



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 08:05 AM UTC

PDB ID : 8C23 / pdb_00008c23
Title : Structure of E. coli Class 2 L-asparaginase EcAIII, mutant M200T (monoclinic form M200T#m)
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Deposited on : 2022-12-21
Resolution : 1.84 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

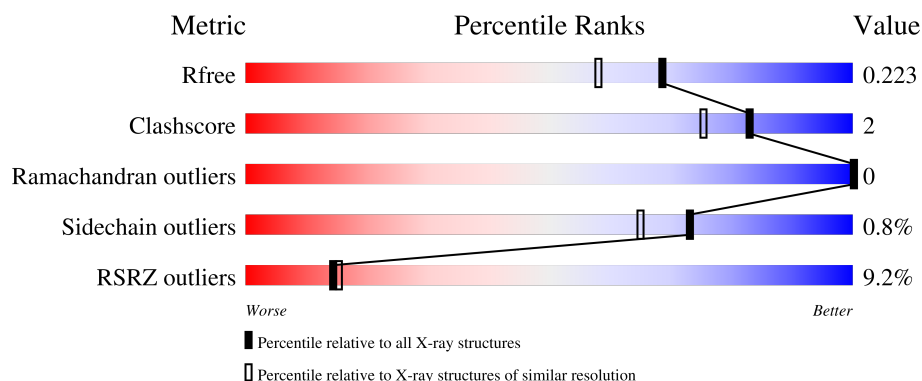
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



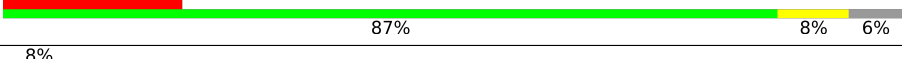
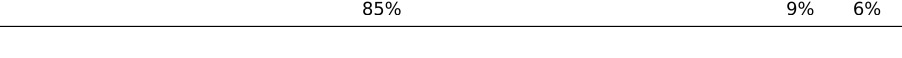
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	AAA	178	4% 86% 11%
1	CCC	178	7% 83% 5% 12%
1	EEE	178	15% 80% 7% 13%
1	GGG	178	7% 80% 8% 12%
2	BBB	143	3% 89% 6% 6%

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Mol	Chain	Length	Quality of chain
2	DDD	143	 3% 89% 6% 6%
2	FFF	143	 20% 87% 8% 6%
2	HHH	143	 8% 85% 9% 6%

2 Entry composition

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			

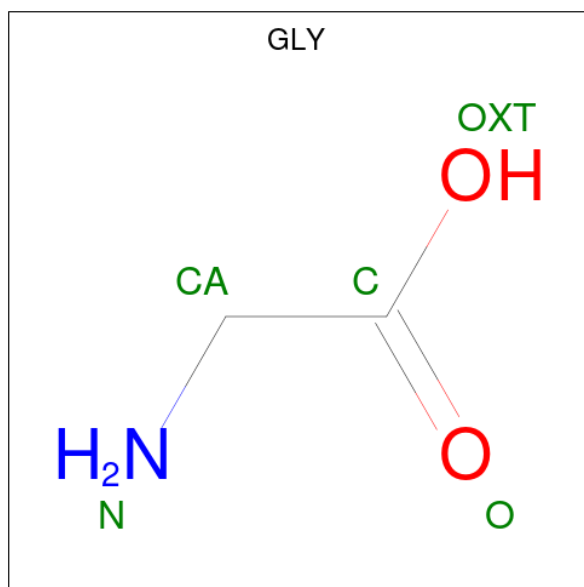
There are 4 discrepancies between the modelled and reference sequences:

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 (CCD ID: NA) (formula: Na).

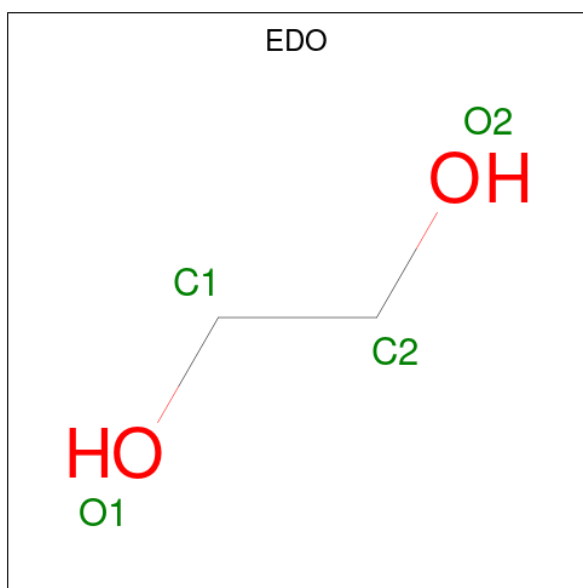
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0
3	CCC	2	Total Na 2 2	0	0
3	EEE	1	Total Na 1 1	0	0
3	GGG	2	Total Na 2 2	0	0

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (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 (CCD ID: EDO) (formula: $C_2H_6O_2$).

