



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:29 AM UTC

PDB ID : 8IBS / pdb_00008ibs
Title : Crystal structure of GH42 beta-galactosidase BiBga42A from Bifidobacterium longum subspecies infantis E160A/E318A mutant in complex with galactose
Authors : Hidaka, M.; Fushinobu, S.; Gotoh, A.; Katayama, T.
Deposited on : 2023-02-10
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

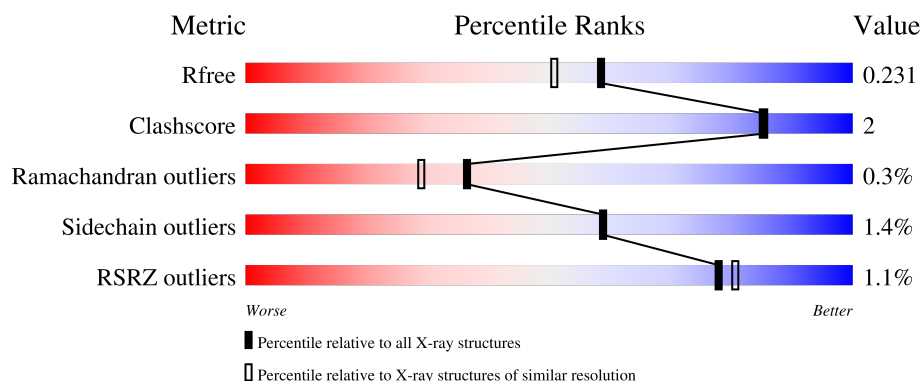
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	702	91% 7%
1	B	702	90% 8%
1	C	702	92% 6%
1	D	702	91% 7%
1	E	702	92% 6%

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Mol	Chain	Length	Quality of chain
1	F	702	2% 92% 5% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35731 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5464	3475	934	1033	22			
1	B	691	Total	C	N	O	S	0	0	0
			5464	3475	934	1033	22			
1	C	691	Total	C	N	O	S	0	0	0
			5464	3475	934	1033	22			
1	D	691	Total	C	N	O	S	0	0	0
			5464	3475	934	1033	22			
1	E	691	Total	C	N	O	S	0	1	0
			5469	3478	934	1035	22			
1	F	691	Total	C	N	O	S	0	0	0
			5464	3475	934	1033	22			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	GLU	engineered mutation	UNP B7GUD7
A	318	ALA	GLU	engineered mutation	UNP B7GUD7
A	692	ALA	-	expression tag	UNP B7GUD7
A	693	ALA	-	expression tag	UNP B7GUD7
A	694	ALA	-	expression tag	UNP B7GUD7
A	695	LEU	-	expression tag	UNP B7GUD7
A	696	GLU	-	expression tag	UNP B7GUD7
A	697	HIS	-	expression tag	UNP B7GUD7
A	698	HIS	-	expression tag	UNP B7GUD7
A	699	HIS	-	expression tag	UNP B7GUD7
A	700	HIS	-	expression tag	UNP B7GUD7
A	701	HIS	-	expression tag	UNP B7GUD7
A	702	HIS	-	expression tag	UNP B7GUD7
B	160	ALA	GLU	engineered mutation	UNP B7GUD7
B	318	ALA	GLU	engineered mutation	UNP B7GUD7
B	692	ALA	-	expression tag	UNP B7GUD7
B	693	ALA	-	expression tag	UNP B7GUD7

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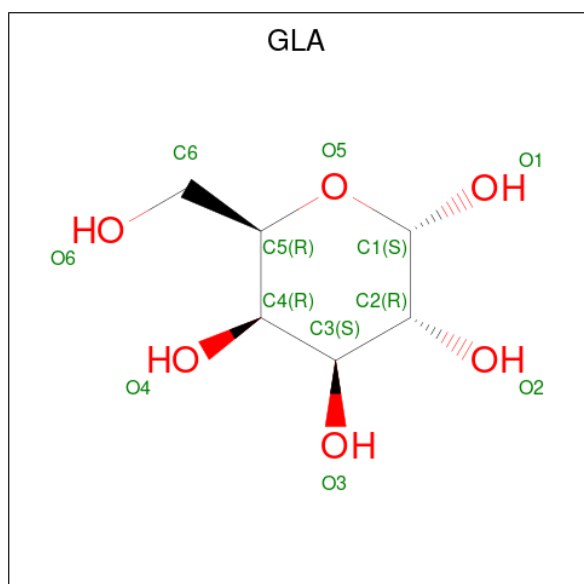
Chain	Residue	Modelled	Actual	Comment	Reference
B	694	ALA	-	expression tag	UNP B7GUD7
B	695	LEU	-	expression tag	UNP B7GUD7
B	696	GLU	-	expression tag	UNP B7GUD7
B	697	HIS	-	expression tag	UNP B7GUD7
B	698	HIS	-	expression tag	UNP B7GUD7
B	699	HIS	-	expression tag	UNP B7GUD7
B	700	HIS	-	expression tag	UNP B7GUD7
B	701	HIS	-	expression tag	UNP B7GUD7
B	702	HIS	-	expression tag	UNP B7GUD7
C	160	ALA	GLU	engineered mutation	UNP B7GUD7
C	318	ALA	GLU	engineered mutation	UNP B7GUD7
C	692	ALA	-	expression tag	UNP B7GUD7
C	693	ALA	-	expression tag	UNP B7GUD7
C	694	ALA	-	expression tag	UNP B7GUD7
C	695	LEU	-	expression tag	UNP B7GUD7
C	696	GLU	-	expression tag	UNP B7GUD7
C	697	HIS	-	expression tag	UNP B7GUD7
C	698	HIS	-	expression tag	UNP B7GUD7
C	699	HIS	-	expression tag	UNP B7GUD7
C	700	HIS	-	expression tag	UNP B7GUD7
C	701	HIS	-	expression tag	UNP B7GUD7
C	702	HIS	-	expression tag	UNP B7GUD7
D	160	ALA	GLU	engineered mutation	UNP B7GUD7
D	318	ALA	GLU	engineered mutation	UNP B7GUD7
D	692	ALA	-	expression tag	UNP B7GUD7
D	693	ALA	-	expression tag	UNP B7GUD7
D	694	ALA	-	expression tag	UNP B7GUD7
D	695	LEU	-	expression tag	UNP B7GUD7
D	696	GLU	-	expression tag	UNP B7GUD7
D	697	HIS	-	expression tag	UNP B7GUD7
D	698	HIS	-	expression tag	UNP B7GUD7
D	699	HIS	-	expression tag	UNP B7GUD7
D	700	HIS	-	expression tag	UNP B7GUD7
D	701	HIS	-	expression tag	UNP B7GUD7
D	702	HIS	-	expression tag	UNP B7GUD7
E	160	ALA	GLU	engineered mutation	UNP B7GUD7
E	318	ALA	GLU	engineered mutation	UNP B7GUD7
E	692	ALA	-	expression tag	UNP B7GUD7
E	693	ALA	-	expression tag	UNP B7GUD7
E	694	ALA	-	expression tag	UNP B7GUD7
E	695	LEU	-	expression tag	UNP B7GUD7
E	696	GLU	-	expression tag	UNP B7GUD7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	697	HIS	-	expression tag	UNP B7GUD7
E	698	HIS	-	expression tag	UNP B7GUD7
E	699	HIS	-	expression tag	UNP B7GUD7
E	700	HIS	-	expression tag	UNP B7GUD7
E	701	HIS	-	expression tag	UNP B7GUD7
E	702	HIS	-	expression tag	UNP B7GUD7
F	160	ALA	GLU	engineered mutation	UNP B7GUD7
F	318	ALA	GLU	engineered mutation	UNP B7GUD7
F	692	ALA	-	expression tag	UNP B7GUD7
F	693	ALA	-	expression tag	UNP B7GUD7
F	694	ALA	-	expression tag	UNP B7GUD7
F	695	LEU	-	expression tag	UNP B7GUD7
F	696	GLU	-	expression tag	UNP B7GUD7
F	697	HIS	-	expression tag	UNP B7GUD7
F	698	HIS	-	expression tag	UNP B7GUD7
F	699	HIS	-	expression tag	UNP B7GUD7
F	700	HIS	-	expression tag	UNP B7GUD7
F	701	HIS	-	expression tag	UNP B7GUD7
F	702	HIS	-	expression tag	UNP B7GUD7

- Molecule 2 is alpha-D-galactopyranose (CCD ID: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

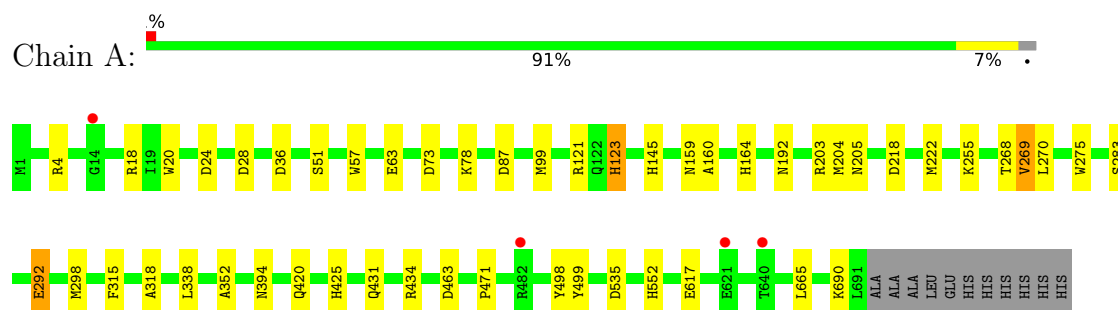
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	525	Total	O	0	0
			525	525		
3	B	505	Total	O	0	0
			505	505		
3	C	519	Total	O	0	0
			519	519		
3	D	490	Total	O	0	0
			490	490		
3	E	422	Total	O	0	0
			422	422		
3	F	409	Total	O	0	0
			409	409		

