



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:19 PM UTC

PDB ID : 7ZZI / pdb\_00007zzi  
Title : Plasmodium falciparum hexokinase complexed with glucose and citrate  
Authors : Fritz-Wolf, K.; Dillenberger, M.; Rahlfs, S.; Becker, K.  
Deposited on : 2022-05-25  
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

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

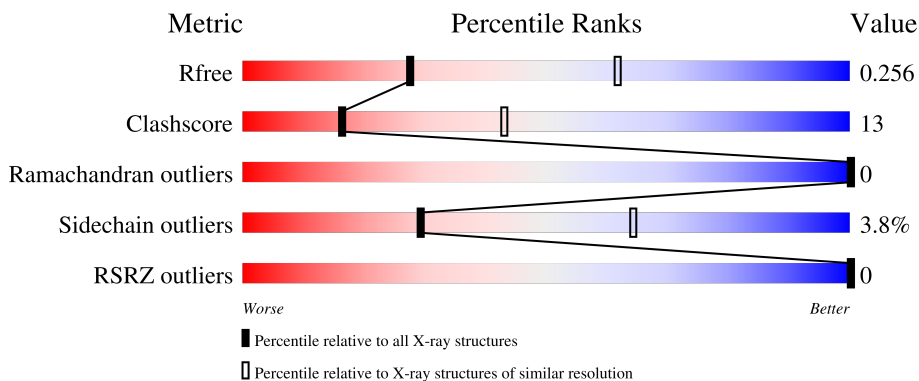
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	493	
1	B	493	

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
3	CIT	A	504	-	X	-	-

## 2 Entry composition [i](#)

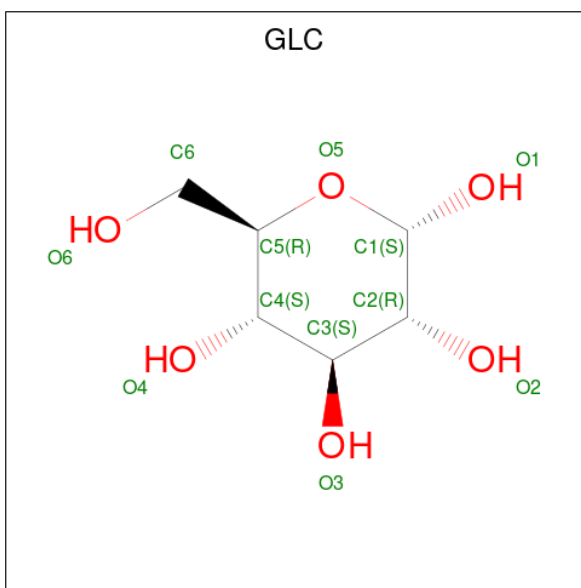
There are 6 unique types of molecules in this entry. The entry contains 7421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	Total 3646	C 2323	N 620	O 680	S 23	0	0	0
1	B	467	Total 3675	C 2342	N 624	O 686	S 23	0	0	0

- Molecule 2 is alpha-D-glucopyranose (CCD ID: 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
			Total	C	O		
2	A	1	Total 12	C 6	O 6	0	0
2	B	1	Total 12	C 6	O 6	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



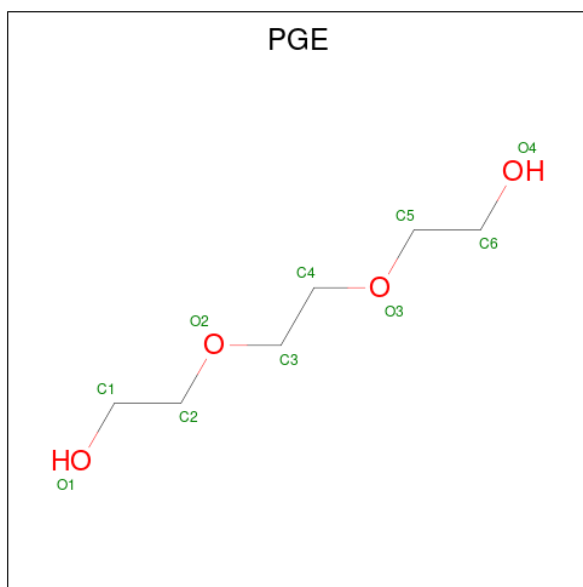
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

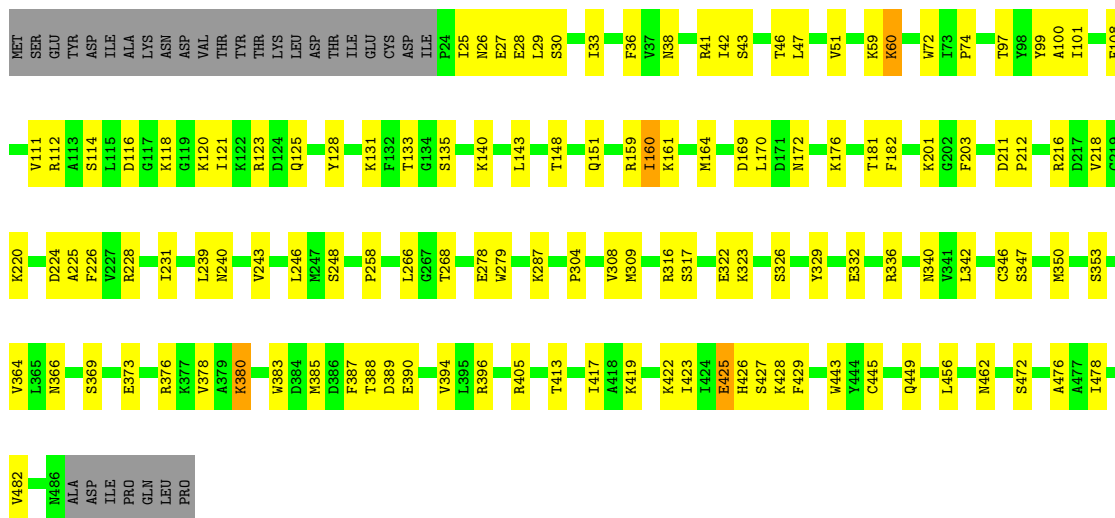
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	15	Total	O	0	0
			15	15		

### 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.

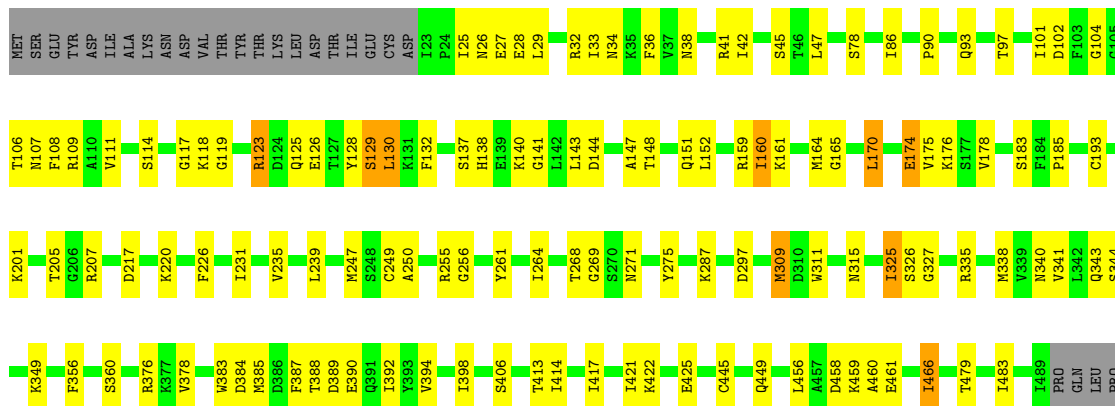
- Molecule 1: Phosphotransferase

Chain A: 