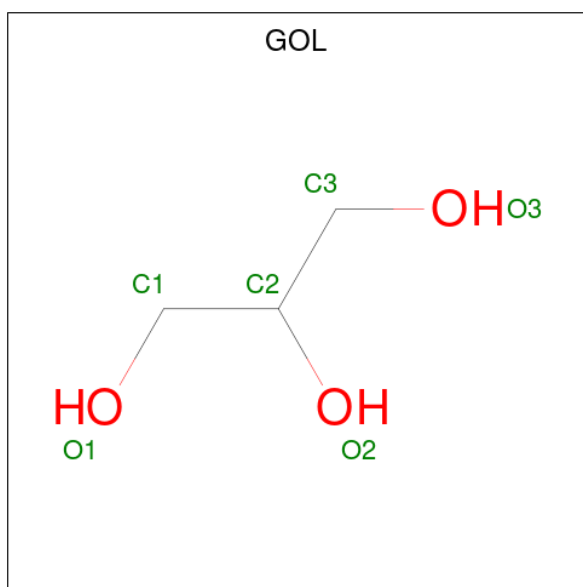


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	C	O	0	0
			4	2	2		
5	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

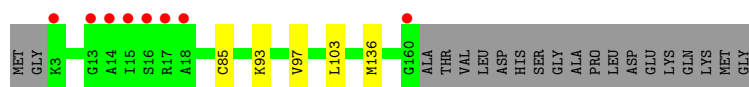
- Molecule 8 is water.

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

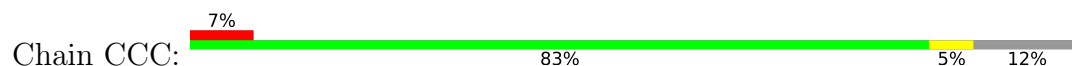
3 Residue-property plots [i](#)

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.

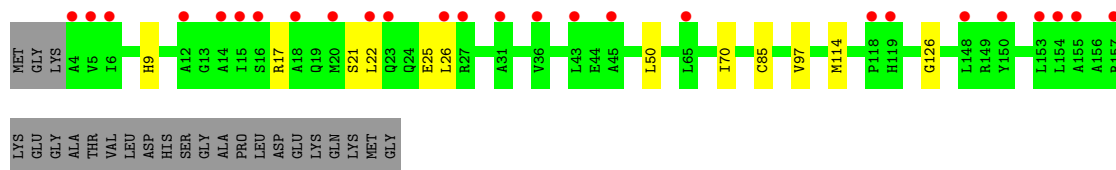
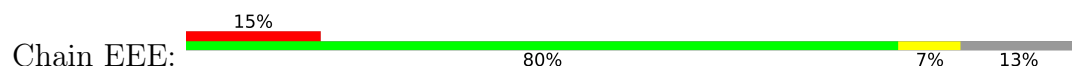
- Molecule 1: Isoaspartyl peptidase subunit alpha



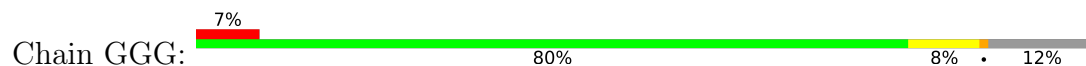
- Molecule 1: Isoaspartyl peptidase subunit alpha



- Molecule 1: Isoaspartyl peptidase subunit alpha



- Molecule 1: Isoaspartyl peptidase subunit alpha

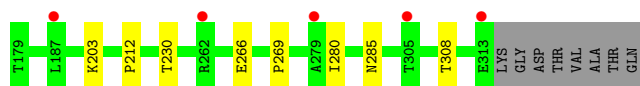


- Molecule 2: Isoaspartyl peptidase subunit beta



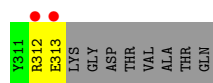
- Molecule 2: Isoaspartyl peptidase subunit beta

Chain DDD:  3% 89% 6% 6%



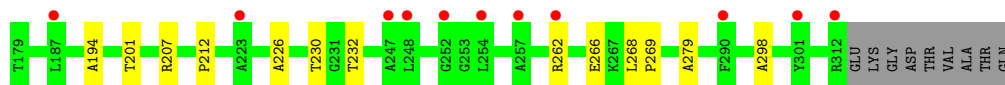
- Molecule 2: Isoaspartyl peptidase subunit beta

Chain FFF:  20% 87% 8% 6%



- Molecule 2: Isoaspartyl peptidase subunit beta

Chain HHH:  8% 85% 9% 6%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (0.80%)	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 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: NA, EDO, CL, GOL

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	1.19	0/1230	1.29	0/1656
1	CCC	1.12	0/1206	1.34	2/1626 (0.1%)
1	EEE	1.09	1/1185 (0.1%)	1.39	0/1599
1	GGG	1.21	1/1216 (0.1%)	1.29	1/1639 (0.1%)
2	BBB	1.12	0/984	1.34	1/1340 (0.1%)
2	DDD	1.13	0/984	1.31	0/1340
2	FFF	1.15	1/966 (0.1%)	1.35	0/1316
2	HHH	1.17	1/964 (0.1%)	1.38	3/1314 (0.2%)
All	All	1.15	4/8735 (0.0%)	1.34	7/11830 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	HHH	298	ALA	C-O	5.79	1.30	1.23
2	FFF	213	LEU	C-O	5.64	1.30	1.24
1	EEE	126	GLY	C-O	5.40	1.30	1.23
1	GGG	13	GLY	C-O	5.28	1.30	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	83	ASP	CA-CB-CG	7.40	120.00	112.60
1	CCC	120	VAL	N-CA-C	-5.51	107.44	111.90
2	HHH	201	THR	CA-CB-OG1	-5.31	101.63	109.60
2	BBB	179	THR	CA-CB-OG1	-5.18	101.83	109.60
1	GGG	54	THR	N-CA-C	-5.02	105.70	111.07
2	HHH	232	THR	CA-C-N	5.01	125.64	120.03
2	HHH	232	THR	C-N-CA	5.01	125.64	120.03