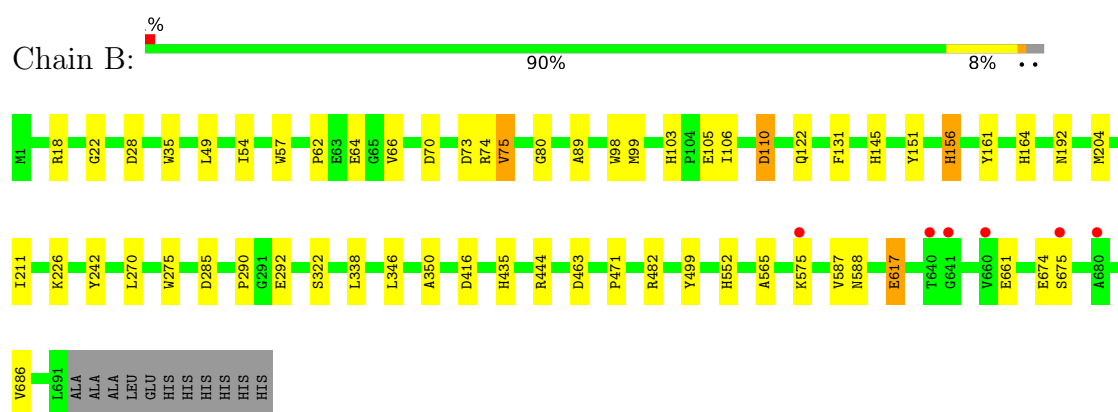
3 Residue-property plots [i](#)

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.

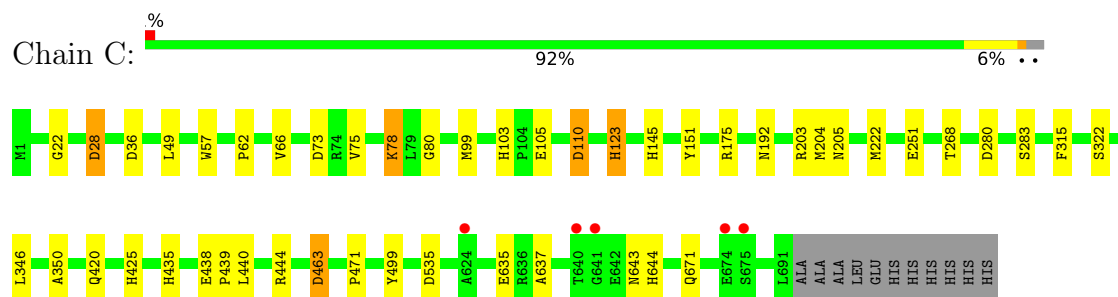
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase

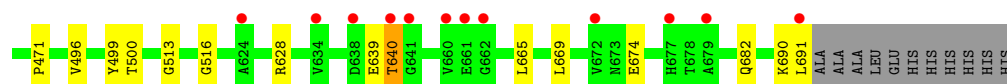


• Molecule 1: Beta-galactosidase





• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	234.47Å 182.69Å 143.26Å 90.00° 125.73° 90.00°	Depositor
Resolution (Å)	48.61 – 1.90 48.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.61-1.90) 98.3 (48.61-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.187 , 0.228 0.194 , 0.231	Depositor DCC
R_{free} test set	18712 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.005 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35731	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

5.1 Standard geometry

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

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	0.66	0/5623	0.99	6/7670 (0.1%)
1	B	0.64	0/5623	1.00	6/7670 (0.1%)
1	C	0.64	0/5623	0.99	5/7670 (0.1%)
1	D	0.61	0/5623	0.97	5/7670 (0.1%)
1	E	0.57	0/5631	0.94	4/7681 (0.1%)
1	F	0.57	0/5623	0.96	2/7670 (0.0%)
All	All	0.62	0/33746	0.97	28/46031 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	28	ASP	CA-CB-CG	9.01	121.61	112.60
1	E	28	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	28	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	110	ASP	CA-CB-CG	7.56	120.16	112.60
1	E	463	ASP	CA-CB-CG	6.75	119.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	280	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	28	ASP	CA-CB-CG	6.15	118.75	112.60
1	A	463	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	463	ASP	CA-CB-CG	5.99	118.59	112.60
1	D	156	HIS	CA-CB-CG	5.93	119.73	113.80
1	C	463	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	28	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	255	LYS	N-CA-C	-5.58	103.20	108.22
1	D	315	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	24	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	392	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	285	ASP	CA-CB-CG	5.36	117.95	112.60
1	A	535	ASP	CB-CA-C	-5.33	100.43	110.67
1	F	296	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	156	HIS	CA-CB-CG	5.26	119.06	113.80
1	D	556	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	535	ASP	CB-CA-C	5.20	119.36	110.56
1	E	296	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	218	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	251	GLU	CB-CG-CD	5.11	121.29	112.60
1	B	290	PRO	N-CA-C	5.11	119.33	111.21
1	E	24	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ARG	Sidechain
1	C	175	ARG	Sidechain
1	D	4	ARG	Sidechain
1	D	628	ARG	Sidechain
1	E	628	ARG	Sidechain
1	F	74	ARG	Sidechain

5.2 Too-close contacts

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	5464	0	5169	25	0
1	B	5464	0	5169	29	0
1	C	5464	0	5169	22	0
1	D	5464	0	5169	24	0
1	E	5469	0	5173	21	0
1	F	5464	0	5169	21	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
2	E	12	0	12	0	0
2	F	12	0	12	0	0
3	A	525	0	0	4	0
3	B	505	0	0	3	0
3	C	519	0	0	2	0
3	D	490	0	0	2	0
3	E	422	0	0	0	0
3	F	409	0	0	2	0
All	All	35731	0	31090	142	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 2.