- Molecule 1: Phosphotransferase

Chain B: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.24Å 125.24Å 120.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.48 – 2.80 49.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.48-2.80) 99.9 (49.48-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.199 , 0.268 (Not available) , 0.256	Depositor DCC
$R_{free}$ test set	2746 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.7	Xtrriage
Anisotropy	0.159	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CIT, EDO, GLC, PGE

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	0.44	1/3725 (0.0%)	0.63	1/5026 (0.0%)
1	B	0.45	0/3754	0.68	1/5067 (0.0%)
All	All	0.44	1/7479 (0.0%)	0.65	2/10093 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	LYS	CE-NZ	8.49	1.74	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	LYS	CD-CE-NZ	-5.90	93.01	111.90
1	B	130	LEU	N-CA-C	-5.85	98.33	110.80

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	3646	0	3618	93	0
1	B	3675	0	3648	98	1
2	A	12	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	11	3	0
3	A	26	0	10	4	0
4	A	8	0	12	0	0
4	B	8	0	12	3	0
5	B	10	0	14	4	0
6	A	9	0	0	2	0
6	B	15	0	0	1	0
All	All	7421	0	7336	192	1

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 (192) 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:380:LYS:CE	1:A:380:LYS:NZ	1.74	1.47
1:A:380:LYS:NZ	1:A:380:LYS:HG3	1.74	1.02
1:A:33:ILE:HD11	1:A:394:VAL:HG22	1.51	0.92
1:A:25:ILE:HG22	1:A:390:GLU:HG2	1.51	0.92
1:A:380:LYS:NZ	1:A:380:LYS:CG	2.34	0.91
1:A:380:LYS:HG3	1:A:380:LYS:HZ2	1.35	0.89
1:A:181:THR:HG23	1:A:476:ALA:HB2	1.57	0.85
1:A:426:HIS:HE1	1:A:462:ASN:HD22	1.27	0.83
1:B:126:GLU:HB3	1:B:128:TYR:CE2	2.16	0.80
1:A:380:LYS:NZ	1:A:380:LYS:CD	2.47	0.78
1:B:111:VAL:HG22	1:B:125:GLN:HG3	1.66	0.77
1:B:108:PHE:H	1:B:129:SER:HB3	1.50	0.77
1:B:217:ASP:HB3	5:B:502:PGE:H3	1.67	0.75
1:A:278:GLU:OE2	6:A:601:HOH:O	2.07	0.73
1:B:174:GLU:OE1	1:B:174:GLU:N	2.20	0.72
3:A:504:CIT:O1	3:A:504:CIT:O7	2.06	0.71
1:A:42:ILE:HD11	1:A:405:ARG:HG3	1.74	0.69
1:A:426:HIS:CE1	1:A:462:ASN:HD22	2.10	0.69
1:A:164:MET:HB3	1:A:170:LEU:HB2	1.75	0.69
1:B:165:GLY:HA2	1:B:170:LEU:HB3	1.76	0.68
1:A:380:LYS:CG	1:A:380:LYS:HZ2	2.02	0.68
1:B:338:MET:HE1	1:B:394:VAL:HG12	1.76	0.68
1:A:309:MET:CE	1:A:336:ARG:HD2	2.25	0.67
1:A:133:THR:HG23	1:A:135:SER:H	1.60	0.67
1:A:220:LYS:NZ	1:A:224:ASP:OD2	2.24	0.66
1:B:25:ILE:HD13	1:B:390:GLU:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:HH12	4:B:504:EDO:H12	1.63	0.64
1:B:217:ASP:H	5:B:502:PGE:H22	1.63	0.64
1:A:287:LYS:NZ	6:A:602:HOH:O	2.26	0.63
1:B:118:LYS:HD3	1:B:119:GLY:H	1.63	0.63
1:A:164:MET:HE1	1:A:231:ILE:HG23	1.80	0.62
1:A:419:LYS:O	1:A:423:ILE:HG13	1.99	0.62
1:A:161:LYS:HB2	1:A:231:ILE:HD11	1.81	0.62
1:B:102:ASP:OD2	1:B:109:ARG:NH2	2.32	0.62
1:A:160:ILE:HG23	1:A:164:MET:HE2	1.82	0.61
1:A:148:THR:HG22	1:A:151:GLN:HG3	1.81	0.61
1:A:380:LYS:HG3	1:A:380:LYS:HZ3	1.63	0.60
1:B:338:MET:HA	1:B:338:MET:HE2	1.83	0.59
1:A:422:LYS:HE3	1:A:429:PHE:HE1	1.67	0.59
1:B:101:ILE:HD11	1:B:160:ILE:HD13	1.84	0.59
1:B:456:LEU:HB3	1:B:460:ALA:HA	1.85	0.59
1:B:140:LYS:HB2	1:B:143:LEU:HB2	1.84	0.59
1:A:160:ILE:HG21	1:A:226:PHE:HE1	1.68	0.58
1:B:458:ASP:OD1	1:B:459:LYS:NZ	2.36	0.58
3:A:504:CIT:O7	3:A:504:CIT:O4	2.19	0.57
1:B:325:ILE:HG22	1:B:406:SER:HA	1.86	0.57
1:B:160:ILE:HG21	1:B:226:PHE:HE1	1.68	0.57
1:B:387:PHE:HB3	1:B:392:ILE:HG12	1.86	0.57
1:A:316:ARG:O	1:A:317:SER:OG	2.15	0.57
1:A:385:MET:HE2	1:A:387:PHE:CE1	2.39	0.57
1:A:364:VAL:O	1:A:396:ARG:NH1	2.38	0.57
1:B:86:ILE:HD13	1:B:247:MET:HE2	1.87	0.56
1:B:123:ARG:HH12	1:B:125:GLN:HB2	1.70	0.56
1:A:258:PRO:HB2	1:A:429:PHE:HA	1.87	0.56
1:A:304:PRO:HD3	1:B:311:TRP:CE2	2.41	0.56
1:B:255:ARG:HD2	1:B:255:ARG:C	2.30	0.56
1:A:268:THR:O	1:A:326:SER:OG	2.23	0.56
1:A:160:ILE:HG21	1:A:226:PHE:CE1	2.40	0.55
1:B:160:ILE:HG21	1:B:226:PHE:CE1	2.42	0.55
1:A:38:ASN:HA	1:A:41:ARG:HG3	1.87	0.55
1:A:201:LYS:NZ	2:A:501:GLC:O6	2.37	0.55
1:B:126:GLU:HB3	1:B:128:TYR:HE2	1.70	0.55
1:B:201:LYS:HD3	1:B:269:GLY:HA3	1.88	0.55
1:B:275:TYR:OH	1:B:287:LYS:NZ	2.37	0.55
1:B:108:PHE:H	1:B:129:SER:CB	2.19	0.54
1:B:164:MET:HE1	1:B:176:LYS:HG3	1.89	0.54
1:B:107:ASN:HA	1:B:132:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASN:HA	1:B:132:PHE:CE1	2.43	0.54
1:B:207:ARG:HH12	4:B:504:EDO:C1	2.21	0.54
1:A:172:ASN:OD1	1:A:176:LYS:NZ	2.41	0.53
1:B:36:PHE:CZ	1:B:340:ASN:HB3	2.43	0.53
1:B:34:ASN:O	1:B:38:ASN:ND2	2.40	0.52
1:A:99:TYR:CZ	1:A:164:MET:HG2	2.45	0.52
1:B:249:CYS:SG	1:B:466:ILE:HD11	2.50	0.52
1:A:148:THR:HG23	1:A:151:GLN:H	1.75	0.51
1:B:78:SER:OG	1:B:297:ASP:OD1	2.26	0.51
1:A:148:THR:OG1	1:A:211:ASP:HB3	2.10	0.51
1:B:140:LYS:O	1:B:144:ASP:N	2.44	0.51
1:B:32:ARG:CZ	1:B:343:GLN:HE21	2.23	0.51
1:B:97:THR:HG22	1:B:114:SER:OG	2.11	0.51
1:B:93:GLN:HA	1:B:117:GLY:O	2.11	0.50
1:B:315:ASN:HB3	4:B:504:EDO:O1	2.11	0.50