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	7	0
2	BBB	966	0	946	6	0
2	DDD	966	0	946	7	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	41	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 (41) 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
1:CCC:119:HIS:CE1	8:CCC:303:HOH:O	2.61	0.53
8:CCC:304:HOH:O	2:DDD:203:LYS:HE3	2.10	0.50
2:FFF:263:VAL:O	2:FFF:268:LEU:HG	2.11	0.50
1:CCC:85:CYS:HB2	2:DDD:212:PRO:HA	1.93	0.50
2:HHH:268:LEU:HB2	2:HHH:269:PRO:HD3	1.96	0.47
1:CCC:9:HIS:CE1	2:DDD:230:THR:HB	2.50	0.46
1:EEE:9:HIS:CE1	2:FFF:230:THR:HB	2.50	0.46
2:FFF:262:ARG:O	2:FFF:266:GLU:HB2	2.16	0.45
1:AAA:103:LEU:HD22	1:AAA:136[B]:MET:HE2	1.98	0.45
2:BBB:207:ARG:NH1	5:BBB:402:EDO:H21	2.29	0.45
2:HHH:207:ARG:C	2:HHH:207:ARG:HD3	2.41	0.44
2:BBB:226:ALA:O	2:BBB:279:ALA:HA	2.18	0.44
1:GGG:112:LEU:HD22	1:GGG:136:MET:HE3	1.98	0.44
2:FFF:268:LEU:HB2	2:FFF:269:PRO:HD3	1.99	0.44
1:GGG:111:ARG:O	1:GGG:115:GLU:HG3	2.18	0.44
1:EEE:70:ILE:HD12	8:EEE:323:HOH:O	2.18	0.43
8:CCC:304:HOH:O	2:DDD:203:LYS:CE	2.66	0.43
1:CCC:113:VAL:O	1:CCC:117[B]:SER:HB3	2.19	0.43
2:HHH:226:ALA:O	2:HHH:279:ALA:HA	2.18	0.43
2:BBB:233:GLY:HA3	5:BBB:402:EDO:H12	2.00	0.43
1:EEE:85:CYS:HB2	2:FFF:212:PRO:HA	1.99	0.43
1:CCC:33:SER:OG	2:DDD:308:THR:HG21	2.19	0.42
2:FFF:312:ARG:O	2:FFF:313:GLU:HB2	2.19	0.42
1:GGG:85:CYS:HB2	2:HHH:212:PRO:HA	2.00	0.42
2:DDD:266:GLU:C	2:DDD:269:PRO:HD2	2.44	0.42
1:EEE:50:LEU:HD21	1:EEE:114:MET:HE1	2.01	0.42
2:BBB:235:VAL:HG11	2:BBB:273:GLY:HA3	2.02	0.42
1:GGG:28:TYR:CE1	1:GGG:65:LEU:HB3	2.55	0.42
1:AAA:93:LYS:NZ	8:AAA:303:HOH:O	2.48	0.41
1:GGG:86[A]:VAL:HG23	2:HHH:194:ALA:HB2	2.01	0.41
2:DDD:280:ILE:HA	2:DDD:285:ASN:O	2.20	0.41
2:HHH:262:ARG:O	2:HHH:266:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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%)	53	37
1	GGG	124/136 (91%)	121 (98%)	3 (2%)	43	25
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%)	65	54
2	HHH	93/99 (94%)	92 (99%)	1 (1%)	65	54
All	All	868/940 (92%)	861 (99%)	7 (1%)	73	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	17	ARG
1	EEE	21	SER
2	FFF	224	SER
1	GGG	16	SER
1	GGG	17	ARG
1	GGG	142	GLU
2	HHH	230	THR

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 oligosaccharides 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	DDD	402	-	4,4,4	1.21	1 (25%)	3,4,4	1.54	1 (33%)
4	GLY	AAA	202	-	4,4,4	0.76	0	3,4,4	0.55	0
5	EDO	BBB	402	-	3,3,3	0.44	0	2,2,2	0.66	0
4	GLY	HHH	501	-	4,4,4	0.98	0	3,4,4	1.21	0
5	EDO	AAA	203	-	3,3,3	0.06	0	2,2,2	0.18	0
7	GOL	CCC	201	-	5,5,5	0.17	0	5,5,5	0.68	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	DDD	402	-	-	0/2/2/2	-
4	GLY	AAA	202	-	-	2/2/2/2	-
5	EDO	BBB	402	-	-	0/1/1/1	-
4	GLY	HHH	501	-	-	2/2/2/2	-
5	EDO	AAA	203	-	-	1/1/1/1	-
7	GOL	CCC	201	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	402	GLY	OXT-C	-2.33	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DDD	402	GLY	OXT-C-CA	2.14	121.88	113.38

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
4	HHH	501	GLY	OXT-C-CA-N
7	CCC	201	GOL	C1-C2-C3-O3
7	CCC	201	GOL	O2-C2-C3-O3
5	AAA	203	EDO	O1-C1-C2-O2