All (142) 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:B:416:ASP:H	1:B:435:HIS:HE1	1.34	0.75
1:E:192:ASN:HD21	1:E:204:MET:H	1.33	0.75
1:F:298:MET:HE2	3:F:1081:HOH:O	1.88	0.72
1:E:32:GLU:OE2	1:E:74:ARG:NH1	2.25	0.70
1:A:36:ASP:OD1	1:A:78:LYS:NZ	2.23	0.66
1:A:192:ASN:HD21	1:A:204:MET:H	1.42	0.66
1:C:192:ASN:HD21	1:C:204:MET:H	1.43	0.66
1:B:35:TRP:CE3	1:B:75:VAL:HG13	2.32	0.64
1:D:103:HIS:HD2	1:D:105:GLU:OE2	1.81	0.64
1:B:192:ASN:HD21	1:B:204:MET:H	1.46	0.64
1:D:57:TRP:CZ2	1:D:99:MET:HE1	2.35	0.62
1:A:203:ARG:HH12	1:A:205:ASN:ND2	1.99	0.61
1:C:203:ARG:HH12	1:C:205:ASN:ND2	2.00	0.60
1:B:292:GLU:OE2	1:B:444:ARG:NH2	2.35	0.60
1:F:625:GLU:O	1:F:628:ARG:HD3	2.03	0.58
1:D:36:ASP:OD1	1:D:78:LYS:NZ	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:TRP:CZ2	1:F:99:MET:HE1	2.39	0.56
1:B:122:GLN:NE2	1:B:164:HIS:H	2.04	0.55
1:C:222:MET:O	1:C:425:HIS:HE1	1.88	0.55
1:C:57:TRP:CZ2	1:C:99:MET:HE1	2.42	0.55
1:C:123:HIS:HE1	3:C:1221:HOH:O	1.90	0.54
1:B:35:TRP:CZ3	1:B:75:VAL:HG13	2.42	0.54
1:B:18:ARG:HD3	3:B:1355:HOH:O	2.07	0.53
1:E:57:TRP:CZ2	1:E:99:MET:HE1	2.43	0.52
1:D:194:ALA:O	1:D:508:HIS:HE1	1.92	0.52
1:E:283:SER:HA	1:E:315:PHE:O	2.10	0.52
1:B:552:HIS:HE1	3:B:1363:HOH:O	1.92	0.52
1:C:283:SER:HA	1:C:315:PHE:O	2.10	0.52
1:B:22:GLY:HA3	1:B:49:LEU:O	2.11	0.51
1:D:338:LEU:C	1:D:338:LEU:HD23	2.35	0.51
1:C:36:ASP:OD1	1:C:78:LYS:NZ	2.44	0.51
1:D:63:GLU:HG2	3:D:1081:HOH:O	2.12	0.50
1:E:32:GLU:CD	1:E:74:ARG:HH12	2.19	0.50
1:B:70:ASP:OD2	1:B:74:ARG:NH2	2.42	0.50
1:E:22:GLY:HA3	1:E:49:LEU:O	2.12	0.50
1:B:416:ASP:H	1:B:435:HIS:CE1	2.22	0.50
1:F:269:VAL:HG12	1:F:270:LEU:HG	1.93	0.50
1:A:123:HIS:HE1	3:A:1176:HOH:O	1.95	0.49
1:C:145:HIS:HD2	3:C:1388:HOH:O	1.95	0.49
1:F:362:LYS:NZ	3:F:914:HOH:O	2.47	0.48
1:B:49:LEU:HD23	1:B:49:LEU:C	2.39	0.48
1:B:62:PRO:HD2	1:B:66:VAL:O	2.14	0.48
1:D:73:ASP:OD2	1:D:145:HIS:HE1	1.97	0.48
1:B:103:HIS:HD2	1:B:105:GLU:OE2	1.97	0.47
1:F:575:LYS:HE2	1:F:580:ASP:HB3	1.96	0.47
1:E:27:PRO:HG3	1:E:75:VAL:HG21	1.97	0.47
1:A:552:HIS:HE1	3:A:1371:HOH:O	1.97	0.47
1:D:27:PRO:HG3	1:D:75:VAL:HG21	1.96	0.47
1:F:625:GLU:O	1:F:628:ARG:CD	2.62	0.47
1:E:77:ASP:O	1:E:81:LYS:HG2	2.15	0.46
1:A:18:ARG:HH21	1:A:394:ASN:HD22	1.63	0.46
1:C:73:ASP:OD2	1:C:145:HIS:HE1	1.98	0.46
1:C:440:LEU:O	1:C:444:ARG:HG3	2.16	0.45
1:A:269:VAL:HG12	1:A:270:LEU:HG	1.99	0.45
1:B:211:ILE:O	1:B:226:LYS:HE2	2.16	0.45
1:C:635:GLU:OE1	1:C:644:HIS:HE1	1.99	0.45
1:D:292:GLU:OE2	1:D:444:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TRP:CZ2	1:B:99:MET:HE1	2.51	0.45
1:C:80:GLY:HA3	1:C:151:TYR:CG	2.52	0.45
1:C:268:THR:HG21	1:C:420:GLN:HG2	1.99	0.45
1:A:123:HIS:CD2	1:A:123:HIS:H	2.35	0.45
1:B:346:LEU:HD12	1:B:350:ALA:O	2.16	0.45
1:B:80:GLY:HA3	1:B:151:TYR:CG	2.52	0.44
1:D:669:LEU:HB3	1:D:682:GLN:HB2	2.00	0.44
1:E:49:LEU:C	1:E:49:LEU:HD23	2.42	0.44
1:F:479:GLN:HG3	1:F:480:THR:N	2.32	0.44
1:B:64:GLU:HB2	1:B:98:TRP:CZ3	2.53	0.44
1:A:431:GLN:HE21	1:A:434:ARG:HH22	1.65	0.44
1:B:54:ILE:HA	1:B:89:ALA:CB	2.48	0.44
1:E:222:MET:O	1:E:425:HIS:HE1	2.01	0.44
1:C:22:GLY:HA3	1:C:49:LEU:O	2.18	0.43
1:D:222:MET:O	1:D:425:HIS:HE1	2.01	0.43
1:D:552:HIS:HE1	3:D:1353:HOH:O	2.01	0.43
1:F:58:ALA:HB2	1:F:96:PRO:HB3	2.00	0.43
1:A:73:ASP:OD2	1:A:145:HIS:HE1	2.00	0.43
1:B:73:ASP:OD2	1:B:145:HIS:HE1	2.01	0.43
1:B:106:ILE:HG12	1:B:131:PHE:HB2	2.00	0.43
1:B:145:HIS:HD2	3:B:1379:HOH:O	2.00	0.43
1:F:518:ILE:O	1:F:522:VAL:HG22	2.18	0.43
1:C:438:GLU:N	1:C:439:PRO:HD2	2.33	0.43
1:D:268:THR:HG21	1:D:420:GLN:HG2	1.99	0.43
1:A:222:MET:O	1:A:425:HIS:HE1	2.02	0.43
1:F:51:SER:HA	1:F:87:ASP:O	2.18	0.43
1:F:482:ARG:HB2	1:F:482:ARG:NH1	2.34	0.43
1:B:270:LEU:HD13	1:B:275:TRP:CE2	2.54	0.43
1:E:639:GLU:O	1:E:640:THR:C	2.61	0.43
1:F:467:ALA:HA	1:F:493:LYS:O	2.18	0.43
1:A:338:LEU:C	1:A:338:LEU:HD23	2.44	0.43
1:C:637:ALA:HA	1:C:643:ASN:O	2.18	0.43
1:E:428:THR:HB	1:E:429:PRO:HD2	2.01	0.42
1:E:496:VAL:HG13	1:E:500:THR:HG21	2.02	0.42
1:B:338:LEU:HD23	1:B:338:LEU:C	2.44	0.42
1:D:438:GLU:N	1:D:439:PRO:HD2	2.33	0.42
1:C:103:HIS:HD2	1:C:105:GLU:OE2	2.02	0.42
1:D:556:ASP:OD2	1:D:597:TYR:OH	2.33	0.42
1:E:420:GLN:HA	1:E:435:HIS:HB3	2.00	0.42
1:A:292:GLU:O	1:A:292:GLU:HG2	2.15	0.42
1:C:62:PRO:HD2	1:C:66:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ARG:HH11	1:E:394:ASN:HD22	1.67	0.42
1:B:565:ALA:HB2	1:B:588:ASN:OD1	2.19	0.42
1:C:346:LEU:HD12	1:C:350:ALA:O	2.20	0.42
1:A:552:HIS:HD2	3:A:1114:HOH:O	2.03	0.42
1:D:103:HIS:CD2	1:D:105:GLU:OE2	2.68	0.42
1:E:35:TRP:O	1:E:39:VAL:HG23	2.20	0.42
1:B:161:TYR:CE2	1:B:242:TYR:HB2	2.55	0.41
1:C:420:GLN:HA	1:C:435:HIS:HB3	2.02	0.41
1:E:513:GLY:O	1:E:516:GLY:HA2	2.19	0.41
1:F:356:PHE:HA	1:F:357:GLN:HA	1.84	0.41
1:A:20:TRP:HB2	1:A:352:ALA:CB	2.49	0.41
1:A:51:SER:HA	1:A:87:ASP:O	2.20	0.41
1:A:57:TRP:CZ2	1:A:99:MET:HE1	2.54	0.41
1:F:159:ASN:O	1:F:160:ALA:C	2.63	0.41
1:B:587:VAL:HG11	1:B:617:GLU:HG2	2.01	0.41
1:C:110:ASP:OD1	1:C:110:ASP:C	2.62	0.41
1:D:292:GLU:CD	1:D:444:ARG:HH22	2.28	0.41
1:E:665:LEU:HD11	1:E:690:LYS:HB2	2.03	0.41
1:A:283:SER:HA	1:A:315:PHE:O	2.21	0.41
1:C:49:LEU:C	1:C:49:LEU:HD23	2.45	0.41
1:E:188:ILE:HD12	1:E:188:ILE:HA	1.95	0.41
1:D:319:HIS:CE1	1:D:355:TYR:CE1	3.09	0.41
1:F:623:SER:HB3	1:F:628:ARG:CG	2.51	0.41
1:D:18:ARG:HH11	1:D:394:ASN:HD22	1.67	0.41
1:F:346:LEU:HD12	1:F:350:ALA:O	2.21	0.41
1:A:318:ALA:HB2	3:A:918:HOH:O	2.20	0.41
1:D:7:LYS:HB2	1:D:280:ASP:HB3	2.02	0.41
1:D:22:GLY:O	1:D:354:CYS:HA	2.21	0.41
1:D:211:ILE:O	1:D:226:LYS:HE3	2.20	0.41
1:E:268:THR:HG21	1:E:420:GLN:HG2	2.02	0.41
1:F:439:PRO:HD3	1:F:471:PRO:HB2	2.03	0.41
1:A:121:ARG:HE	1:A:164:HIS:HE2	1.69	0.41
1:A:298:MET:HE2	1:A:298:MET:HB3	1.96	0.41
1:B:292:GLU:CD	1:B:444:ARG:HH22	2.28	0.41
1:A:665:LEU:HD11	1:A:690:LYS:HB2	2.03	0.40
1:D:161:TYR:CE2	1:D:242:TYR:HB2	2.56	0.40
1:F:53:ALA:HA	1:F:56:SER:OG	2.20	0.40
1:F:264:SER:O	1:F:265:ALA:C	2.64	0.40
1:F:660:VAL:HG21	1:F:672:VAL:HG13	2.03	0.40
1:A:270:LEU:HD13	1:A:275:TRP:CE2	2.57	0.40
1:D:298:MET:HB3	1:D:298:MET:HE2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:LEU:HB3	1:E:682:GLN:HB2	2.03	0.40
1:A:268:THR:HG21	1:A:420:GLN:HG2	2.03	0.40
1:A:159:ASN:O	1:A:160:ALA:C	2.65	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	689/702 (98%)	672 (98%)	15 (2%)	2 (0%)	36	29
1	B	689/702 (98%)	666 (97%)	21 (3%)	2 (0%)	36	29
1	C	689/702 (98%)	672 (98%)	15 (2%)	2 (0%)	36	29
1	D	689/702 (98%)	671 (97%)	16 (2%)	2 (0%)	36	29
1	E	690/702 (98%)	672 (97%)	17 (2%)	1 (0%)	48	40
1	F	689/702 (98%)	666 (97%)	21 (3%)	2 (0%)	36	29
All	All	4135/4212 (98%)	4019 (97%)	105 (2%)	11 (0%)	36	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	SER
1	C	322	SER
1	C	471	PRO
1	D	322	SER
1	D	471	PRO
1	F	322	SER
1	A	471	PRO
1	A	498	TYR
1	E	471	PRO

