wwPDB X-ray Structure Validation Summary Report (i)

Apr 27, 2023 – 07:51 pm BST

PDB ID	:	8C23
Title	:	Structure of E. coli Class 2 L-asparaginase EcAIII, mutant M200T (monoclinic form M200T#m)
Authors	:	Sciuk, A.; Ruszkowski, M.; Jaskolski, M.; Loch, J.I.
Deposited on	:	2022-12-21
Resolution	:	1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

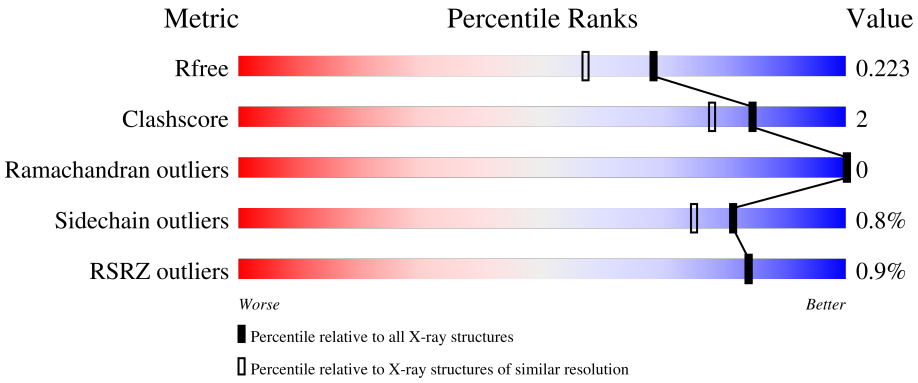
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 <=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	AAA	178	86% · 11%
1	CCC	178	84% · 12%
1	EEE	178	81% 6% 13%
1	GGG	178	82% 6% · 12%
2	BBB	143	90% 5% 6%

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Mol	Chain	Length	Quality of chain
2	DDD	143	
2	FFF	143	
2	HHH	143	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9143 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 Isoaspartyl peptidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	158	Total	C	N	O	S	0	4	0
			1213	755	213	234	11			
1	CCC	157	Total	C	N	O	S	0	2	0
			1189	741	210	228	10			
1	EEE	154	Total	C	N	O	S	0	2	0
			1167	730	205	222	10			
1	GGG	157	Total	C	N	O	S	0	3	0
			1199	748	211	230	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P37595
CCC	1	MET	-	initiating methionine	UNP P37595
EEE	1	MET	-	initiating methionine	UNP P37595
GGG	1	MET	-	initiating methionine	UNP P37595

- Molecule 2 is a protein called Isoaspartyl peptidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	135	Total	C	N	O	S	0	2	0
			966	602	165	193	6			
2	DDD	135	Total	C	N	O	S	0	2	0
			966	602	165	193	6			
2	FFF	135	Total	C	N	O	S	0	0	0
			951	592	161	192	6			
2	HHH	134	Total	C	N	O	S	0	1	0
			946	591	160	189	6			

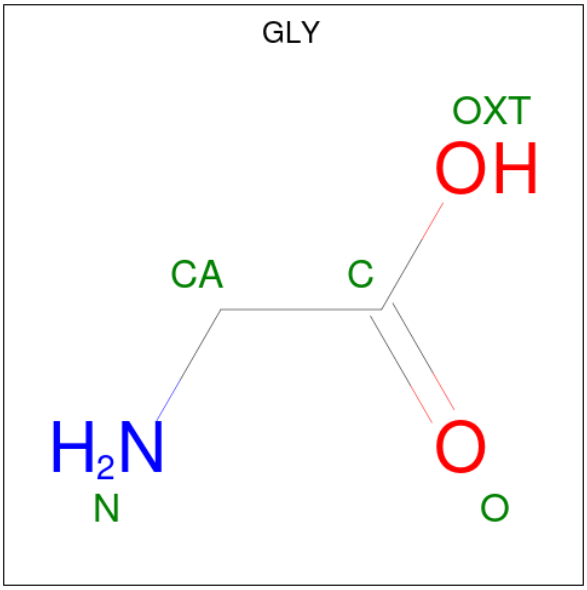
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	200	THR	MET	engineered mutation	UNP P37595
DDD	200	THR	MET	engineered mutation	UNP P37595
FFF	200	THR	MET	engineered mutation	UNP P37595
HHH	200	THR	MET	engineered mutation	UNP P37595