1:B:255:ARG:HD2	1:B:256:GLY:N	2.27	0.50
1:B:264:ILE:HG13	1:B:414:ILE:HG12	1.93	0.50
1:A:225:ALA:HA	1:A:228:ARG:HH11	1.75	0.50
1:A:309:MET:HE3	1:A:336:ARG:HD2	1.93	0.50
1:B:268:THR:O	1:B:326:SER:OG	2.30	0.50
1:A:181:THR:HG22	1:A:239:LEU:HG	1.93	0.49
1:A:131:LYS:HE2	1:A:140:LYS:HE2	1.95	0.49
1:B:338:MET:HE3	1:B:398:ILE:HB	1.95	0.49
1:B:193:CYS:SG	5:B:502:PGE:H5	2.52	0.49
1:B:413:THR:O	1:B:417:ILE:HG13	2.13	0.49
1:B:161:LYS:CD	1:B:231:ILE:HD11	2.42	0.48
1:A:148:THR:CG2	1:A:151:GLN:HG3	2.43	0.48
1:B:132:PHE:CD2	1:B:143:LEU:HD11	2.48	0.48
1:B:137:SER:O	1:B:140:LYS:HG2	2.14	0.48
1:B:161:LYS:HD3	1:B:231:ILE:HD11	1.95	0.48
1:A:26:ASN:OD1	1:A:28:GLU:N	2.46	0.48
1:B:108:PHE:N	1:B:129:SER:HB3	2.26	0.47
1:A:25:ILE:HG22	1:A:390:GLU:CG	2.35	0.47
1:A:116:ASP:OD1	1:A:120:LYS:HB2	2.14	0.47
1:A:164:MET:HE1	1:A:231:ILE:CG2	2.42	0.47
1:B:38:ASN:HA	1:B:41:ARG:HG3	1.96	0.47
1:A:60:LYS:HA	1:A:60:LYS:HD2	1.63	0.47
1:A:240:ASN:O	1:A:243:VAL:HG22	2.14	0.47
1:A:346:CYS:HB3	1:A:350:MET:HB3	1.96	0.47
1:A:478:ILE:O	1:A:482:VAL:HG23	2.15	0.47
1:A:182:PHE:CD1	1:A:218:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HD3	1:B:343:GLN:NE2	2.29	0.47
1:B:42:ILE:HG22	1:B:47:LEU:HB2	1.96	0.47
1:B:376:ARG:NH1	1:B:387:PHE:O	2.48	0.47
1:A:118:LYS:HD2	1:A:118:LYS:HA	1.55	0.47
1:A:304:PRO:HD3	1:B:311:TRP:CD2	2.50	0.47
1:A:123:ARG:HD2	1:A:125:GLN:HE21	1.80	0.47
1:A:413:THR:O	1:A:417:ILE:HG13	2.15	0.46
1:B:130:LEU:HD23	1:B:143:LEU:HD13	1.97	0.46
1:B:161:LYS:HG3	1:B:170:LEU:HD11	1.97	0.46
1:B:271:ASN:HB2	2:B:501:GLC:H5	1.97	0.46
1:A:422:LYS:HA	1:A:425:GLU:O	2.15	0.46
1:A:118:LYS:O	1:A:120:LYS:N	2.40	0.46
1:A:212:PRO:O	1:A:216:ARG:HD3	2.16	0.46
1:B:90:PRO:HG2	1:B:250:ALA:HB3	1.98	0.46
1:A:445:CYS:O	1:A:449:GLN:HG3	2.16	0.45
1:B:335:ARG:O	1:B:338:MET:HB2	2.16	0.45
1:B:104:GLY:HA2	1:B:183:SER:OG	2.15	0.45
1:A:29:LEU:HD12	1:A:29:LEU:HA	1.74	0.45
1:A:123:ARG:HD2	1:A:125:GLN:NE2	2.32	0.45
1:A:148:THR:HG22	1:A:151:GLN:CG	2.47	0.45
1:A:385:MET:HE3	1:A:385:MET:HB3	1.92	0.45
1:B:461:GLU:H	1:B:461:GLU:HG2	1.24	0.45
1:B:106:THR:HG21	6:B:615:HOH:O	2.17	0.45
1:B:140:LYS:HD3	1:B:144:ASP:HA	1.99	0.45
1:B:118:LYS:HD3	1:B:119:GLY:N	2.29	0.44
1:B:185:PRO:HD3	2:B:501:GLC:O2	2.17	0.44
1:B:201:LYS:NZ	2:B:501:GLC:O5	2.46	0.44
1:B:178:VAL:HG13	1:B:235:VAL:HA	1.99	0.44
1:A:309:MET:HE1	1:A:332:GLU:HG3	1.99	0.44
3:A:502:CIT:O4	3:A:502:CIT:O7	2.33	0.44
1:B:159:ARG:HD3	1:B:159:ARG:HA	1.80	0.44
1:A:366:ASN:OD1	1:A:443:TRP:HB2	2.17	0.44
1:A:99:TYR:CE2	1:A:164:MET:HG2	2.53	0.43
1:B:164:MET:CE	1:B:176:LYS:HG3	2.48	0.43
1:A:159:ARG:HD3	1:A:159:ARG:HA	1.32	0.43
1:A:143:LEU:HG	1:A:203:PHE:CG	2.53	0.43
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.87	0.43
1:B:356:PHE:HB2	1:B:383:TRP:CZ2	2.53	0.43
1:A:248:SER:HA	1:A:478:ILE:CD1	2.47	0.43
1:A:426:HIS:CE1	1:A:462:ASN:ND2	2.83	0.43
1:A:72:TRP:CZ2	1:A:74:PRO:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG21	3:A:504:CIT:H22	2.00	0.43
1:B:376:ARG:HH22	1:B:389:ASP:CG	2.26	0.43
1:A:369:SER:OG	1:A:373:GLU:N	2.52	0.43
1:B:479:THR:O	1:B:483:ILE:HD12	2.19	0.43
1:A:347:SER:OG	1:A:383:TRP:O	2.35	0.43
1:B:385:MET:HE2	1:B:387:PHE:CE1	2.54	0.43
1:B:309:MET:HE2	1:B:309:MET:HB3	1.61	0.43
1:B:138:HIS:C	1:B:140:LYS:H	2.27	0.42
1:A:97:THR:HA	1:A:114:SER:HA	2.01	0.42
1:A:100:ALA:HB3	1:A:111:VAL:CG1	2.49	0.42
1:B:141:GLY:O	1:B:147:ALA:HB2	2.19	0.42
1:A:128:TYR:CD1	1:A:159:ARG:HG3	2.55	0.42
1:A:181:THR:HG21	1:A:472:SER:O	2.19	0.42
1:A:36:PHE:CZ	1:A:340:ASN:HB3	2.55	0.42
1:A:112:ARG:NH2	1:A:169:ASP:OD2	2.38	0.42
1:B:326:SER:OG	1:B:327:GLY:N	2.52	0.42
1:B:349:LYS:HE3	1:B:384:ASP:OD1	2.18	0.42
1:A:376:ARG:NH2	1:A:389:ASP:OD1	2.42	0.42
1:B:445:CYS:O	1:B:449:GLN:HG3	2.19	0.42
1:B:201:LYS:HD2	1:B:268:THR:HG22	2.01	0.42
1:A:323:LYS:HA	1:A:329:TYR:CD2	2.54	0.42
1:B:118:LYS:CD	1:B:119:GLY:H	2.30	0.42
1:A:25:ILE:O	1:A:25:ILE:HD12	2.20	0.41
1:B:422:LYS:HZ2	1:B:422:LYS:HG2	1.63	0.41
1:A:47:LEU:O	1:A:51:VAL:HG23	2.20	0.41
1:B:456:LEU:HD23	1:B:456:LEU:HA	1.93	0.41
1:A:322:GLU:O	1:A:326:SER:HB3	2.20	0.41
1:B:220:LYS:HG3	5:B:502:PGE:H32	2.02	0.41
1:B:261:TYR:HB3	1:B:421:ILE:HD13	2.01	0.41
1:B:33:ILE:HG22	1:B:341:VAL:HG11	2.02	0.41
1:B:360:SER:HB3	1:B:378:VAL:CG1	2.51	0.41
1:B:376:ARG:HG2	1:B:392:ILE:HG13	2.02	0.41
1:B:349:LYS:HE3	1:B:384:ASP:HB2	2.02	0.41
1:A:350:MET:HE3	1:A:383:TRP:CE3	2.55	0.41
1:B:148:THR:OG1	1:B:151:GLN:HG3	2.20	0.41
1:B:152:LEU:HD22	1:B:205:THR:HG21	2.02	0.41
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.93	0.41
1:A:279:TRP:NE1	1:A:287:LYS:HG2	2.36	0.41
1:A:160:ILE:HD12	1:A:160:ILE:HA	1.78	0.40
1:B:456:LEU:HB3	1:B:460:ALA:CA	2.48	0.40
1:B:239:LEU:HD23	1:B:239:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:OG	1:A:46:THR:HG23	2.21	0.40
1:B:26:ASN:HB3	1:B:29:LEU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLU:N	1:B:461:GLU:OE2[3_664]	2.08	0.12