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Mol	Chain	Res	Type
1	F	471	PRO
1	B	471	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/574 (99%)	560 (99%)	6 (1%)	65	67
1	B	566/574 (99%)	555 (98%)	11 (2%)	50	47
1	C	566/574 (99%)	558 (99%)	8 (1%)	59	59
1	D	566/574 (99%)	562 (99%)	4 (1%)	76	78
1	E	567/574 (99%)	561 (99%)	6 (1%)	65	67
1	F	566/574 (99%)	552 (98%)	14 (2%)	42	37
All	All	3397/3444 (99%)	3348 (99%)	49 (1%)	59	59

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	123	HIS
1	A	269	VAL
1	A	292	GLU
1	A	499	TYR
1	A	617	GLU
1	B	75	VAL
1	B	110	ASP
1	B	156	HIS
1	B	482	ARG
1	B	499	TYR
1	B	575	LYS
1	B	617	GLU
1	B	661	GLU
1	B	674	GLU
1	B	675	SER

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Mol	Chain	Res	Type
1	B	686	VAL
1	C	28	ASP
1	C	75	VAL
1	C	78	LYS
1	C	110	ASP
1	C	123	HIS
1	C	463	ASP
1	C	499	TYR
1	C	671	GLN
1	D	28	ASP
1	D	81	LYS
1	D	289	SER
1	D	499	TYR
1	E	28	ASP
1	E	463	ASP
1	E	499	TYR
1	E	640	THR
1	E	674	GLU
1	E	691	LEU
1	F	28	ASP
1	F	74	ARG
1	F	269	VAL
1	F	292	GLU
1	F	362	LYS
1	F	479	GLN
1	F	482	ARG
1	F	499	TYR
1	F	575	LYS
1	F	623	SER
1	F	631	VAL
1	F	640	THR
1	F	644	HIS
1	F	661	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	123	HIS
1	A	137	ASN
1	A	145	HIS
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	357	GLN
1	A	394	ASN
1	A	425	HIS
1	A	431	GLN
1	A	552	HIS
1	A	682	GLN
1	B	10	GLN
1	B	103	HIS
1	B	122	GLN
1	B	145	HIS
1	B	192	ASN
1	B	345	HIS
1	B	425	HIS
1	B	431	GLN
1	B	435	HIS
1	B	449	ASN
1	B	552	HIS
1	C	29	GLN
1	C	101	GLN
1	C	103	HIS
1	C	123	HIS
1	C	137	ASN
1	C	145	HIS
1	C	192	ASN
1	C	205	ASN
1	C	220	ASN
1	C	345	HIS
1	C	425	HIS
1	C	588	ASN
1	C	644	HIS
1	D	10	GLN
1	D	26	ASN
1	D	103	HIS
1	D	117	GLN
1	D	137	ASN
1	D	145	HIS
1	D	357	GLN
1	D	394	ASN
1	D	425	HIS
1	D	431	GLN
1	D	479	GLN

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Mol	Chain	Res	Type
1	D	508	HIS
1	D	552	HIS
1	E	3	HIS
1	E	26	ASN
1	E	145	HIS
1	E	192	ASN
1	E	394	ASN
1	E	425	HIS
1	E	431	GLN
1	E	508	HIS
1	E	643	ASN
1	F	26	ASN
1	F	145	HIS
1	F	490	ASN
1	F	588	ASN
1	F	653	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	GLA	F	801	-	12,12,12	0.77	0	17,17,17	0.95	1 (5%)
2	GLA	B	801	-	12,12,12	0.82	0	17,17,17	0.79	0
2	GLA	E	801	-	12,12,12	0.73	0	17,17,17	0.72	0
2	GLA	A	801	-	12,12,12	0.78	0	17,17,17	0.57	0
2	GLA	C	801	-	12,12,12	0.82	0	17,17,17	0.76	0
2	GLA	D	801	-	12,12,12	0.61	0	17,17,17	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	F	801	-	-	0/2/22/22	0/1/1/1
2	GLA	B	801	-	-	0/2/22/22	0/1/1/1
2	GLA	E	801	-	-	0/2/22/22	0/1/1/1
2	GLA	A	801	-	-	0/2/22/22	0/1/1/1
2	GLA	C	801	-	-	0/2/22/22	0/1/1/1
2	GLA	D	801	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	GLA	O2-C2-C3	2.40	116.03	110.38
2	F	801	GLA	O1-C1-C2	2.32	115.71	108.98

There are no chirality outliers.

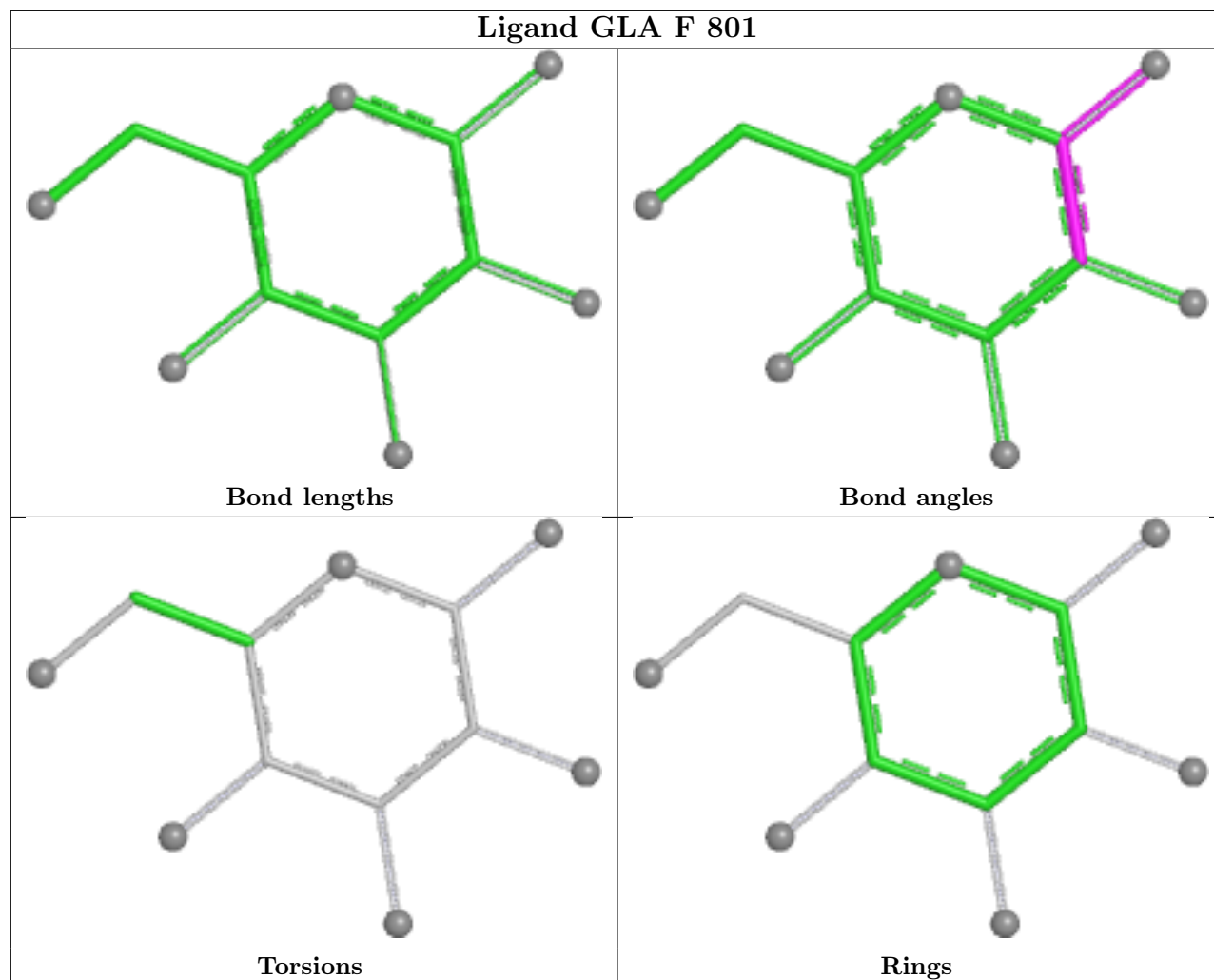
There are no torsion outliers.