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

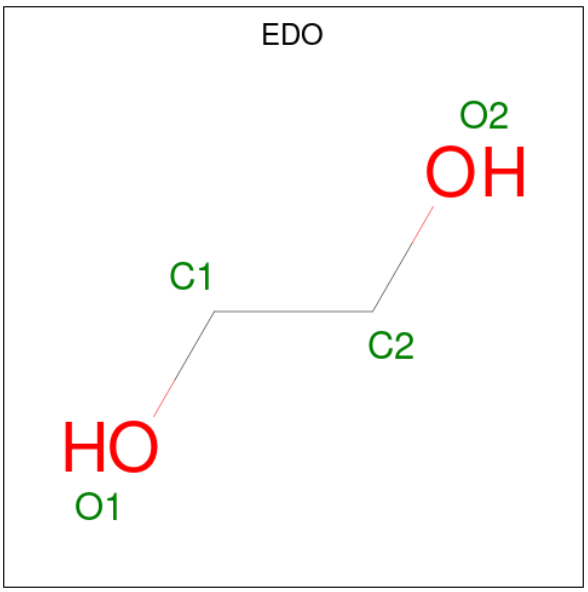
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0
3	CCC	2	Total Na 2 2	0	0
3	EEE	1	Total Na 1 1	0	0
3	GGG	2	Total Na 2 2	0	0

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C N O 5 2 1 2	0	0
4	DDD	1	Total C N O 5 2 1 2	0	0
4	HHH	1	Total C N O 5 2 1 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

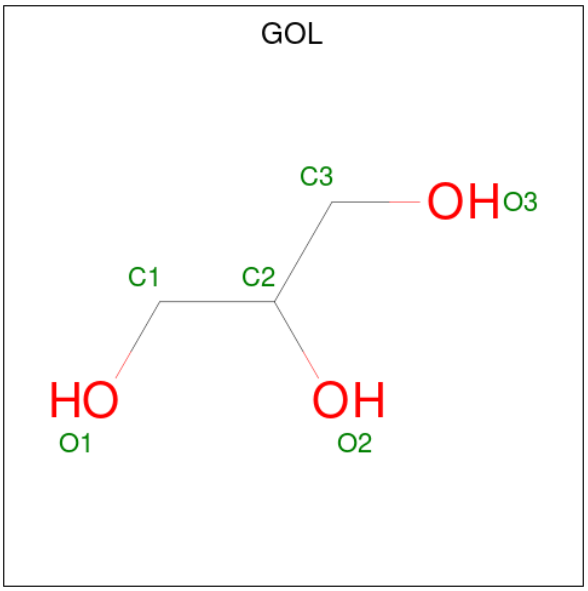


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 4 2 2	0	0
5	BBB	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total Cl 1 1	0	0
6	DDD	1	Total Cl 1 1	0	0
6	EEE	1	Total Cl 1 1	0	0
6	GGG	1	Total Cl 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

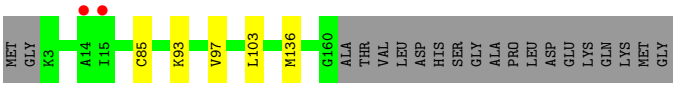
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	112	Total O 112 112	0	0
8	BBB	49	Total O 49 49	0	0
8	CCC	83	Total O 83 83	0	0
8	DDD	31	Total O 31 31	0	0
8	EEE	65	Total O 65 65	0	0
8	FFF	22	Total O 22 22	0	0
8	GGG	110	Total O 110 110	0	0
8	HHH	35	Total O 35 35	0	0

3 Residue-property plots (i)

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

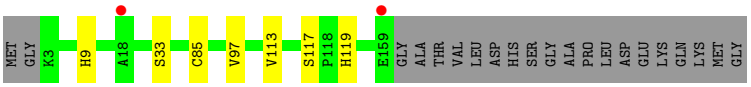
• Molecule 1: Isoaspartyl peptidase subunit alpha

Chain AAA:



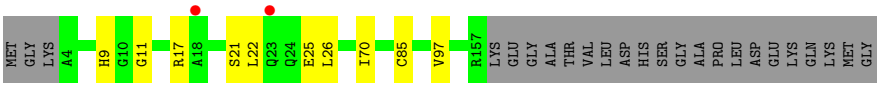
• Molecule 1: Isoaspartyl peptidase subunit alpha

Chain CCC:



• Molecule 1: Isoaspartyl peptidase subunit alpha

Chain EEE:

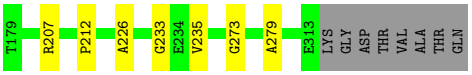


• Molecule 1: Isoaspartyl peptidase subunit alpha

Chain GGG:

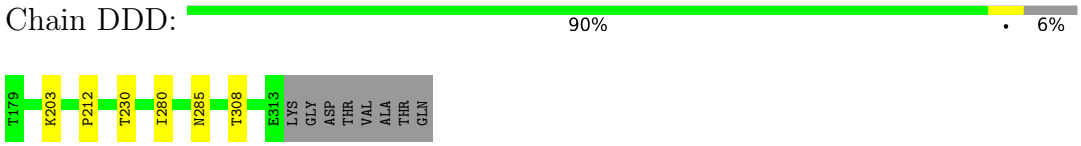
• Molecule 2: Isoaspartyl peptidase subunit beta

Chain BBB:



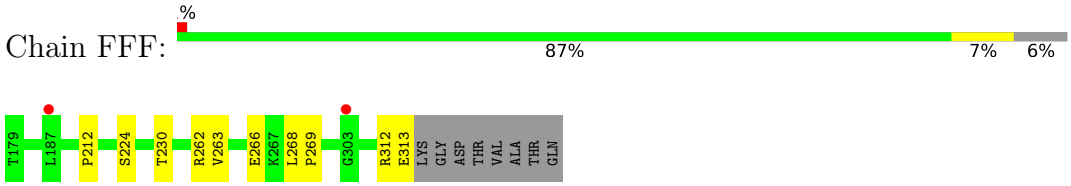
• Molecule 2: Isoaspartyl peptidase subunit beta

Chain DDD:



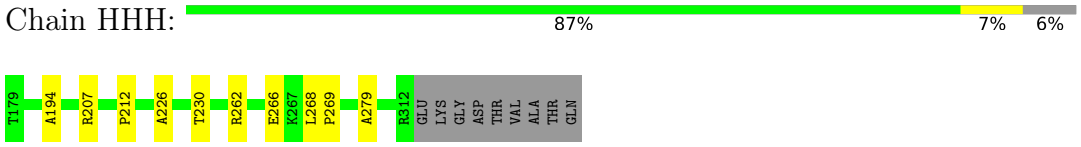
• Molecule 2: Isoaspartyl peptidase subunit beta

Chain FFF:



• Molecule 2: Isoaspartyl peptidase subunit beta

Chain HHH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.46Å 149.65Å 105.13Å 90.00° 126.72° 90.00°	Depositor
Resolution (Å)	84.38 – 1.84 84.38 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.9 (84.38-1.84) 97.9 (84.38-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.216 0.199 , 0.223	Depositor DCC
R_{free} test set	1088 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9143	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, NA, EDO

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	AAA	0.85	0/1230	0.84	0/1656
1	CCC	0.77	0/1206	0.84	0/1626
1	EEE	0.75	0/1185	0.83	0/1599
1	GGG	0.85	0/1216	0.85	0/1639
2	BBB	0.75	0/984	0.88	0/1340
2	DDD	0.77	0/984	0.86	0/1340
2	FFF	0.75	0/966	0.84	0/1316
2	HHH	0.78	0/964	0.88	0/1314
All	All	0.79	0/8735	0.85	0/11830

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

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	AAA	1213	0	1215	4	0
1	CCC	1189	0	1199	6	0
1	EEE	1167	0	1170	7	0
1	GGG	1199	0	1207	6	0
2	BBB	966	0	946	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	966	0	946	6	0
2	FFF	951	0	925	6	0
2	HHH	946	0	928	6	0
3	AAA	1	0	0	0	0
3	CCC	2	0	0	0	0
3	EEE	1	0	0	0	0
3	GGG	2	0	0	0	0
4	AAA	5	0	2	0	0
4	DDD	5	0	2	0	0
4	HHH	5	0	2	0	0
5	AAA	4	0	6	0	0
5	BBB	4	0	6	3	0
6	BBB	1	0	0	0	0
6	DDD	1	0	0	0	0
6	EEE	1	0	0	0	0
6	GGG	1	0	0	0	0
7	CCC	6	0	8	0	0
8	AAA	112	0	0	1	0
8	BBB	49	0	0	0	0
8	CCC	83	0	0	3	0
8	DDD	31	0	0	0	0
8	EEE	65	0	0	1	0
8	FFF	22	0	0	0	0
8	GGG	110	0	0	0	0
8	HHH	35	0	0	0	0
All	All	9143	0	8562	39	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.

The worst 5 of 39 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)
2:BBB:207:ARG:HH12	5:BBB:402:EDO:H21	1.57	0.70
1:GGG:16:SER:HB3	1:GGG:19:GLN:HG2	1.73	0.69
1:EEE:22:LEU:O	1:EEE:26:LEU:HG	2.03	0.58
1:AAA:85:CYS:HB2	2:BBB:212:PRO:HA	1.87	0.55
1:EEE:22:LEU:HA	1:EEE:25:GLU:OE1	2.07	0.54

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	AAA	160/178 (90%)	159 (99%)	1 (1%)	0	100	100
1	CCC	157/178 (88%)	154 (98%)	3 (2%)	0	100	100
1	EEE	154/178 (86%)	151 (98%)	3 (2%)	0	100	100
1	GGG	158/178 (89%)	154 (98%)	4 (2%)	0	100	100
2	BBB	135/143 (94%)	131 (97%)	4 (3%)	0	100	100
2	DDD	135/143 (94%)	131 (97%)	4 (3%)	0	100	100
2	FFF	133/143 (93%)	127 (96%)	6 (4%)	0	100	100
2	HHH	133/143 (93%)	128 (96%)	5 (4%)	0	100	100
All	All	1165/1284 (91%)	1135 (97%)	30 (3%)	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	AAA	125/136 (92%)	125 (100%)	0	100	100
1	CCC	123/136 (90%)	123 (100%)	0	100	100
1	EEE	120/136 (88%)	118 (98%)	2 (2%)	60	47
1	GGG	124/136 (91%)	121 (98%)	3 (2%)	49	32
2	BBB	95/99 (96%)	95 (100%)	0	100	100
2	DDD	95/99 (96%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	FFF	93/99 (94%)	92 (99%)	1 (1%)	73 64
2	HHH	93/99 (94%)	92 (99%)	1 (1%)	73 64
All	All	868/940 (92%)	861 (99%)	7 (1%)	81 75