## 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	461/493 (94%)	448 (97%)	13 (3%)	0	100	100
1	B	465/493 (94%)	442 (95%)	23 (5%)	0	100	100
All	All	926/986 (94%)	890 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	392/420 (93%)	376 (96%)	16 (4%)	27	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	395/420 (94%)	381 (96%)	14 (4%)	32	67
All	All	787/840 (94%)	757 (96%)	30 (4%)	29	64

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	30	SER
1	A	59	LYS
1	A	60	LYS
1	A	101	ILE
1	A	108	PHE
1	A	121	ILE
1	A	160	ILE
1	A	246	LEU
1	A	342	LEU
1	A	353	SER
1	A	378	VAL
1	A	388	THR
1	A	425	GLU
1	A	427	SER
1	A	428	LYS
1	B	28	GLU
1	B	45	SER
1	B	123	ARG
1	B	129	SER
1	B	160	ILE
1	B	170	LEU
1	B	174	GLU
1	B	175	VAL
1	B	309	MET
1	B	325	ILE
1	B	344	SER
1	B	388	THR
1	B	425	GLU
1	B	466	ILE

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	39	GLN

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Mol	Chain	Res	Type
1	A	138	HIS
1	A	319	GLN
1	A	426	HIS
1	B	125	GLN
1	B	151	GLN
1	B	168	ASN
1	B	252	GLN
1	B	343	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

9 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
2	GLC	A	501	-	12,12,12	1.23	1 (8%)	17,17,17	1.22	3 (17%)
4	EDO	A	503	-	3,3,3	0.53	0	2,2,2	0.12	0
5	PGE	B	502	-	9,9,9	0.35	0	8,8,8	0.44	0
4	EDO	B	503	-	3,3,3	0.51	0	2,2,2	0.25	0
3	CIT	A	504	-	12,12,12	1.16	0	17,17,17	2.40	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	B	501	-	12,12,12	1.16	1 (8%)	17,17,17	1.20	1 (5%)
4	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.23	0
4	EDO	B	504	-	3,3,3	0.52	0	2,2,2	0.96	0
3	CIT	A	502	-	12,12,12	1.15	0	17,17,17	1.33	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	GLC	A	501	-	-	2/2/22/22	0/1/1/1
4	EDO	A	503	-	-	1/1/1/1	-
5	PGE	B	502	-	-	7/7/7/7	-
4	EDO	B	503	-	-	0/1/1/1	-
3	CIT	A	504	-	-	13/16/16/16	-
2	GLC	B	501	-	-	0/2/22/22	0/1/1/1
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
3	CIT	A	502	-	-	6/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GLC	O5-C1	3.11	1.50	1.42
2	B	501	GLC	O5-C1	2.73	1.49	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	CIT	O7-C3-C6	6.05	117.54	108.96
3	A	504	CIT	C4-C3-C6	-4.22	100.70	110.03
3	A	504	CIT	C4-C3-C2	3.32	117.82	109.31
2	B	501	GLC	O2-C2-C1	-3.03	102.25	109.25
3	A	504	CIT	O2-C1-C2	2.78	123.16	114.35
2	A	501	GLC	C6-C5-C4	-2.72	106.35	113.02
3	A	502	CIT	C3-C4-C5	-2.44	107.24	113.92
3	A	504	CIT	O4-C5-O3	-2.25	117.55	123.33
2	A	501	GLC	O5-C5-C4	2.18	113.62	109.70
3	A	502	CIT	O4-C5-C4	2.10	121.00	114.35
2	A	501	GLC	O5-C1-C2	2.10	113.98	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	CIT	O1-C1-C2	-2.08	117.05	122.95

There are no chirality outliers.

