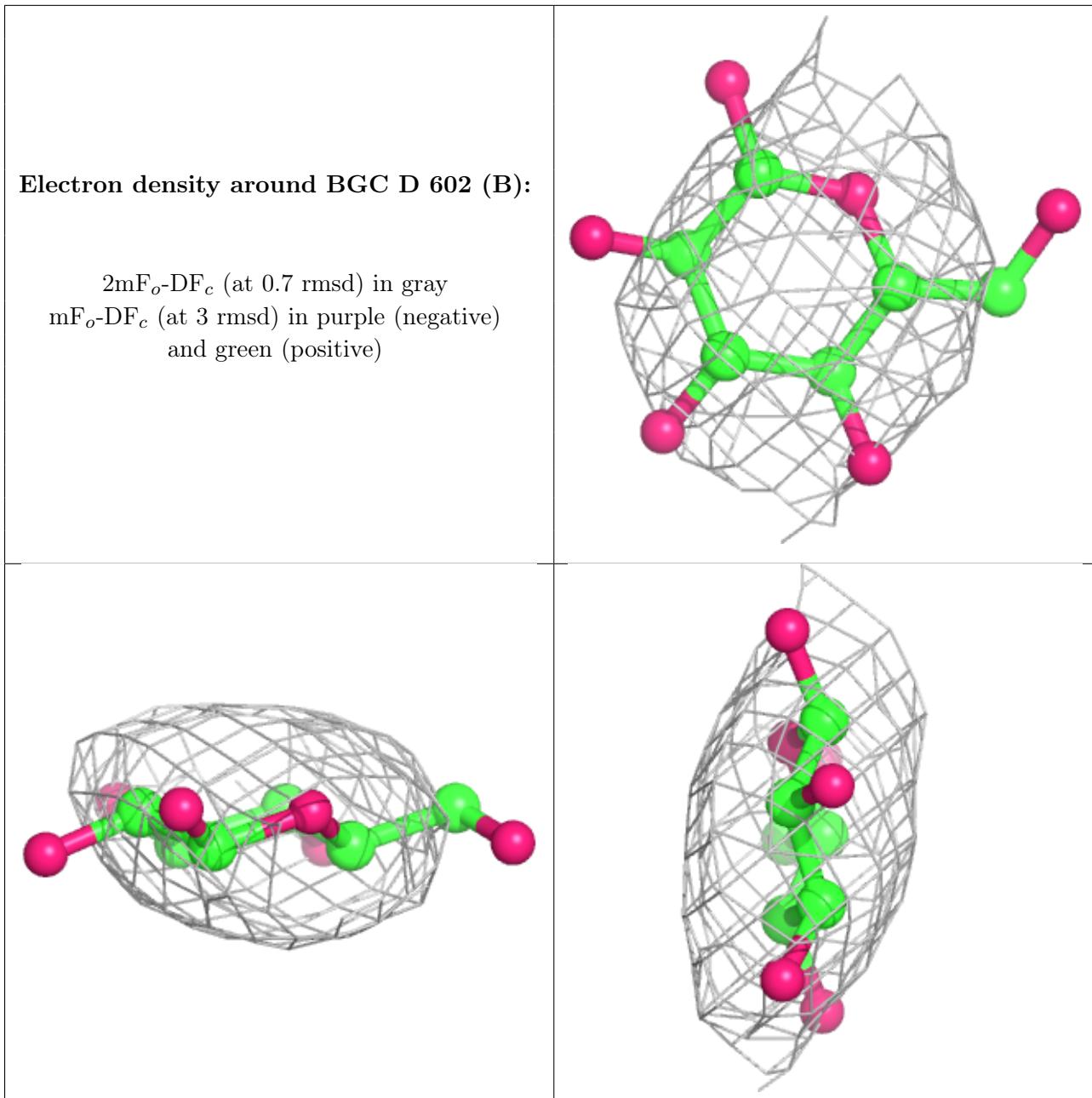


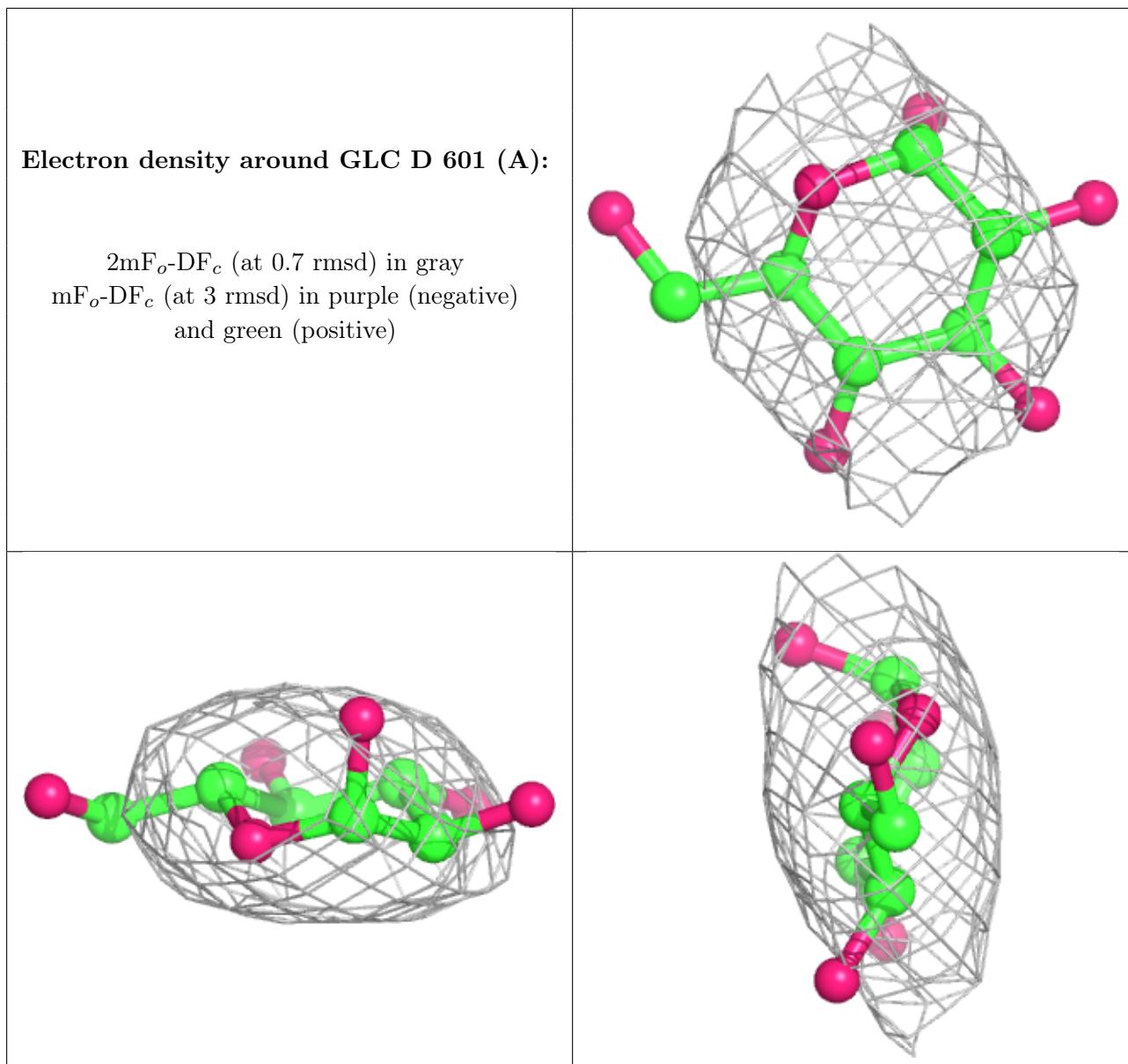












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.