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GGG	16	SER
1	GGG	17	ARG
2	HHH	230	THR
1	GGG	142	GLU
2	FFF	224	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\|>2$
4	GLY	AAA	202	-	4,4,4	0.75	0	3,4,4	0.55	0
7	GOL	CCC	201	-	5,5,5	0.17	0	5,5,5	0.66	0
4	GLY	DDD	402	-	4,4,4	1.18	1 (25%)	3,4,4	1.55	1 (33%)
5	EDO	BBB	402	-	3,3,3	0.43	0	2,2,2	0.73	0
4	GLY	HHH	501	-	4,4,4	0.96	0	3,4,4	1.21	0
5	EDO	AAA	203	-	3,3,3	0.07	0	2,2,2	0.25	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
4	GLY	AAA	202	-	-	2/2/2/2	-
7	GOL	CCC	201	-	-	2/4/4/4	-
4	GLY	DDD	402	-	-	0/2/2/2	-
5	EDO	BBB	402	-	-	0/1/1/1	-
4	GLY	HHH	501	-	-	2/2/2/2	-
5	EDO	AAA	203	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	402	GLY	OXT-C	-2.27	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	DDD	402	GLY	OXT-C-CA	2.12	121.88	113.45

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	202	GLY	O-C-CA-N
4	AAA	202	GLY	OXT-C-CA-N
4	HHH	501	GLY	O-C-CA-N
4	HHH	501	GLY	OXT-C-CA-N
7	CCC	201	GOL	C1-C2-C3-O3

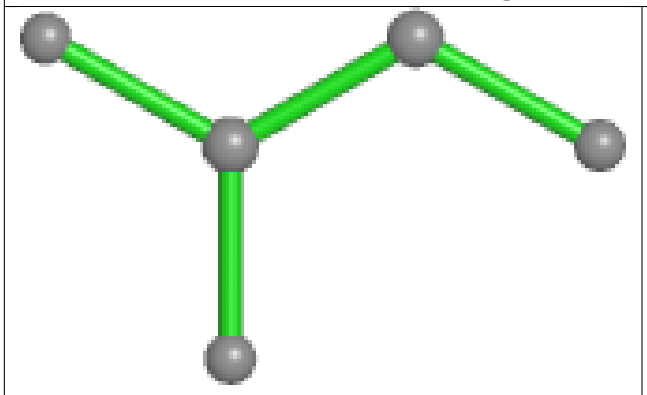
There are no ring outliers.

1 monomer is involved in 3 short contacts:

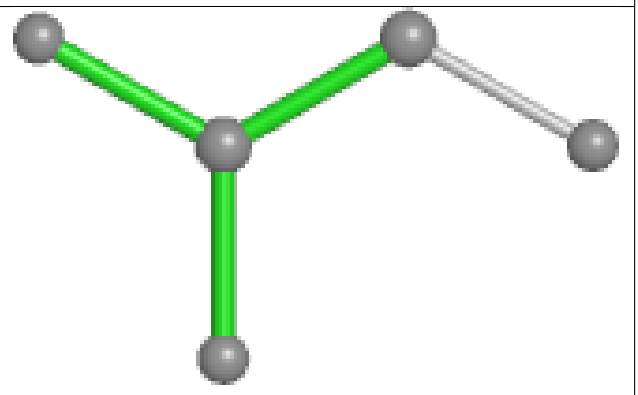
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	402	EDO	3	0

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 then 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.