All (31) torsion outliers are listed below:

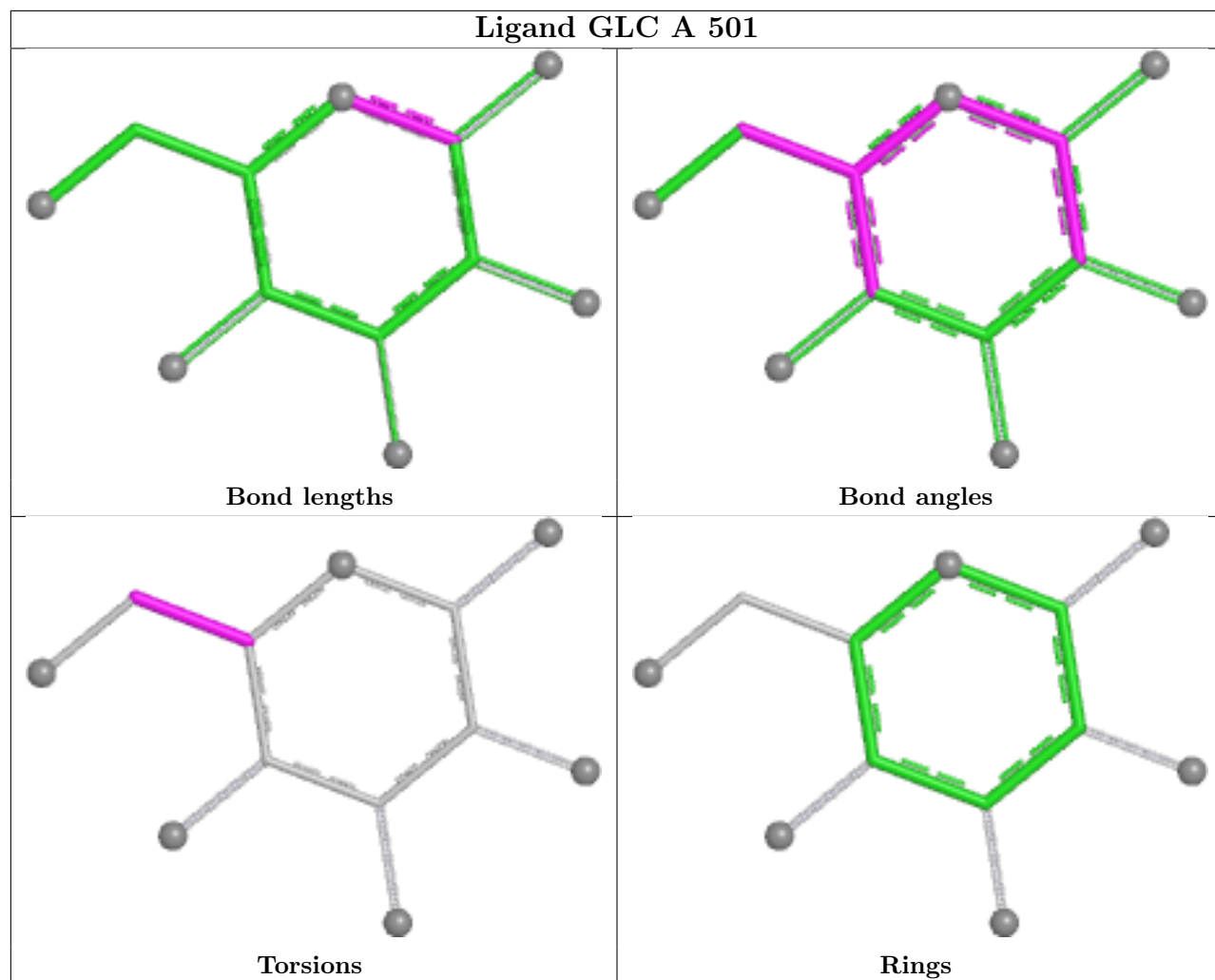
Mol	Chain	Res	Type	Atoms
3	A	502	CIT	O7-C3-C4-C5
3	A	502	CIT	C6-C3-C4-C5
5	B	502	PGE	C1-C2-O2-C3
3	A	502	CIT	C2-C3-C4-C5
5	B	502	PGE	O2-C3-C4-O3
5	B	502	PGE	O3-C5-C6-O4
2	A	501	GLC	C4-C5-C6-O6
2	A	501	GLC	O5-C5-C6-O6
3	A	502	CIT	C1-C2-C3-O7
3	A	502	CIT	C1-C2-C3-C6
3	A	504	CIT	C1-C2-C3-C6
3	A	504	CIT	C6-C3-C4-C5
5	B	502	PGE	O1-C1-C2-O2
3	A	504	CIT	C1-C2-C3-O7
3	A	504	CIT	O7-C3-C4-C5
3	A	502	CIT	C1-C2-C3-C4
4	B	504	EDO	O1-C1-C2-O2
3	A	504	CIT	C2-C3-C4-C5
3	A	504	CIT	C1-C2-C3-C4
3	A	504	CIT	C2-C3-C6-O6
5	B	502	PGE	C3-C4-O3-C5
3	A	504	CIT	C2-C3-C6-O5
4	A	503	EDO	O1-C1-C2-O2
5	B	502	PGE	C6-C5-O3-C4
3	A	504	CIT	C4-C3-C6-O6
4	A	505	EDO	O1-C1-C2-O2
3	A	504	CIT	C3-C4-C5-O4
3	A	504	CIT	O7-C3-C6-O5
3	A	504	CIT	O7-C3-C6-O6
3	A	504	CIT	C3-C4-C5-O3
5	B	502	PGE	C4-C3-O2-C2

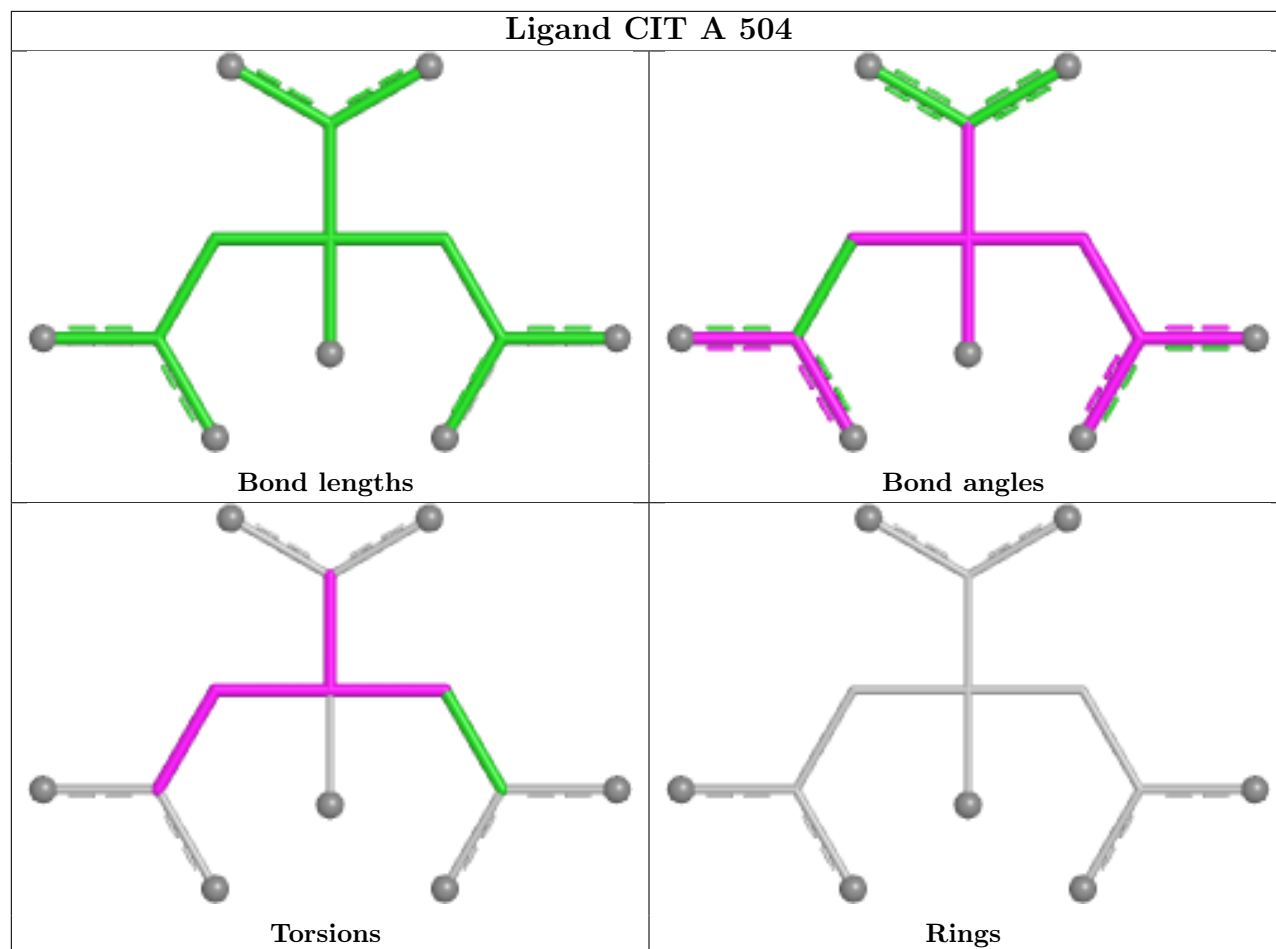
There are no ring outliers.