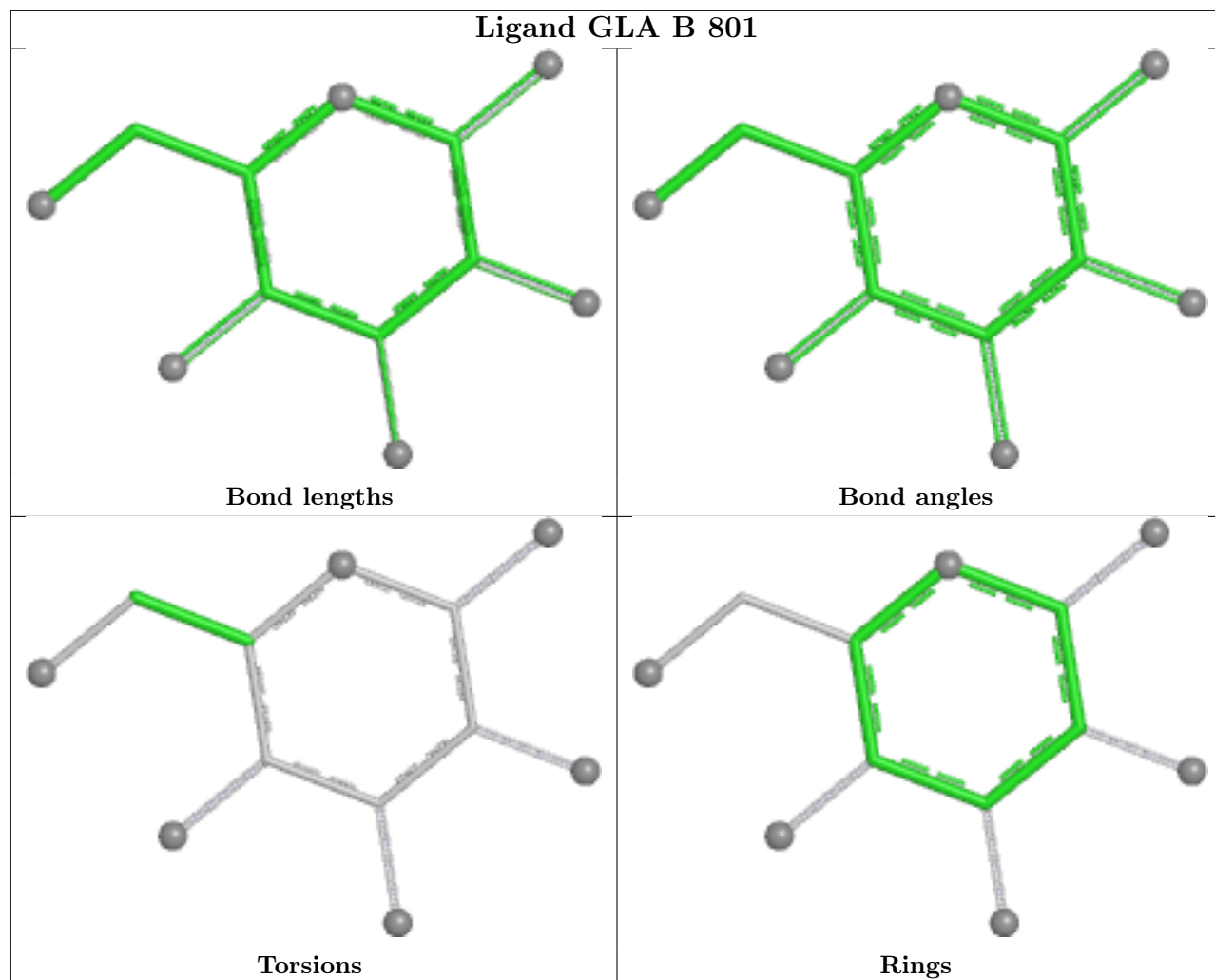
There are no ring outliers.

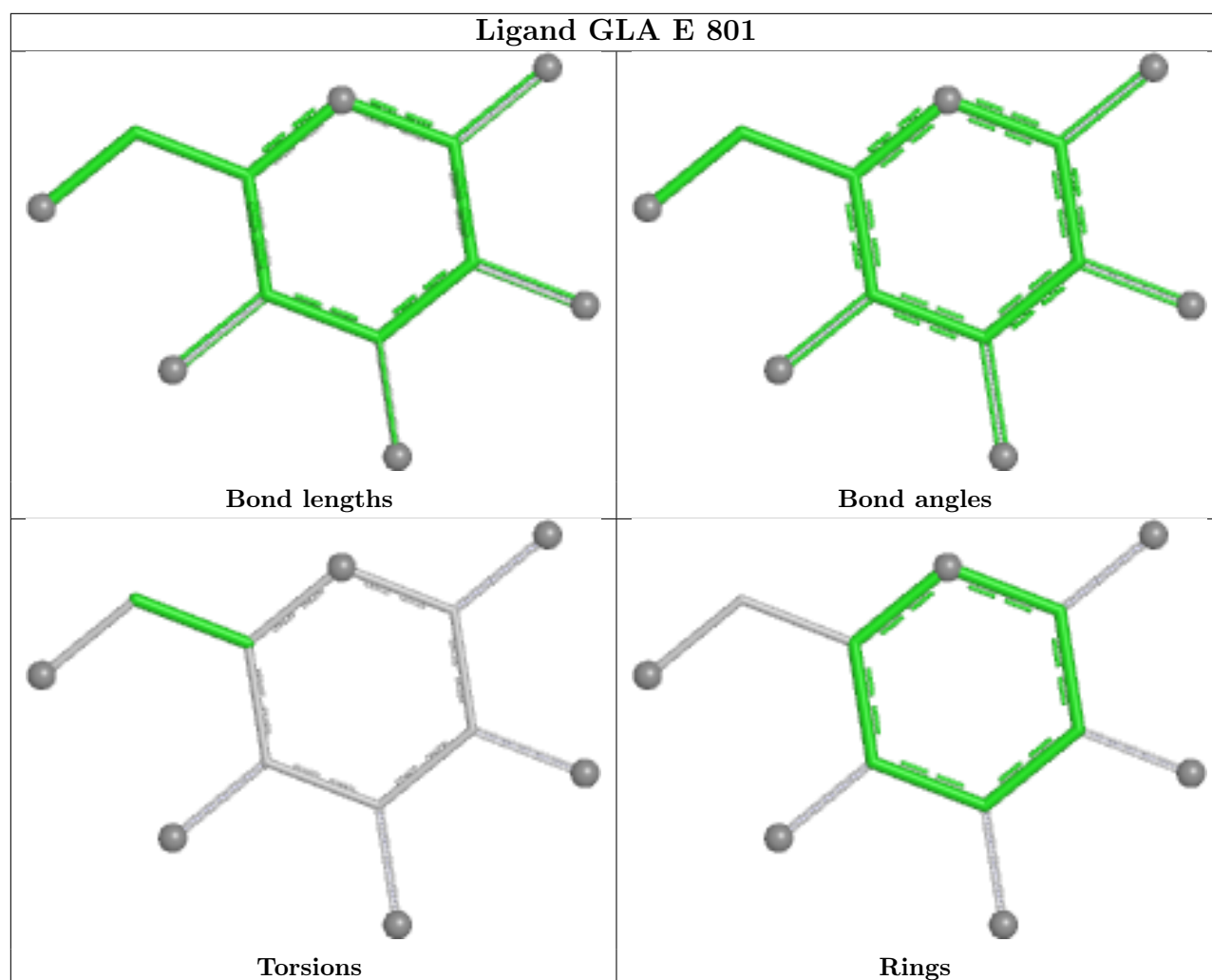
No monomer is involved in short contacts.

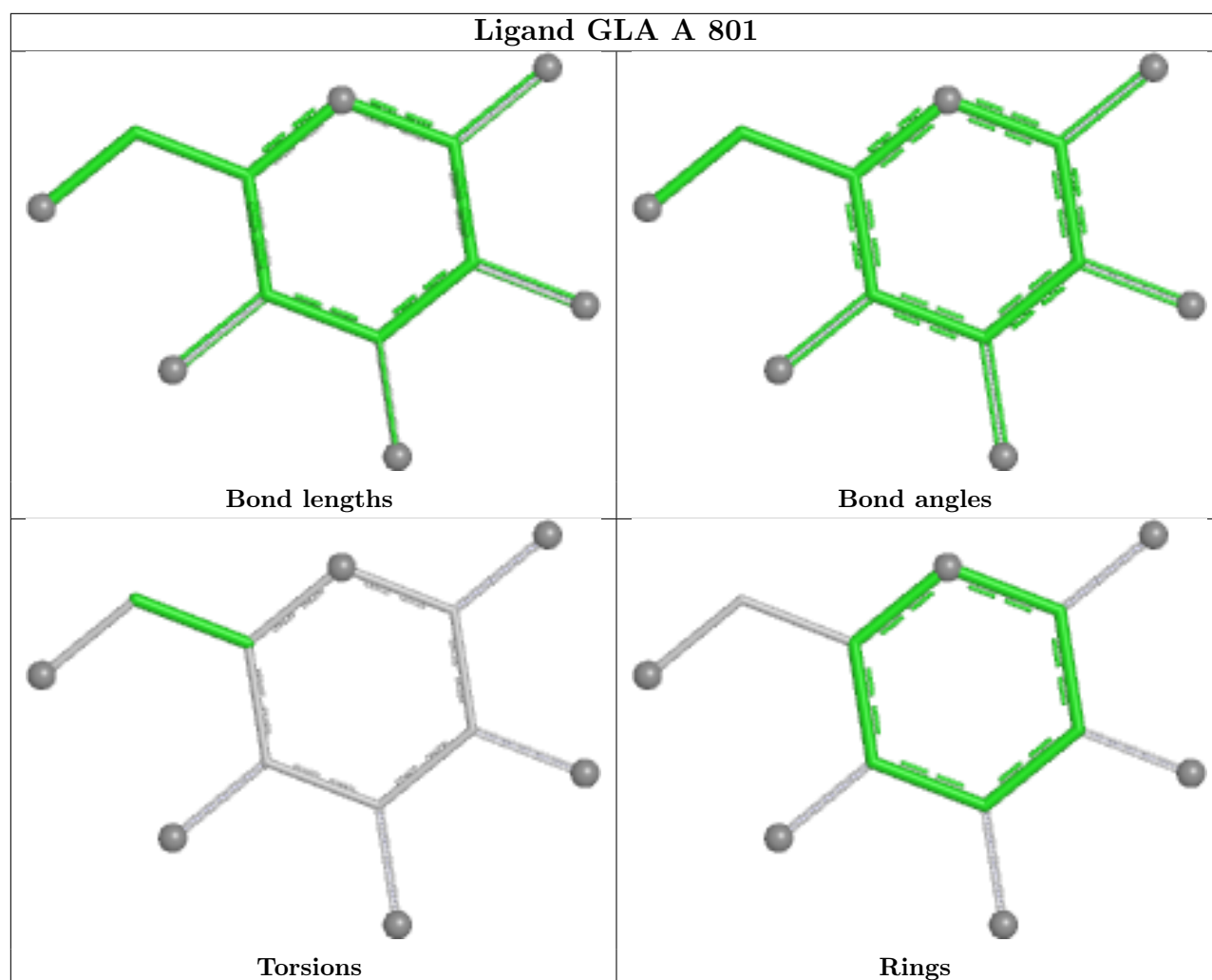
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