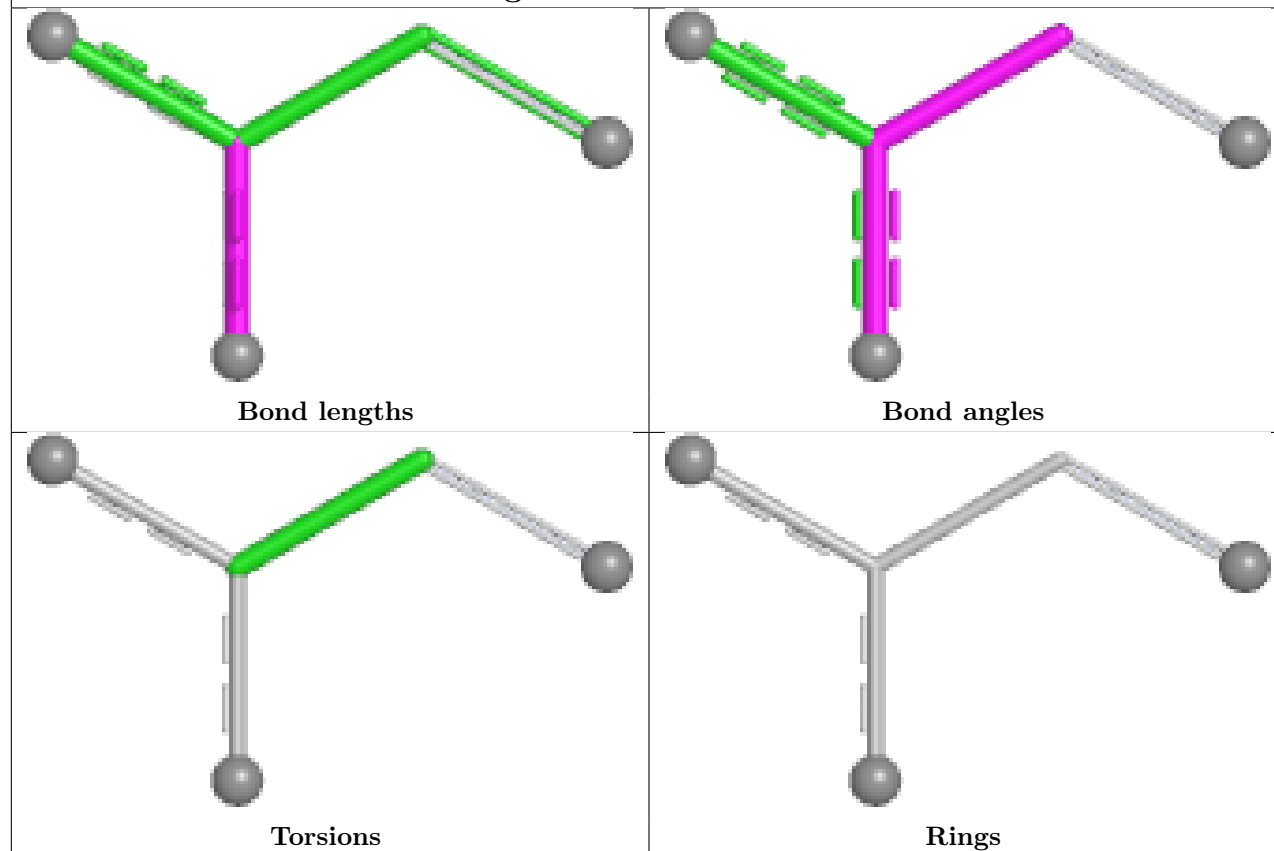
There are no ring outliers.

1 monomer is involved in 3 short contacts:

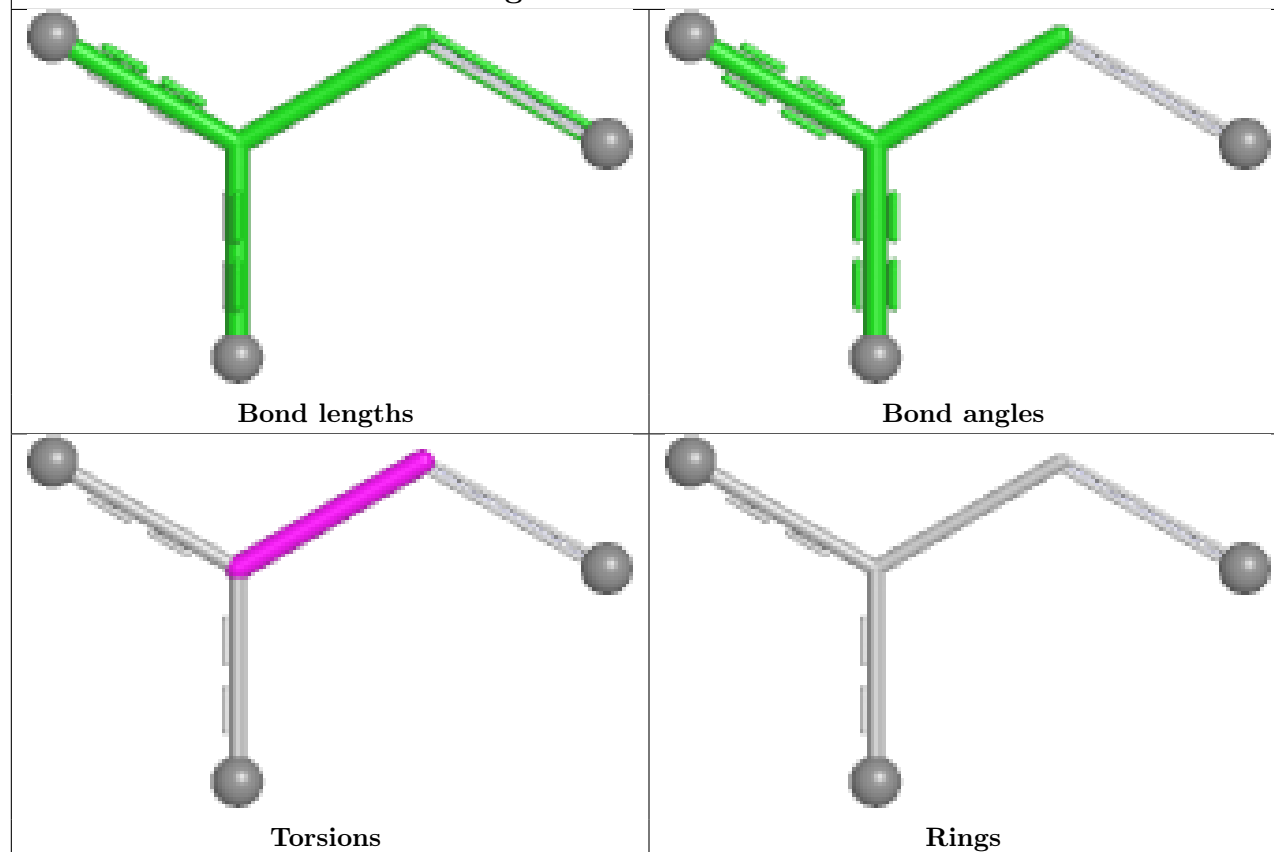
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BBB	402	EDO	3	0