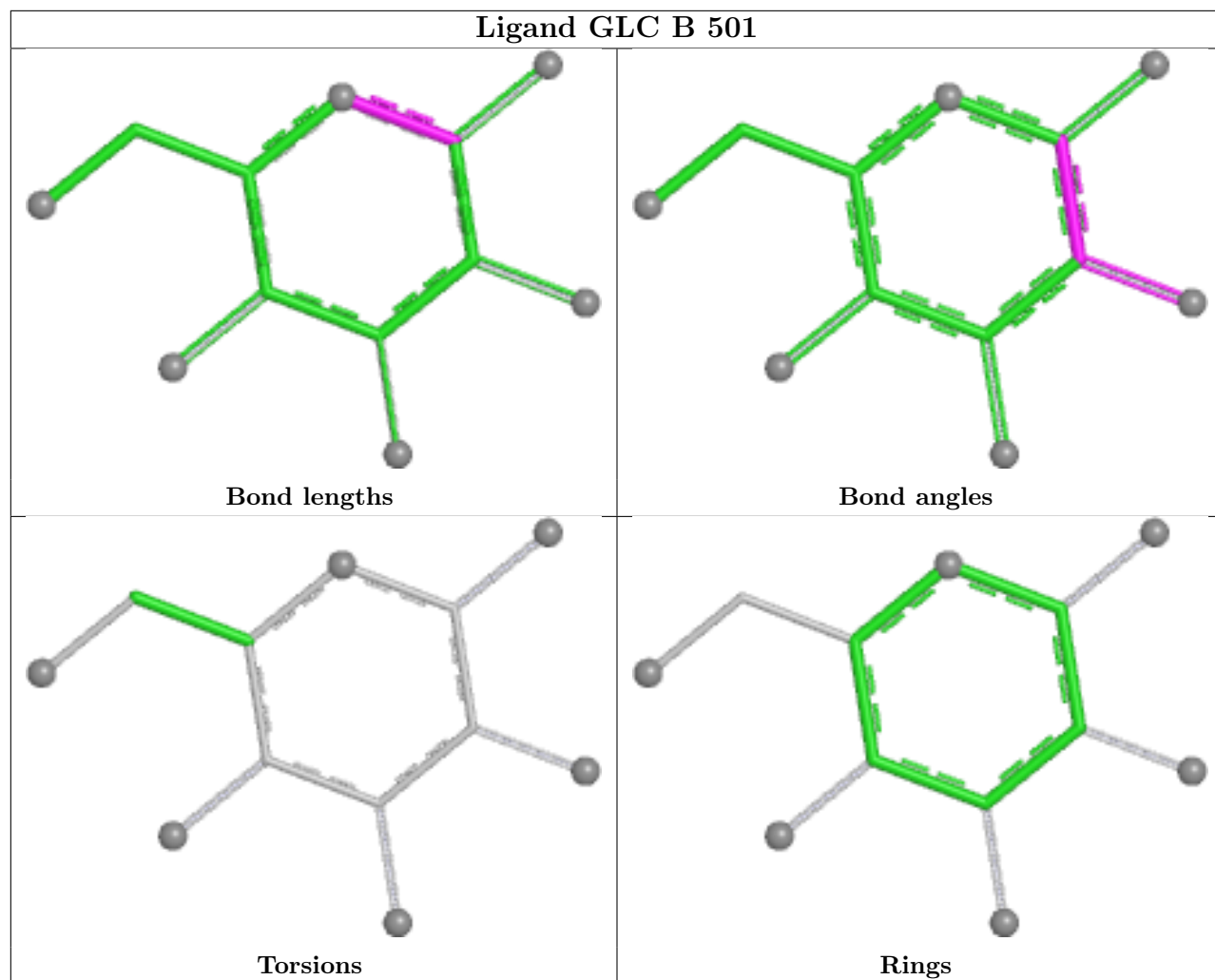
6 monomers are involved in 15 short contacts:

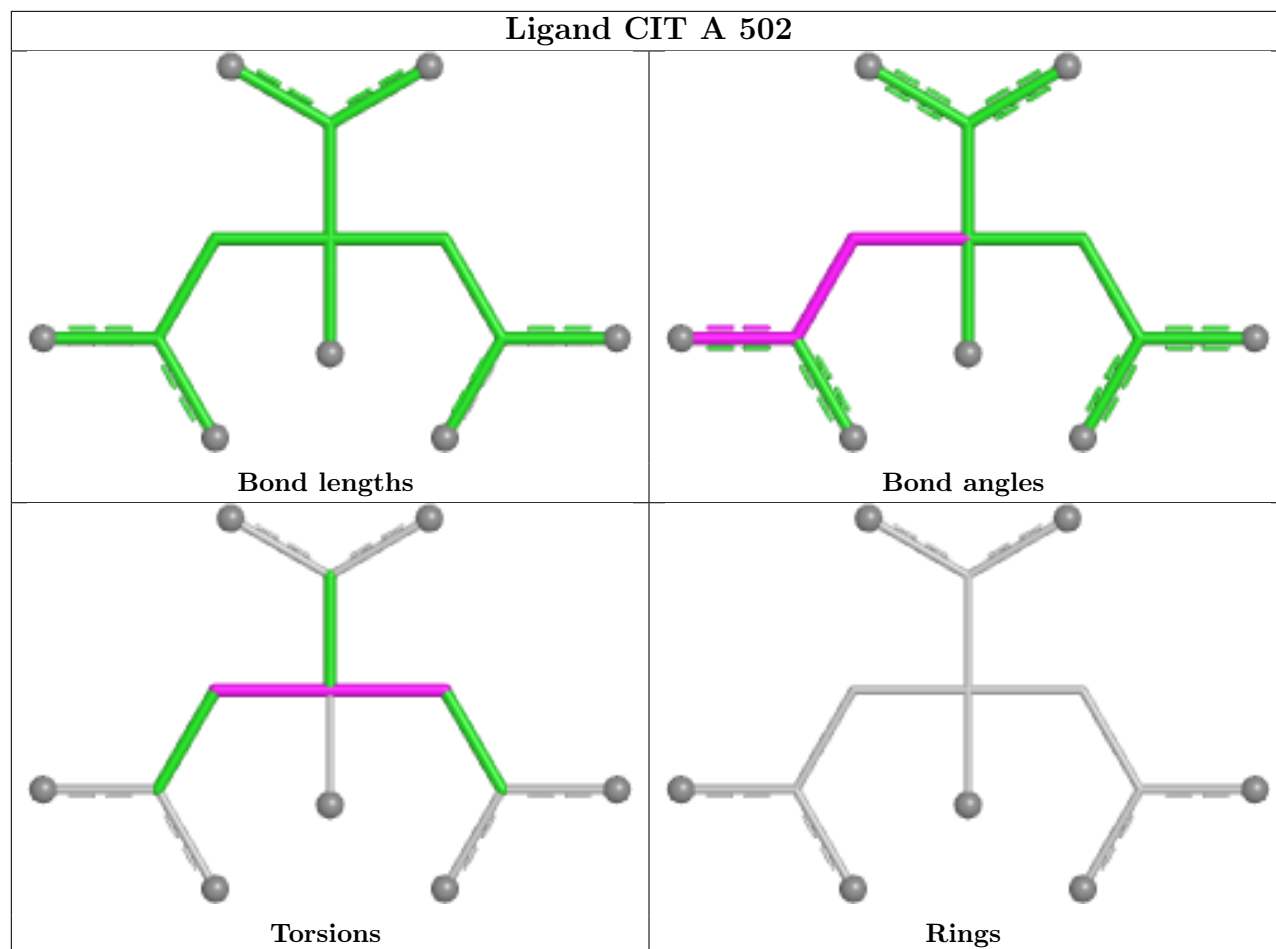
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GLC	1	0
5	B	502	PGE	4	0
3	A	504	CIT	3	0
2	B	501	GLC	3	0
4	B	504	EDO	3	0
3	A	502	CIT	1	0