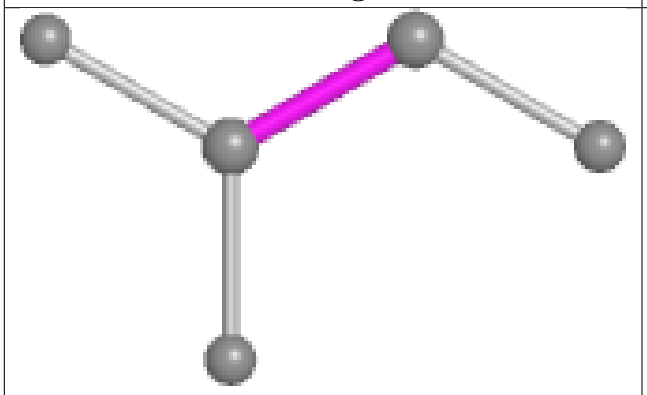
Ligand GLY AAA 202



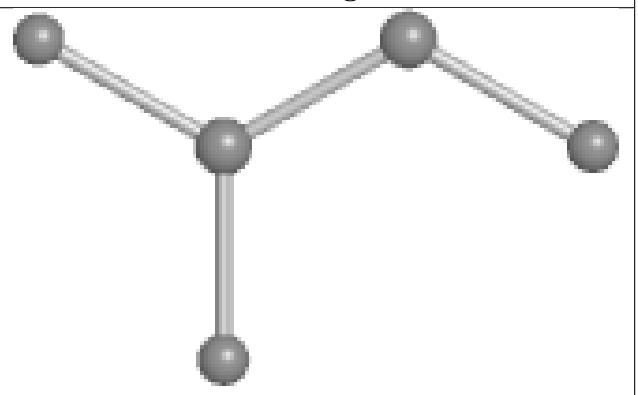
Bond lengths



Bond angles

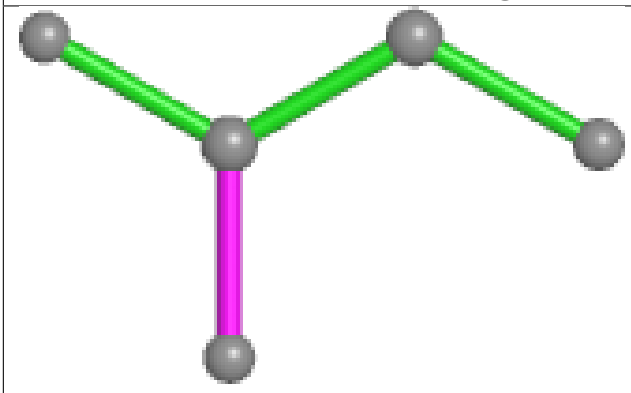


Torsions

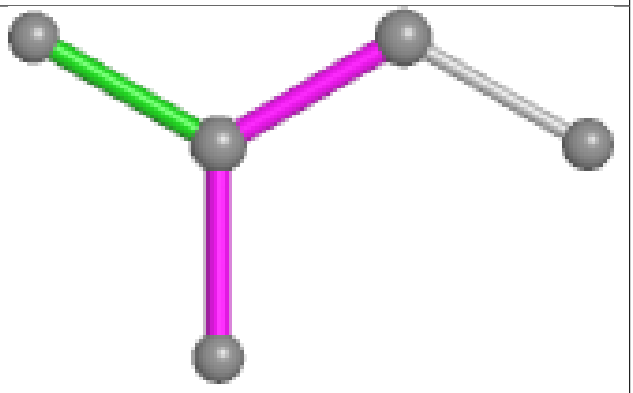


Rings

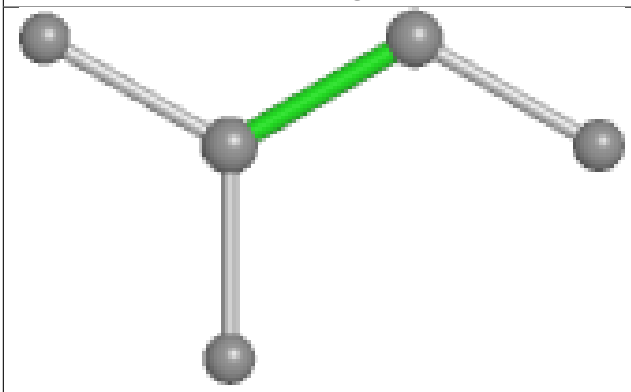
Ligand GLY DDD 402



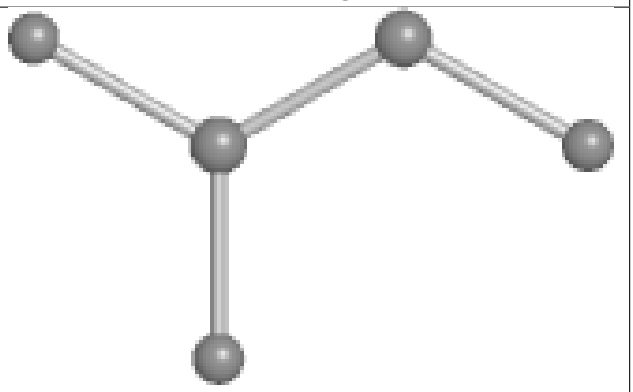
Bond lengths



Bond angles

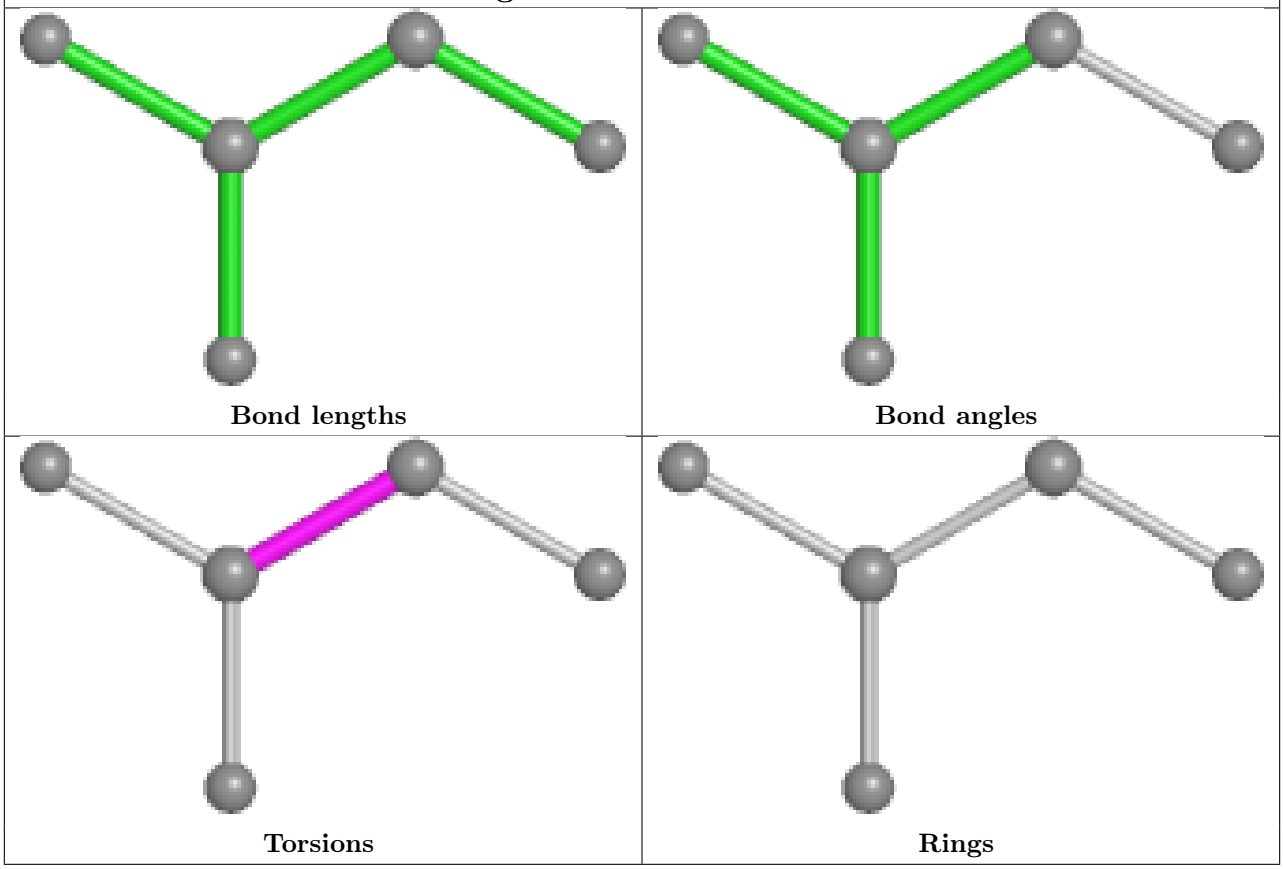


Torsions



Rings

Ligand GLY HHH 501



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, 95^{th} 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	AAA	158/178 (88%)	-0.07	2 (1%) 77 77	20, 31, 66, 86	0
1	CCC	157/178 (88%)	-0.05	2 (1%) 77 77	23, 38, 77, 115	0