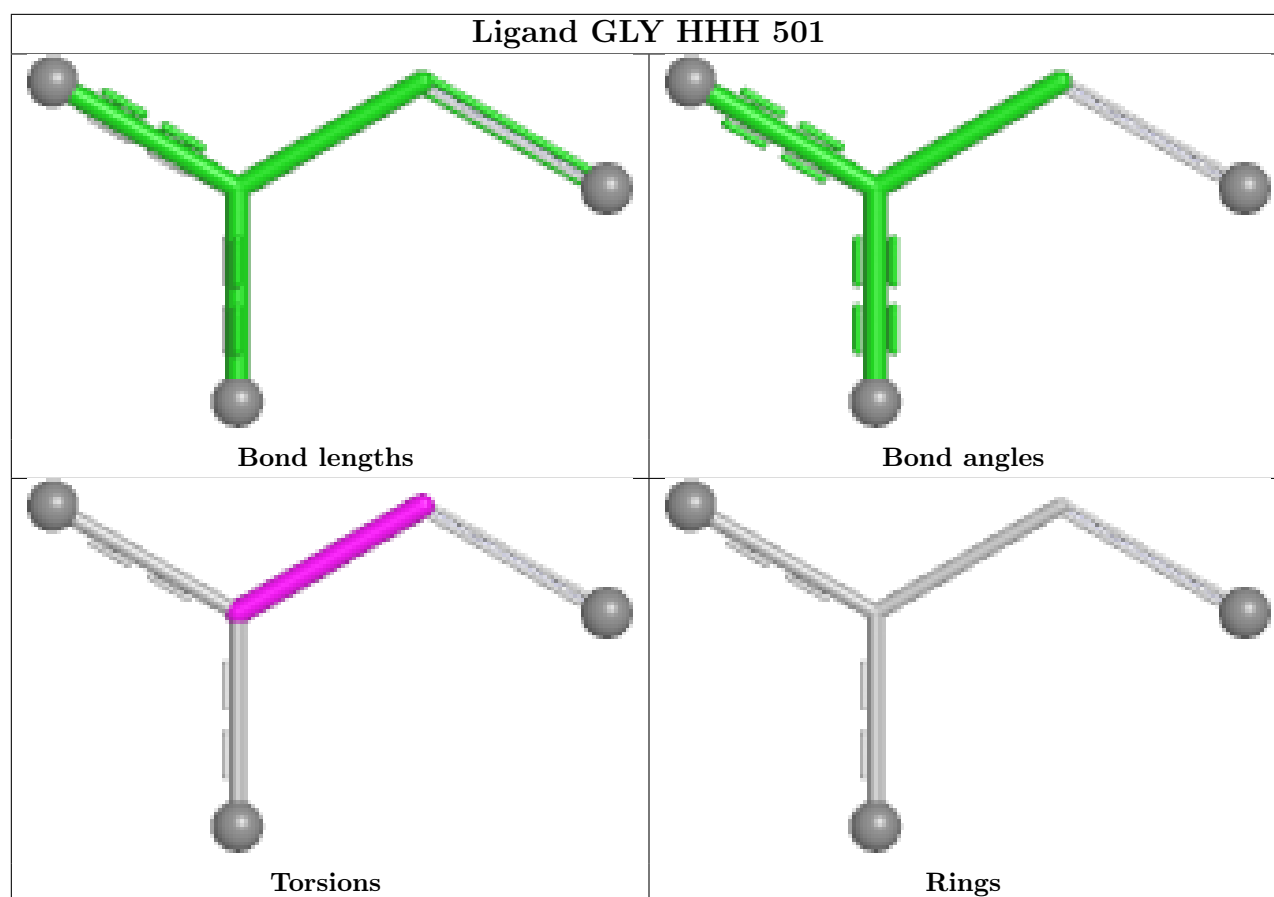
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand GLY DDD 402