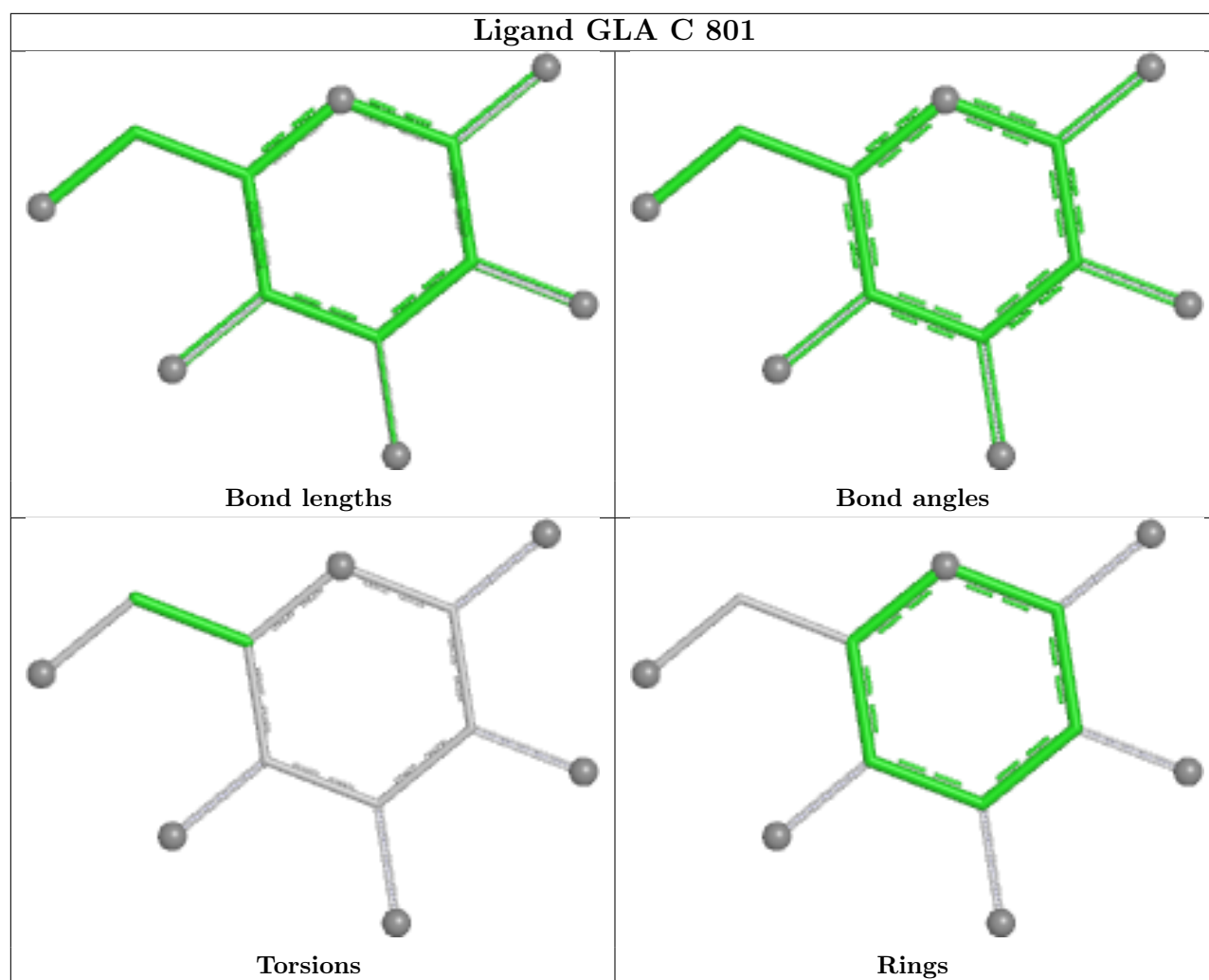
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

