



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:25 AM UTC

PDB ID : 4KNL / pdb_00004knl
Title : Crystal structure of Staphylococcus aureus hydrolase AmiA in complex with its ligand
Authors : Buettner, F.M.; Stehle, T.
Deposited on : 2013-05-10
Resolution : 1.55 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

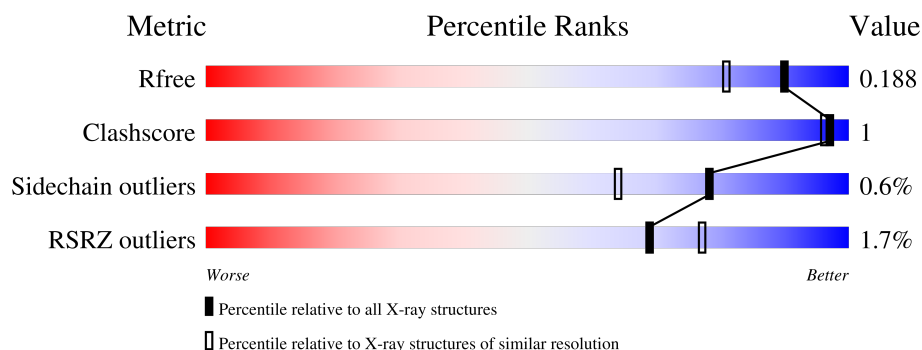
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	225	89% • 9%
1	B	225	2% 90% • 9%
1	C	225	0% 90% • 8%
1	D	225	3% 87% • 9%
2	F	5	60% 20% 20%
2	G	5	60% 40%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7321 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 Bifunctional autolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1631	1039	270	318	4			
1	B	205	Total	C	N	O	S	0	0	0
			1630	1038	270	318	4			
1	C	207	Total	C	N	O	S	0	1	0
			1648	1048	274	322	4			
1	D	204	Total	C	N	O	S	0	0	0
			1622	1033	269	316	4			

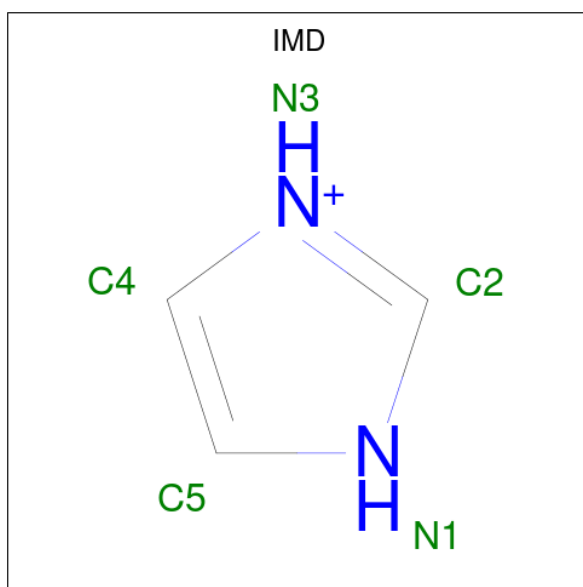
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLY	-	expression tag	UNP Q2FZK7
B	197	GLY	-	expression tag	UNP Q2FZK7
C	197	GLY	-	expression tag	UNP Q2FZK7
D	197	GLY	-	expression tag	UNP Q2FZK7

- Molecule 2 is a protein called Muramyl tetrapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	5	Total	C	N	O	0	0	1
			32	19	7	6			
2	G	5	Total	C	N	O	0	0	1
			32	19	7	6			

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).