1	EEE	154/178 (86%)	0.03	2 (1%) 77 77	26, 47, 81, 100	0
1	GGG	157/178 (88%)	-0.10	2 (1%) 77 77	22, 33, 68, 102	0
2	BBB	135/143 (94%)	-0.22	0 100 100	22, 36, 55, 92	0
2	DDD	135/143 (94%)	-0.17	0 100 100	24, 39, 58, 90	0
2	FFF	135/143 (94%)	0.15	2 (1%) 73 73	32, 48, 69, 92	0
2	HHH	134/143 (93%)	-0.07	0 100 100	23, 41, 61, 78	0
All	All	1165/1284 (90%)	-0.06	10 (0%) 84 84	20, 39, 70, 115	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	159	GLU	4.2
1	GGG	14	ALA	4.1
1	AAA	14	ALA	3.8
1	EEE	18	ALA	3.4
2	FFF	303	GLY	2.7

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 monosaccharides in this entry.

6.4 Ligands (i)

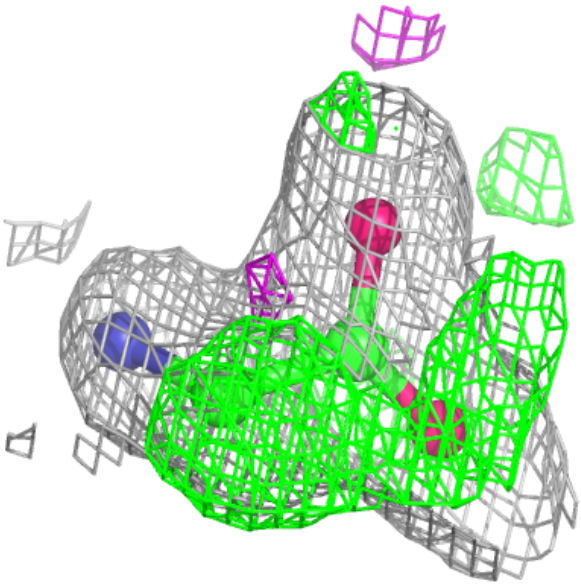
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