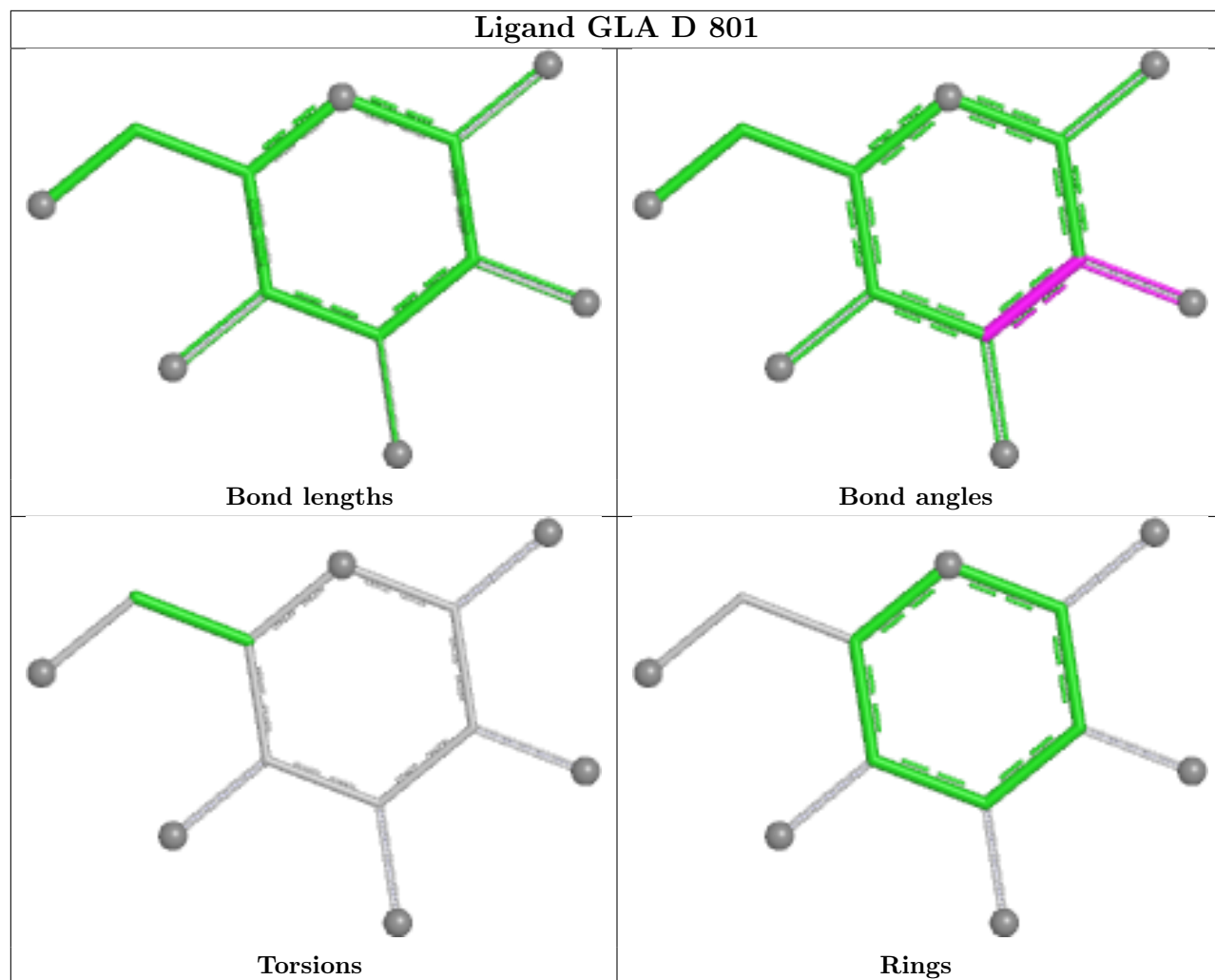












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	691/702 (98%)	-0.05	4 (0%) 85 87	13, 21, 35, 54	0
1	B	691/702 (98%)	0.11	6 (0%) 81 83	14, 23, 39, 69	0
1	C	691/702 (98%)	0.02	5 (0%) 84 86	13, 22, 38, 82	0
1	D	691/702 (98%)	0.06	1 (0%) 92 92	15, 23, 41, 68	0
1	E	691/702 (98%)	0.32	14 (2%) 65 69	16, 28, 47, 77	1 (0%)
1	F	691/702 (98%)	0.36	14 (2%) 65 69	16, 29, 47, 78	0
All	All	4146/4212 (98%)	0.14	44 (1%) 78 80	13, 24, 42, 82	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	640	THR	3.9
1	F	640	THR	3.5
1	E	641	GLY	3.4
1	F	691	LEU	3.1
1	E	1	MET	3.0
1	F	624	ALA	2.9
1	E	624	ALA	2.8
1	F	655	VAL	2.8
1	F	689	VAL	2.7
1	C	641	GLY	2.6
1	F	641	GLY	2.6
1	F	660	VAL	2.6
1	A	640	THR	2.5
1	E	661	GLU	2.5
1	A	14	GLY	2.5
1	B	641	GLY	2.5
1	A	621	GLU	2.4
1	C	675	SER	2.4
1	E	640	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	644	HIS	2.4
1	E	691	LEU	2.3
1	E	679	ALA	2.3
1	E	662	GLY	2.3
1	B	660	VAL	2.3
1	E	660	VAL	2.3
1	B	675	SER	2.2
1	B	680	ALA	2.2
1	F	667	ALA	2.2
1	C	674	GLU	2.1
1	E	638	ASP	2.1
1	A	482	ARG	2.1
1	F	678	THR	2.1
1	B	575	LYS	2.0
1	F	575	LYS	2.0
1	F	661	GLU	2.0
1	F	675	SER	2.0
1	B	640	THR	2.0
1	E	672	VAL	2.0
1	E	451	LEU	2.0
1	C	624	ALA	2.0
1	D	677	HIS	2.0
1	E	677	HIS	2.0
1	F	677	HIS	2.0
1	E	634	VAL	2.0

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

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

6.3 Carbohydrates

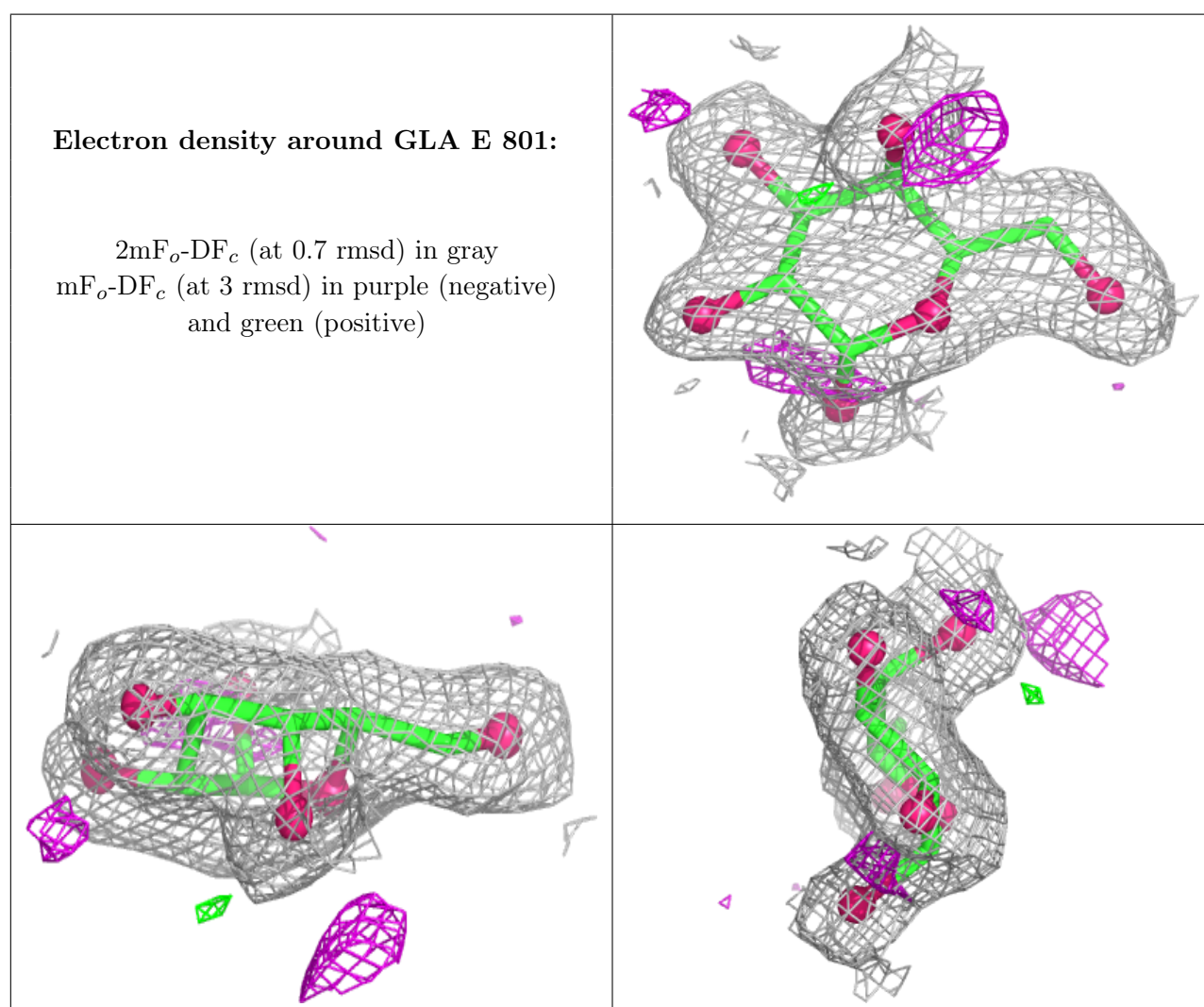
There are no oligosaccharides in this entry.

6.4 Ligands

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

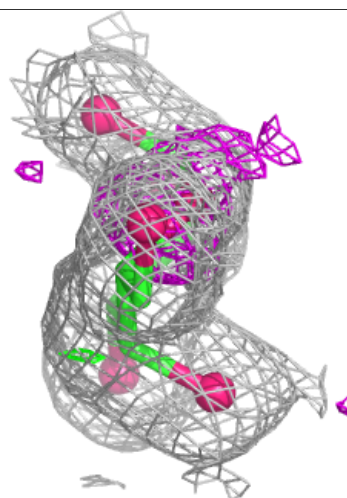
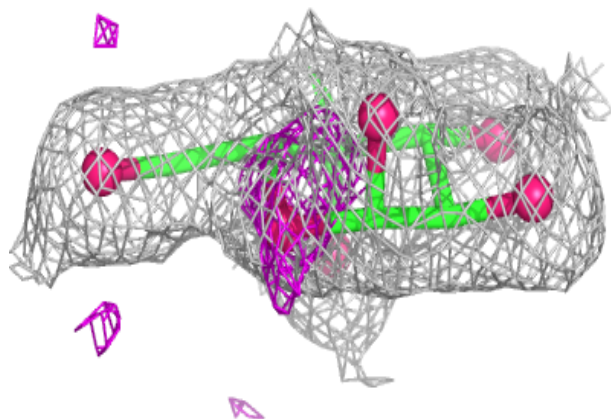
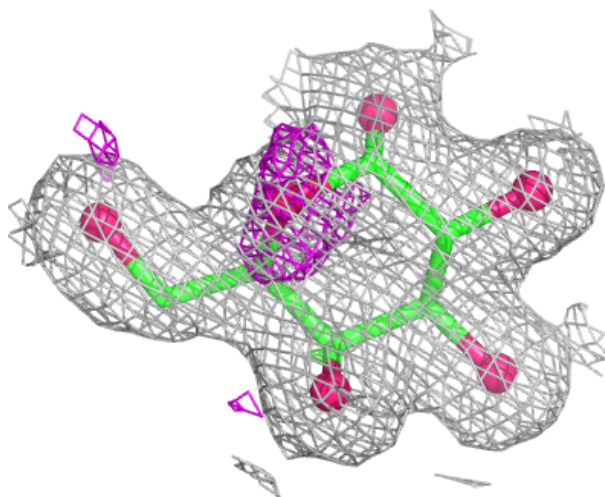
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLA	E	801	12/12	0.92	0.09	22,29,32,32	0
2	GLA	A	801	12/12	0.93	0.08	16,20,23,23	0
2	GLA	D	801	12/12	0.94	0.08	17,20,26,30	0
2	GLA	C	801	12/12	0.94	0.09	20,24,29,31	0
2	GLA	F	801	12/12	0.94	0.08	20,28,35,35	0
2	GLA	B	801	12/12	0.95	0.07	19,23,25,27	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.