Ligand GLY AAA 202





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	AAA	158/178 (88%)	0.35	8 (5%) 33 35	14, 31, 66, 86	4 (2%)
1	CCC	157/178 (88%)	0.62	13 (8%) 17 18	16, 38, 77, 115	2 (1%)
1	EEE	154/178 (86%)	0.98	26 (16%) 4 4	18, 47, 81, 100	2 (1%)
1	GGG	157/178 (88%)	0.50	12 (7%) 20 20	13, 33, 68, 102	3 (1%)
2	BBB	135/143 (94%)	0.43	4 (2%) 52 57	22, 36, 55, 92	2 (1%)
2	DDD	135/143 (94%)	0.53	5 (3%) 45 48	21, 38, 58, 90	2 (1%)
2	FFF	135/143 (94%)	1.24	28 (20%) 2 2	32, 48, 69, 92	0
2	HHH	134/143 (93%)	0.81	11 (8%) 17 18	23, 40, 61, 78	1 (0%)
All	All	1165/1284 (90%)	0.68	107 (9%) 14 15	13, 38, 70, 115	16 (1%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	15	ILE	5.7
1	EEE	18	ALA	5.1
1	EEE	15	ILE	4.9
1	GGG	15	ILE	4.6
1	EEE	22	LEU	4.4
1	AAA	14	ALA	4.4
1	GGG	14	ALA	4.4
1	CCC	18	ALA	4.3
1	AAA	15	ILE	4.1
1	GGG	16	SER	3.7
1	AAA	160	GLY	3.7
1	GGG	18	ALA	3.5
2	FFF	299	TRP	3.5
1	CCC	14	ALA	3.5
1	AAA	3	LYS	3.3
2	FFF	282	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
2	DDD	305	THR	3.2
1	CCC	159	GLU	3.2
1	EEE	14	ALA	3.1
1	EEE	154	LEU	3.1
2	HHH	252	GLY	3.1
1	AAA	17	ARG	3.0
2	FFF	305	THR	3.0
2	HHH	312	ARG	3.0
2	HHH	257	ALA	3.0
1	EEE	23	GLN	3.0
1	GGG	118	PRO	2.9
1	AAA	18	ALA	2.9
1	CCC	20	MET	2.9
2	FFF	187	LEU	2.9
1	EEE	119	HIS	2.8
1	GGG	159	GLU	2.8
1	CCC	22	LEU	2.8
1	CCC	155	ALA	2.8
1	EEE	157	ARG	2.8
1	CCC	3	LYS	2.8
2	FFF	303	GLY	2.7
2	DDD	187	LEU	2.7
1	EEE	155	ALA	2.7
2	FFF	249	MET	2.6
1	CCC	158	LYS	2.6
1	EEE	118	PRO	2.6
2	FFF	312	ARG	2.6
2	HHH	301	TYR	2.6
1	EEE	36	VAL	2.6
1	GGG	13	GLY	2.6
1	AAA	16	SER	2.6
2	BBB	305	THR	2.6
1	EEE	150	TYR	2.5
2	FFF	301	TYR	2.5
1	GGG	3	LYS	2.5
1	EEE	16	SER	2.5
1	EEE	45	ALA	2.5
2	BBB	262[A]	ARG	2.5
1	EEE	20	MET	2.5
2	DDD	262[A]	ARG	2.4
1	EEE	4	ALA	2.4
1	EEE	27	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	156	ALA	2.4
2	FFF	223	ALA	2.4
2	FFF	224	SER	2.4
2	DDD	279	ALA	2.4
1	GGG	20	MET	2.4
1	CCC	154	LEU	2.3
2	BBB	301	TYR	2.3
2	FFF	270	ALA	2.3
2	HHH	247	ALA	2.3
2	FFF	309	GLY	2.3
2	BBB	312	ARG	2.3
1	EEE	12	ALA	2.3
2	FFF	247	ALA	2.3
2	FFF	306	PRO	2.3
1	EEE	6	ILE	2.3
1	EEE	65	LEU	2.3
1	EEE	153	LEU	2.3
2	HHH	187	LEU	2.3
1	GGG	17	ARG	2.2
2	FFF	313	GLU	2.2
2	DDD	313	GLU	2.2
2	FFF	256	LEU	2.2
2	HHH	254	LEU	2.2
2	FFF	279	ALA	2.2
1	GGG	29	ILE	2.2
1	EEE	148	LEU	2.2
2	FFF	189	GLY	2.2
2	FFF	287	ALA	2.2
2	HHH	223	ALA	2.2
1	GGG	44	GLU	2.1
2	FFF	253	GLY	2.1
1	EEE	26	LEU	2.1
2	FFF	184	ALA	2.1
2	FFF	290	PHE	2.1
2	HHH	290	PHE	2.1
1	CCC	147	SER	2.1
2	FFF	308	THR	2.1
1	EEE	5	VAL	2.1
2	FFF	286	VAL	2.1
1	CCC	118	PRO	2.1
1	EEE	43	LEU	2.1
2	HHH	262	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	FFF	181	GLY	2.1
2	HHH	248	LEU	2.1
2	FFF	310	ILE	2.0
2	FFF	251	TYR	2.0
1	EEE	31	ALA	2.0
1	AAA	13	GLY	2.0
2	FFF	272	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