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, 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	463/493 (93%)	-0.63	0 100 100	64, 91, 122, 141	0
1	B	467/493 (94%)	-0.63	0 100 100	60, 84, 119, 140	0
All	All	930/986 (94%)	-0.63	0 100 100	60, 87, 121, 141	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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.

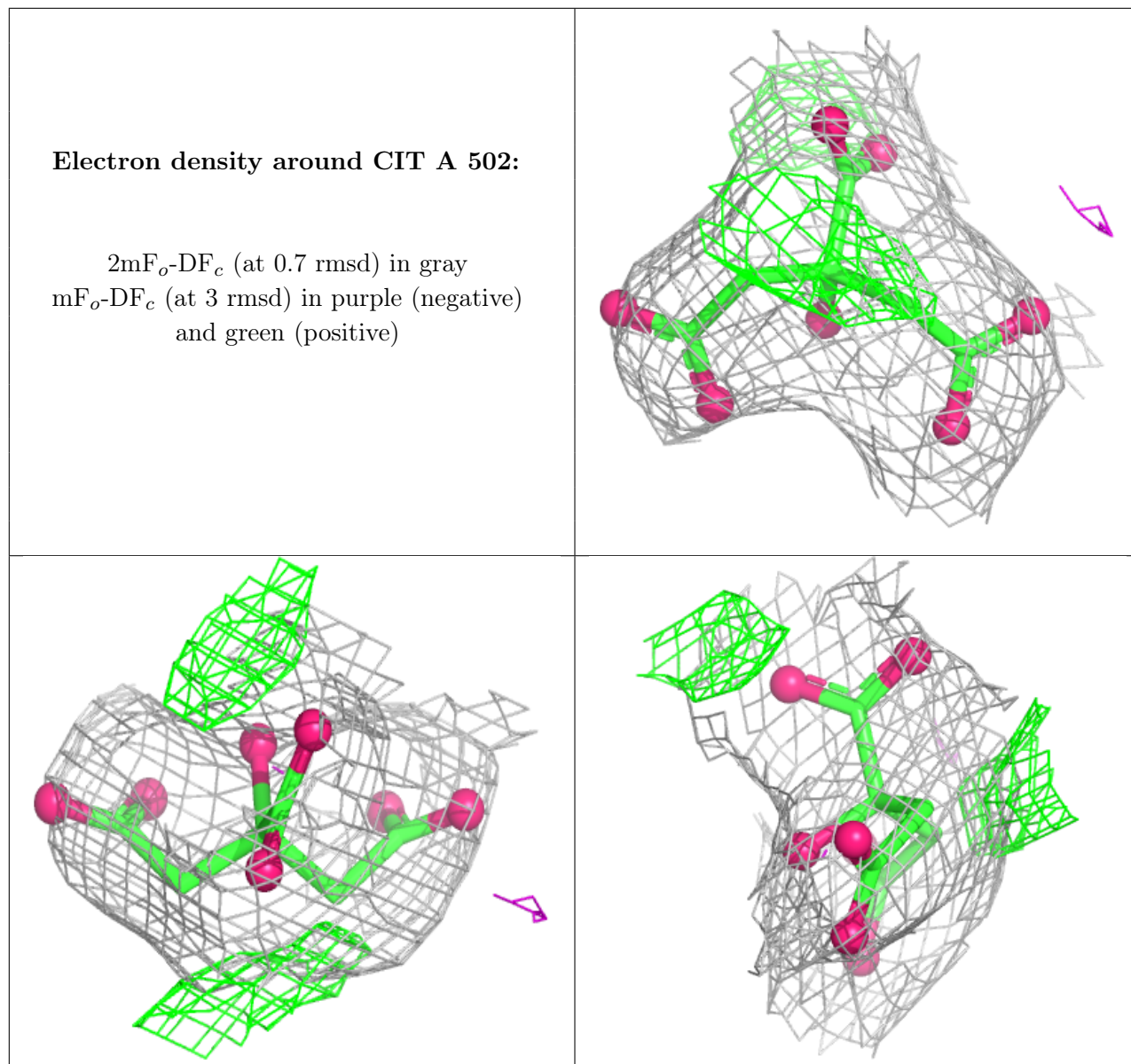
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CIT	A	502	13/13	0.67	0.10	91,98,114,117	0
4	EDO	A	505	4/4	0.71	0.14	86,87,96,99	0
3	CIT	A	504	13/13	0.81	0.11	77,89,103,104	0
4	EDO	B	503	4/4	0.85	0.16	68,76,76,80	4
4	EDO	B	504	4/4	0.90	0.09	66,69,76,84	0
5	PGE	B	502	10/10	0.90	0.11	77,78,79,79	10
4	EDO	A	503	4/4	0.92	0.08	57,70,70,77	4

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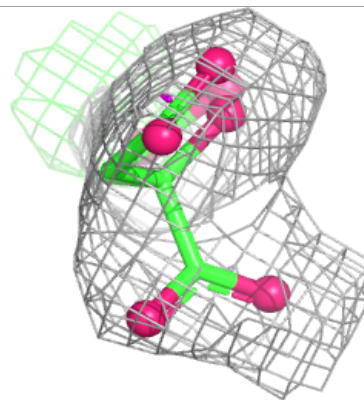
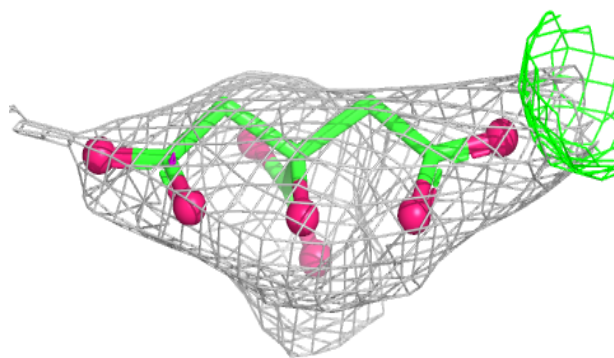
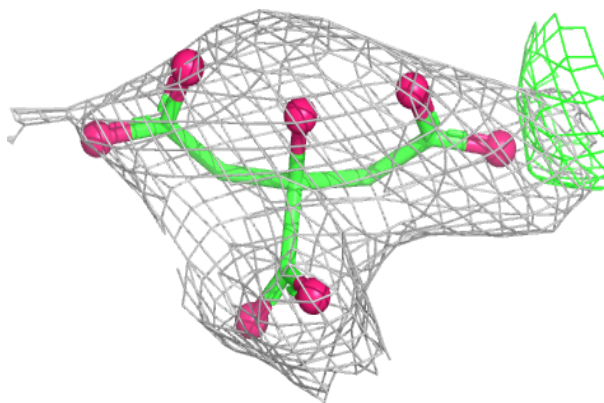
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	B	501	12/12	0.95	0.06	58,64,70,74	0
2	GLC	A	501	12/12	0.95	0.05	73,79,87,89	0

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.