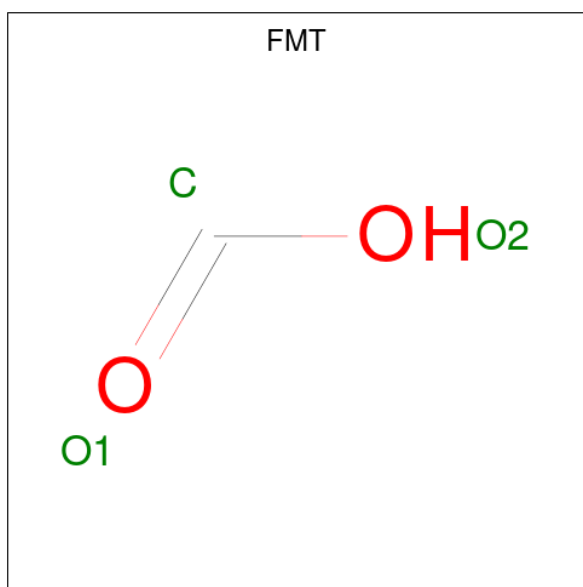


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

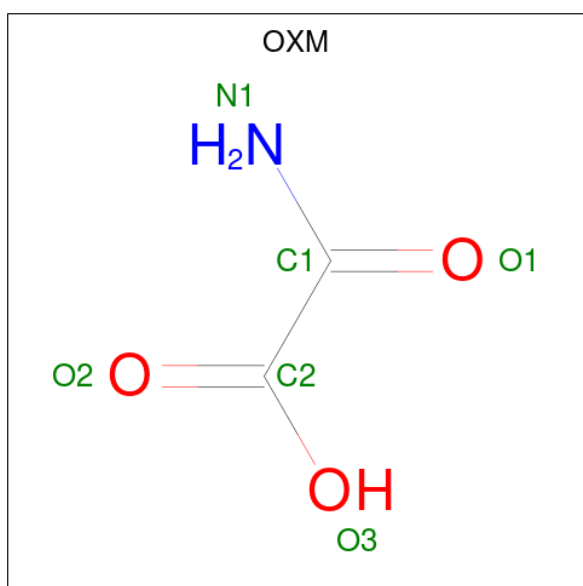
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		
4	C	2	Total	Na	0	0
			2	2		
4	D	2	Total	Na	0	0
			2	2		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



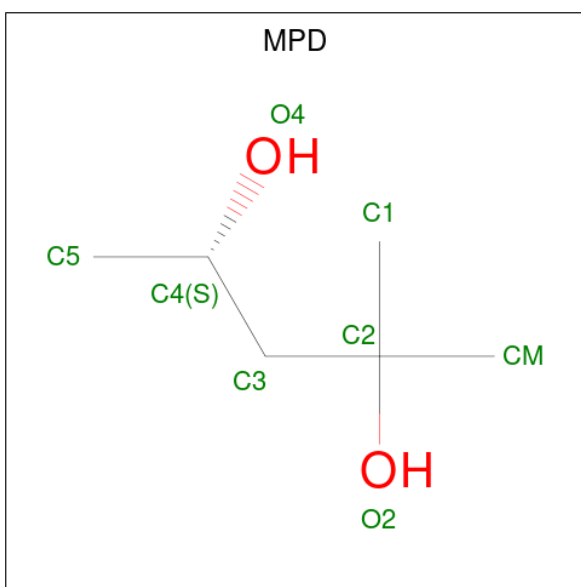
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



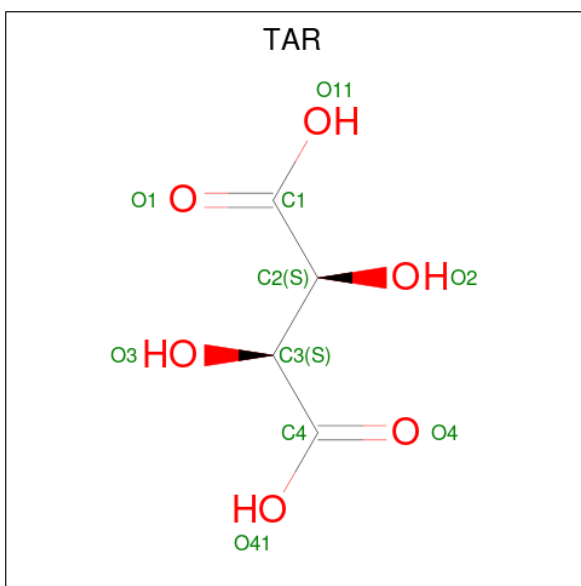
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



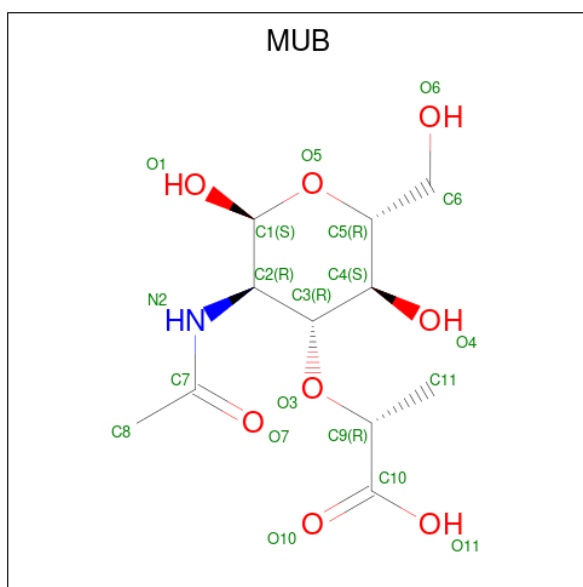
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 9 is N-acetyl-alpha-muramic acid (CCD ID: MUB) (formula: $C_{11}H_{19}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total	C	N	O	0	0
			19	11	1	7		
9	G	1	Total	C	N	O	0	0
			19	11	1	7		

- Molecule 10 is water.