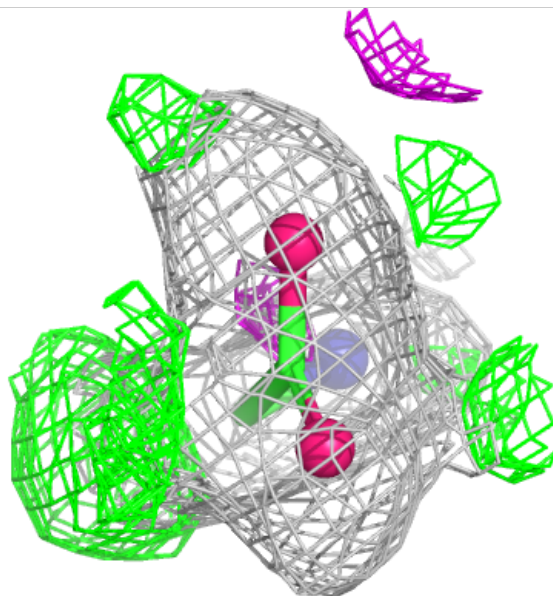
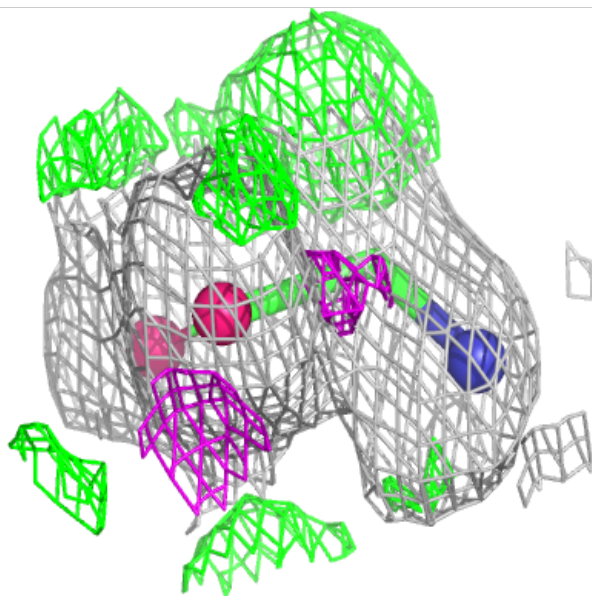
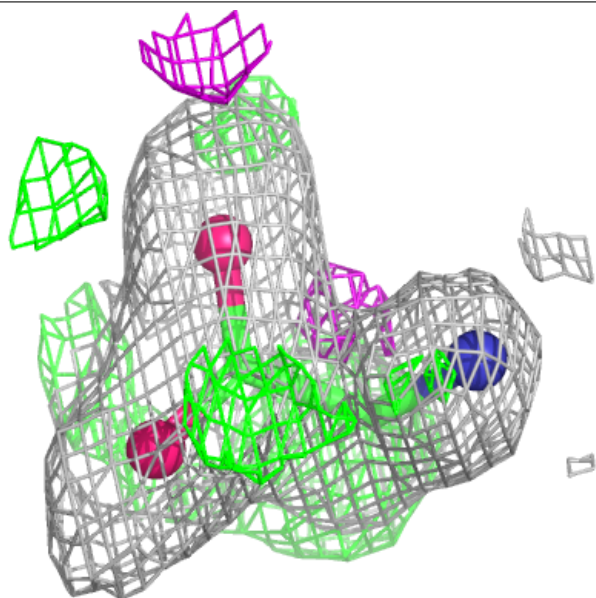
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLY	AAA	202	5/5	0.76	0.16	48,51,52,57	0
5	EDO	AAA	203	4/4	0.82	0.16	76,76,76,78	0
4	GLY	HHH	501	5/5	0.85	0.16	39,48,49,51	0
7	GOL	CCC	201	6/6	0.87	0.14	48,54,55,56	0
5	EDO	BBB	402	4/4	0.88	0.15	40,42,45,46	0
6	CL	GGG	203	1/1	0.92	0.14	59,59,59,59	0
6	CL	EEE	202	1/1	0.92	0.26	76,76,76,76	0
3	NA	GGG	202	1/1	0.95	0.11	41,41,41,41	0
3	NA	CCC	203	1/1	0.96	0.09	42,42,42,42	0
4	GLY	DDD	402	5/5	0.96	0.10	33,35,40,41	0
3	NA	EEE	201	1/1	0.97	0.05	41,41,41,41	0
6	CL	BBB	401	1/1	0.97	0.08	49,49,49,49	0
6	CL	DDD	401	1/1	0.97	0.07	45,45,45,45	0
3	NA	CCC	202	1/1	0.98	0.05	34,34,34,34	0
3	NA	AAA	201	1/1	0.98	0.07	26,26,26,26	0
3	NA	GGG	201	1/1	0.99	0.05	24,24,24,24	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.