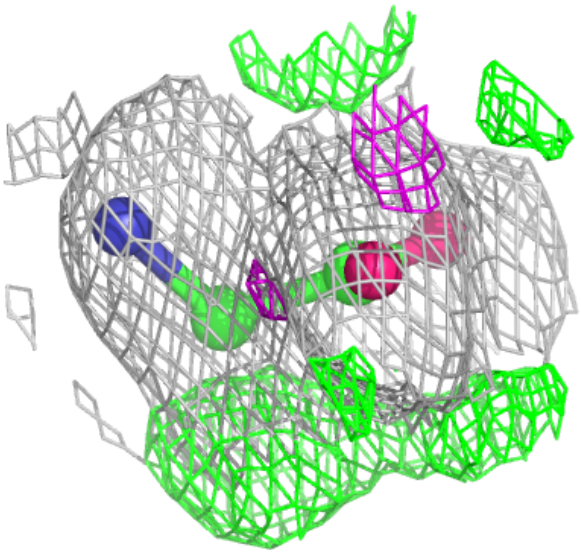
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLY	AAA	202	5/5	0.74	0.16	48,51,52,57	0
5	EDO	BBB	402	4/4	0.89	0.13	40,42,45,46	0
5	EDO	AAA	203	4/4	0.90	0.29	76,76,76,78	0
4	GLY	HHH	501	5/5	0.90	0.16	39,48,49,51	0
6	CL	GGG	203	1/1	0.92	0.07	59,59,59,59	0
7	GOL	CCC	201	6/6	0.93	0.22	48,54,55,56	0
6	CL	BBB	401	1/1	0.95	0.05	49,49,49,49	0
6	CL	DDD	401	1/1	0.96	0.11	45,45,45,45	0
6	CL	EEE	202	1/1	0.97	0.29	76,76,76,76	0
4	GLY	DDD	402	5/5	0.97	0.11	33,35,40,41	0
3	NA	EEE	201	1/1	0.97	0.05	41,41,41,41	0
3	NA	CCC	203	1/1	0.98	0.07	42,42,42,42	0
3	NA	CCC	202	1/1	0.98	0.08	34,34,34,34	0
3	NA	GGG	201	1/1	0.99	0.06	24,24,24,24	0
3	NA	GGG	202	1/1	0.99	0.20	41,41,41,41	0
3	NA	AAA	201	1/1	0.99	0.05	26,26,26,26	0

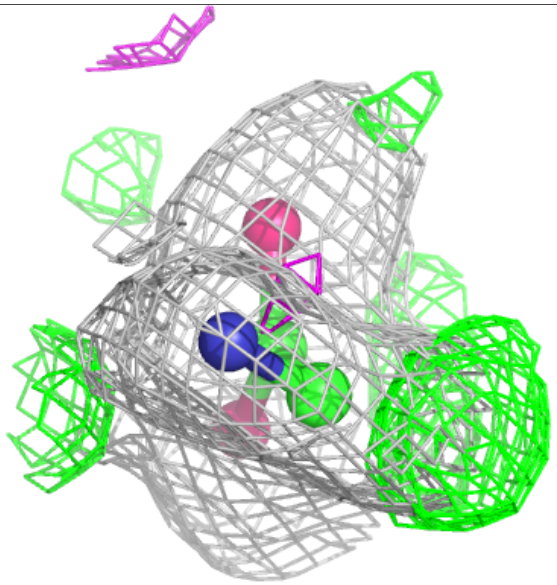
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLY AAA 202:

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

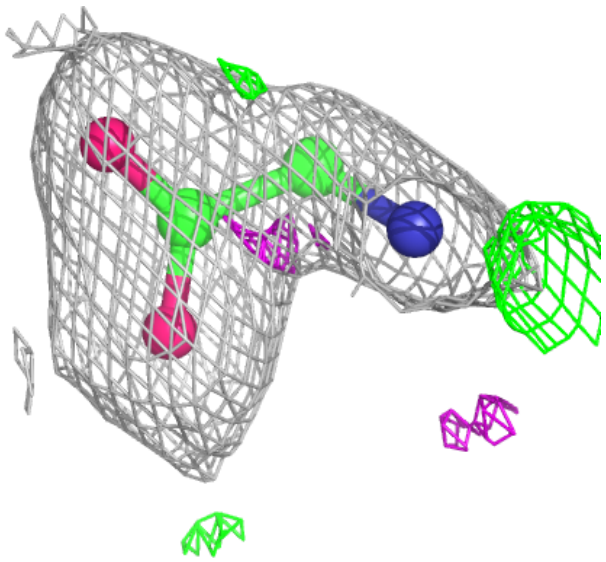


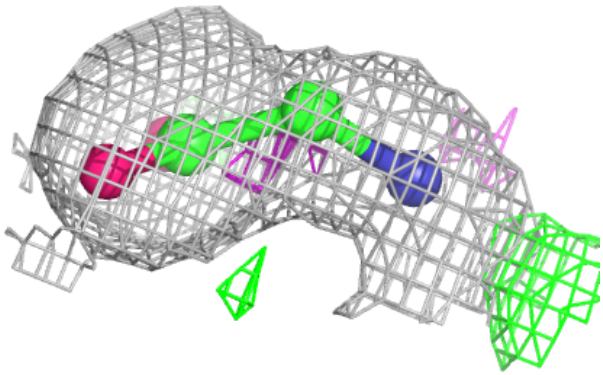


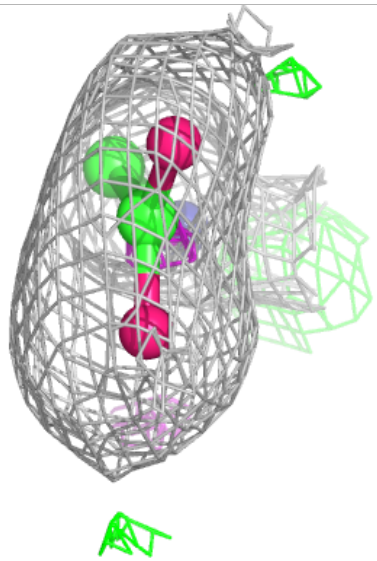


Electron density around GLY HHH 501:

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

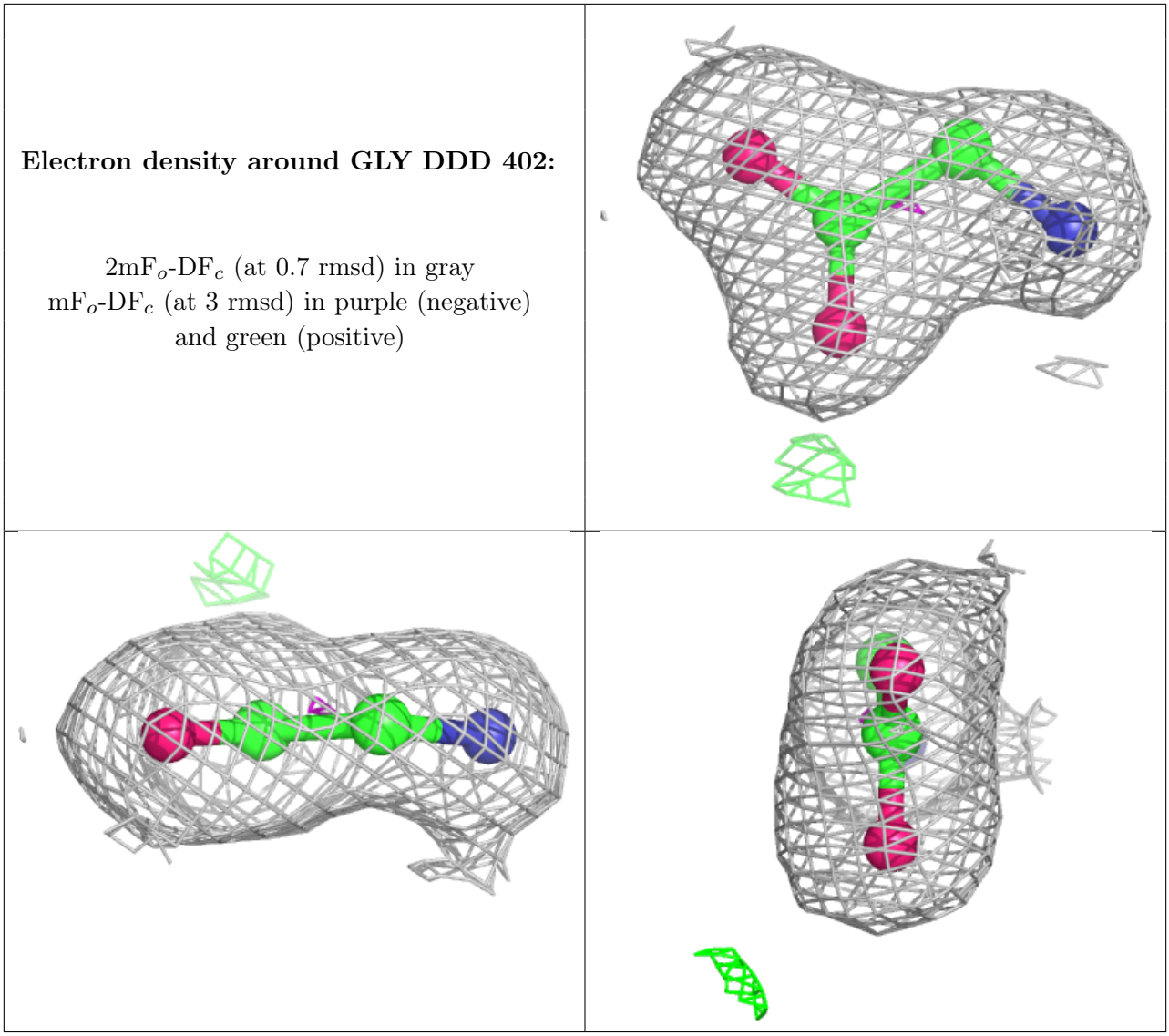






Electron density around GLY DDD 402:

$2mF_o$-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.