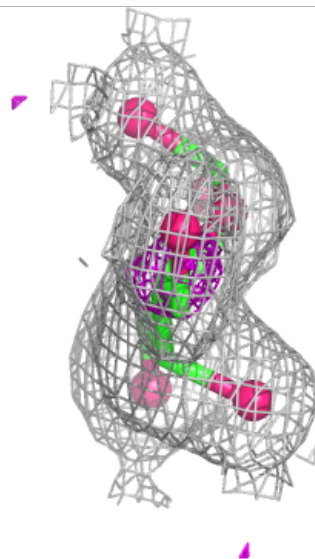
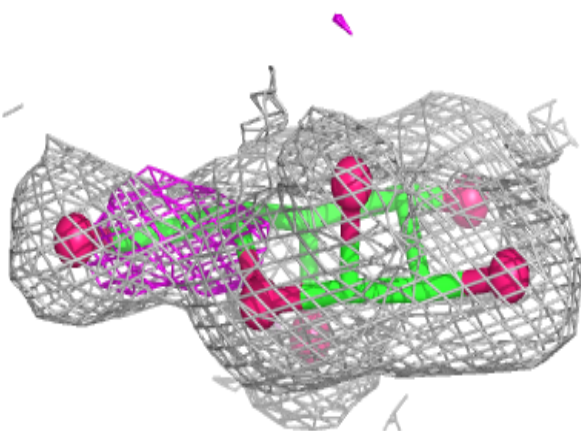
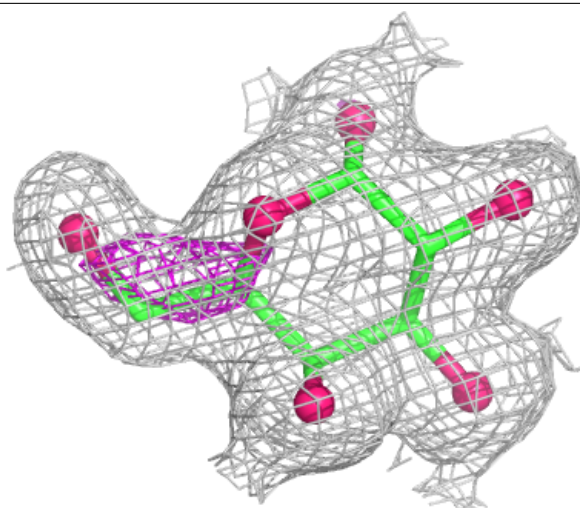
Electron density around GLA A 801:

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



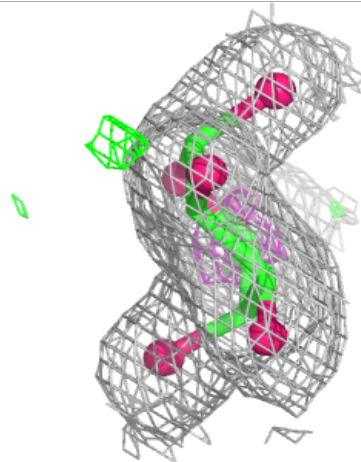
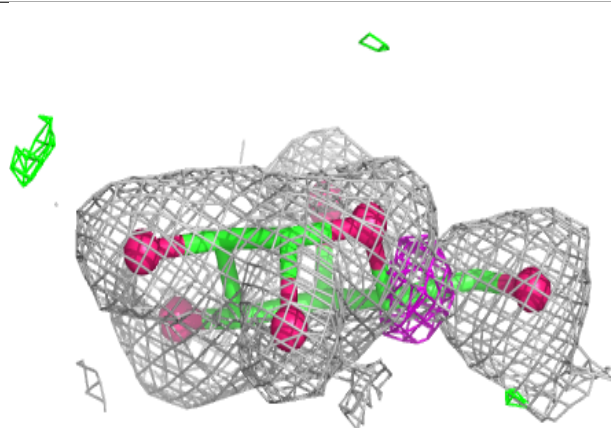
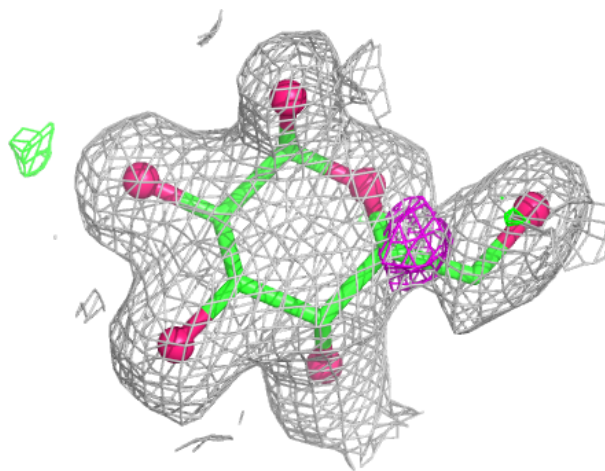
Electron density around GLA D 801:

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



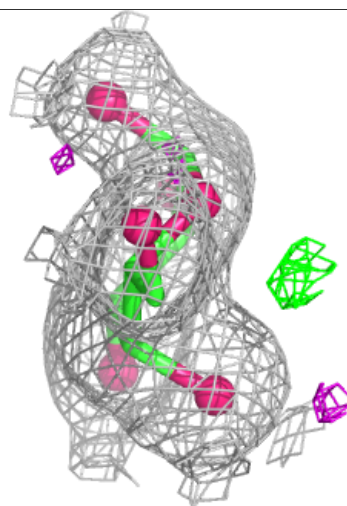
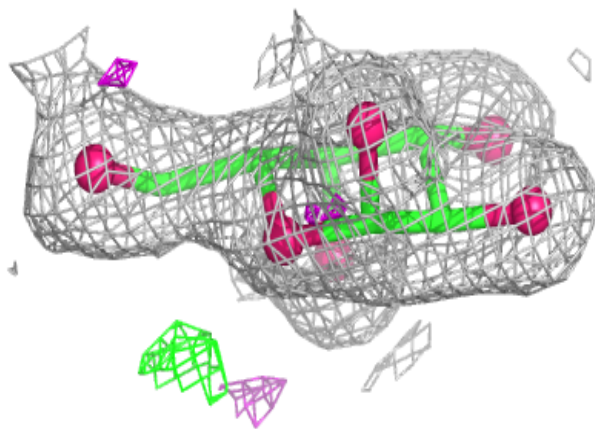
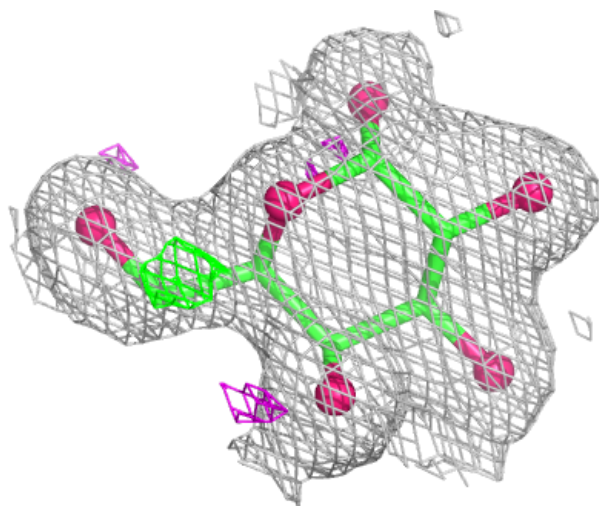
Electron density around GLA C 801:

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



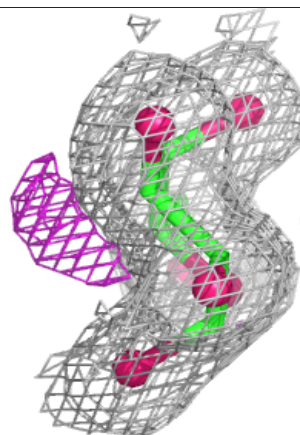
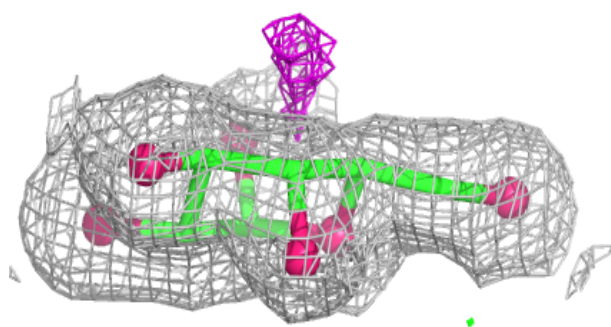
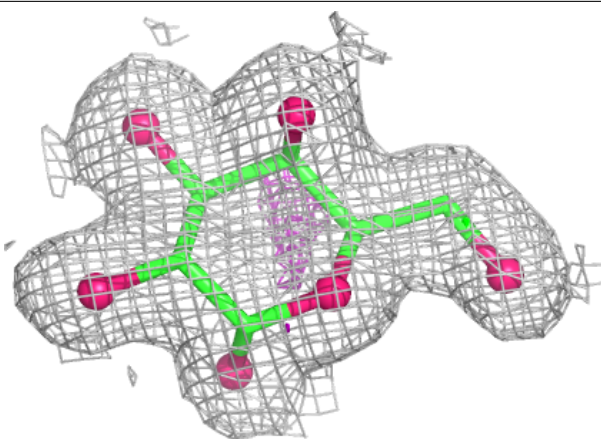
Electron density around GLA F 801:

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



Electron density around GLA B 801:

$2mF_o-DF_c$ (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.