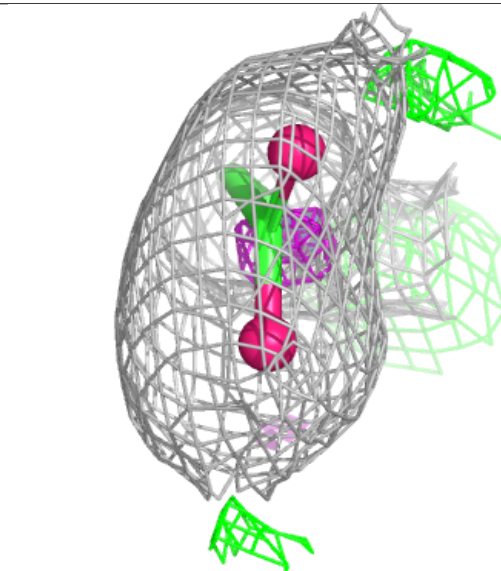
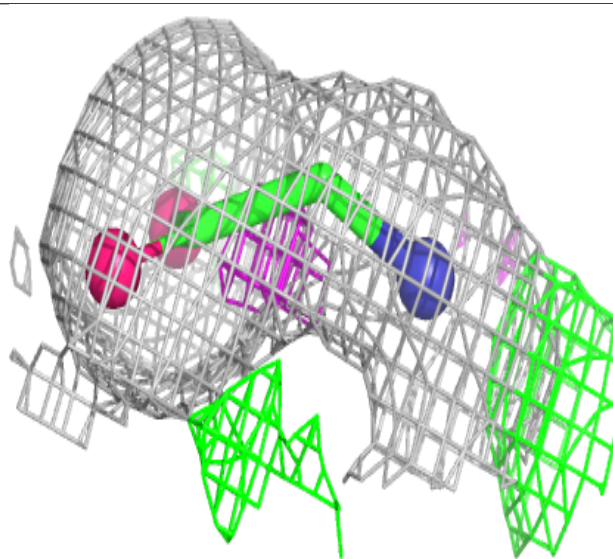
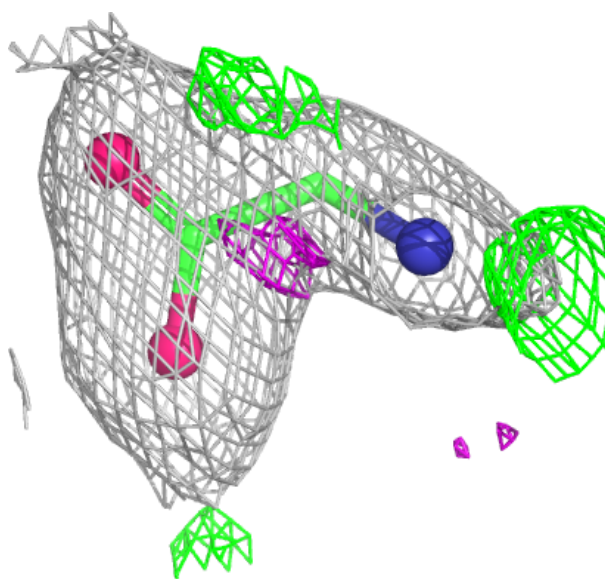
Electron density around GLY AAA 202:

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



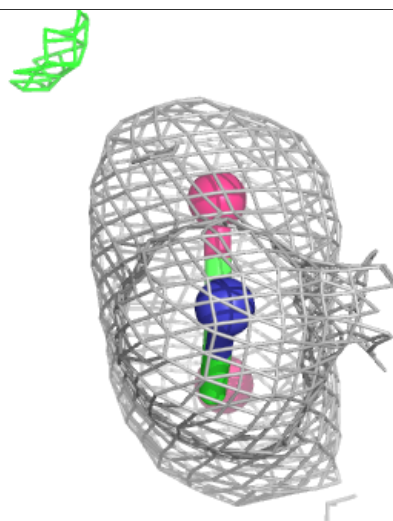
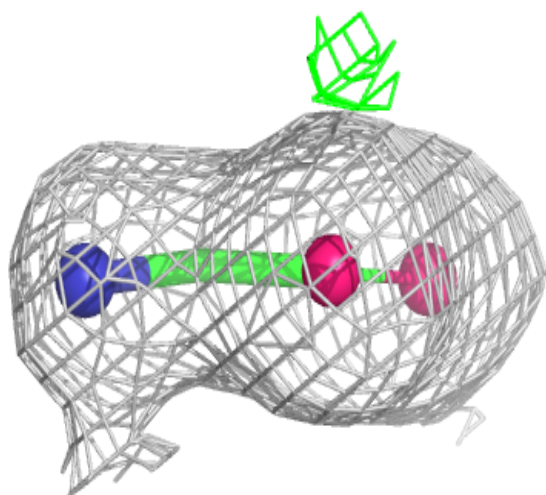
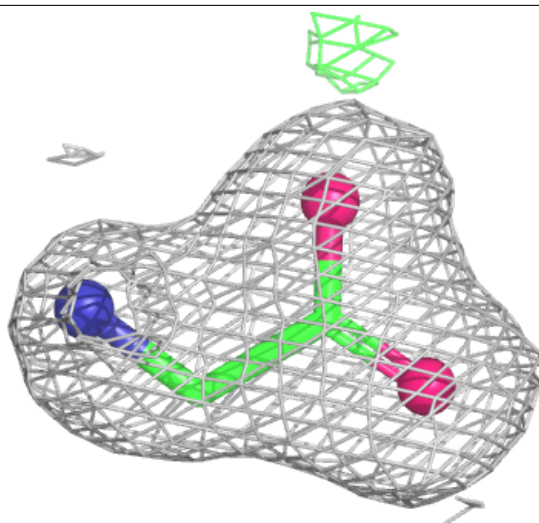
Electron density around GLY HHH 501:

$2mF_o-DF_c$ (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.