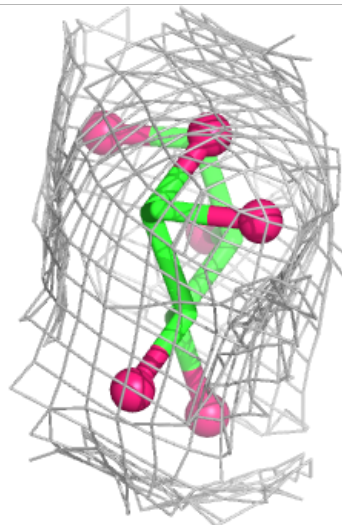
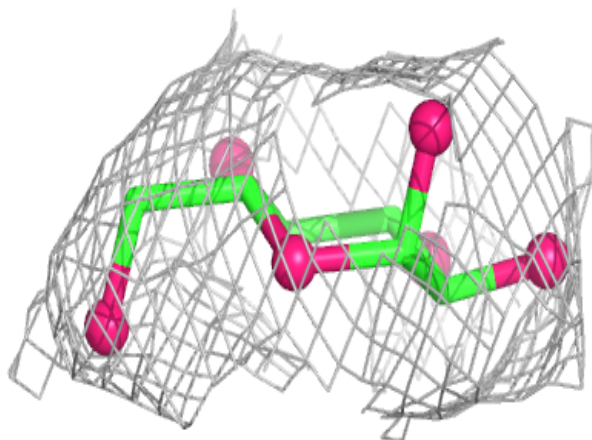
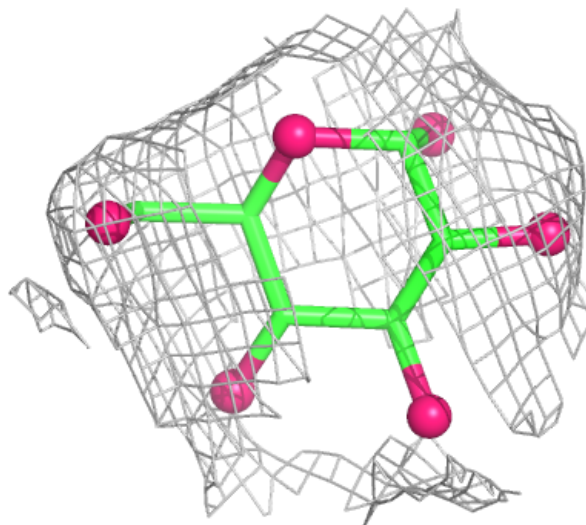
**Electron density around CIT A 504:**

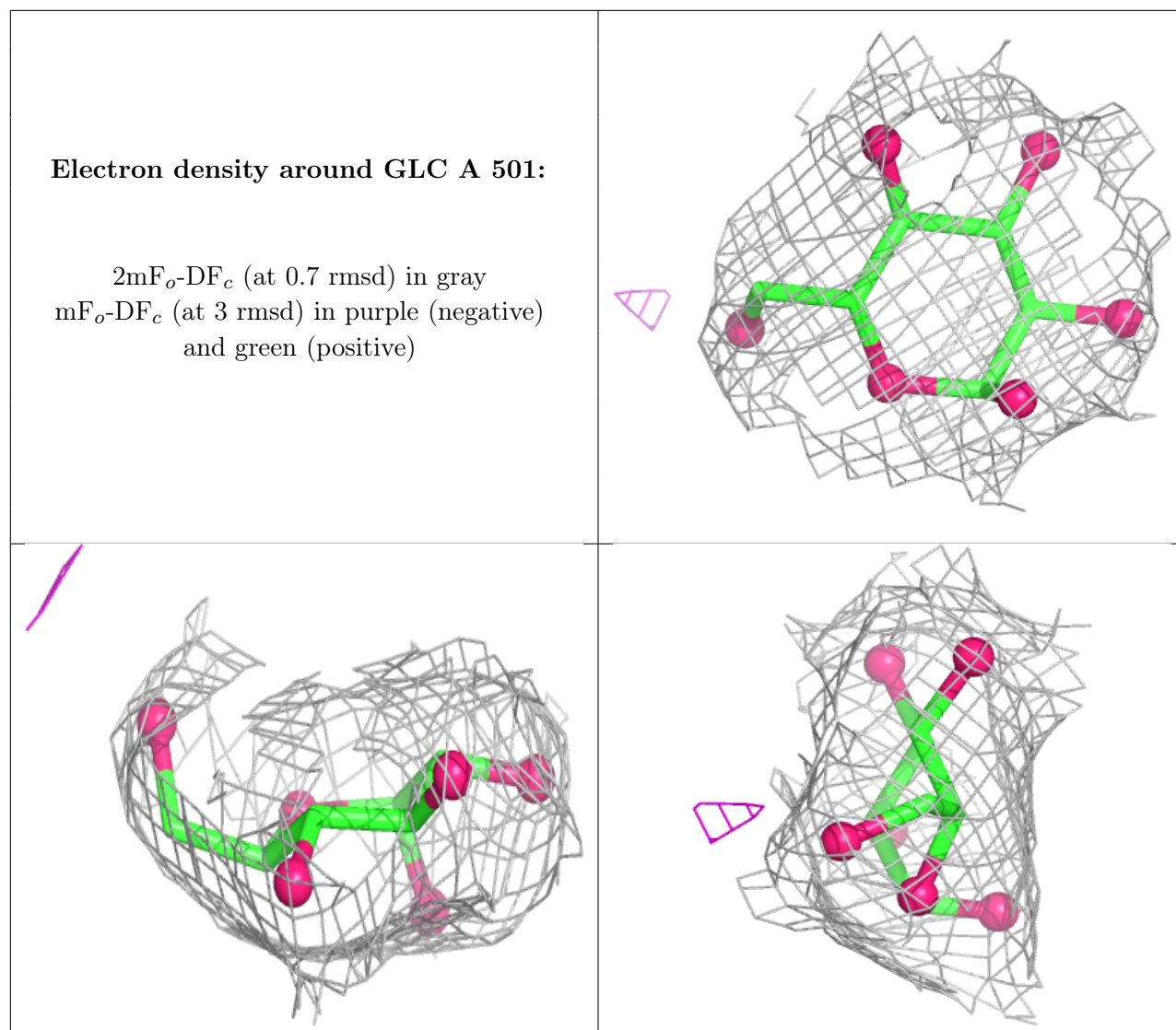
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GLC B 501:**

$2mF_o-DF_c$  (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.