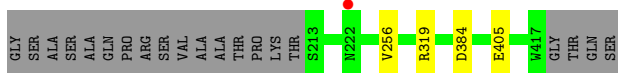
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	169	Total	O	0	0
			169	169		
10	B	134	Total	O	0	0
			134	134		
10	C	174	Total	O	0	0
			174	174		
10	D	144	Total	O	0	0
			144	144		
10	F	5	Total	O	0	0
			5	5		
10	G	4	Total	O	0	0
			4	4		

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.

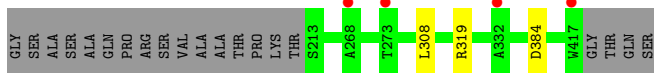
- Molecule 1: Bifunctional autolysin

Chain A:  89% 9%



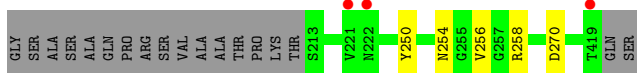
- Molecule 1: Bifunctional autolysin

Chain B:  90% 9%



- Molecule 1: Bifunctional autolysin

Chain C:  90% 8%



- Molecule 1: Bifunctional autolysin

Chain D:  87% 9%



- Molecule 2: Muramyl tetrapeptide

Chain F:  60% 20% 20%



- Molecule 2: Muramyl tetrapeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.81Å 82.83Å 77.43Å 90.00° 96.18° 90.00°	Depositor
Resolution (Å)	48.21 – 1.55 48.21 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.21-1.55) 99.5 (48.21-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.171 , 0.198 (Not available) , 0.188	Depositor DCC
R_{free} test set	6137 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1055e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TAR, IMD, DAL, ZGL, NH2, MUB, FMT, MPD, ALY, OXM, NA

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	0.74	0/1681	0.87	0/2297
1	B	0.62	0/1680	0.84	0/2296
1	C	0.72	0/1701	0.86	0/2324
1	D	0.64	0/1672	0.85	0/2286
2	F	0.41	0/4	1.28	0/4
2	G	0.45	0/4	0.70	0/4
All	All	0.68	0/6742	0.86	0/9211

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
2	F	0	2
2	G	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	3	ZGL	Peptide,Mainchain
2	G	3	ZGL	Peptide,Mainchain

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	1631	0	1482	3	0
1	B	1630	0	1480	2	0
1	C	1648	0	1503	3	0
1	D	1622	0	1471	4	0
2	F	32	0	26	0	0
2	G	32	0	25	1	0
3	A	5	0	5	1	0
3	B	5	0	5	0	0
3	C	5	0	5	0	0
3	D	5	0	5	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	3	0	1	1	0
5	B	3	0	1	1	0
6	B	6	0	2	0	0
7	C	8	0	14	2	0
8	C	10	0	4	0	0
9	F	19	0	18	0	0
9	G	19	0	18	0	0
10	A	169	0	0	0	0
10	B	134	0	0	0	0
10	C	174	0	0	0	0
10	D	144	0	0	0	0
10	F	5	0	0	0	0
10	G	4	0	0	0	0
All	All	7321	0	6065	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:NH1	5:A:503:FMT:O1	2.30	0.61
1:B:319:ARG:NH1	5:B:503:FMT:O1	2.36	0.56
1:C:254:ASN:O	1:C:258:ARG:HD2	2.08	0.54
1:A:405:GLU:OE1	3:A:501:IMD:H5	2.09	0.51
1:C:250:TYR:CE2	7:C:503:MPD:H11	2.51	0.46
7:C:503:MPD:H4	2:G:4:ALY:HH32	1.99	0.45
1:D:254:ASN:O	1:D:258:ARG:HD2	2.17	0.45
1:A:256:VAL:HG11	1:C:256:VAL:HG11	1.98	0.44
1:B:308:LEU:HD12	1:B:308:LEU:C	2.43	0.44
1:D:405:GLU:O	1:D:409:ILE:HG13	2.19	0.43
1:D:325:ILE:HD13	1:D:338:MET:HE1	2.02	0.41
1:D:342:ALA:HA	1:D:403:ILE:HG12	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/188 (89%)	166 (99%)	1 (1%)	78	64
1	B	167/188 (89%)	166 (99%)	1 (1%)	78	64
1	C	170/188 (90%)	169 (99%)	1 (1%)	78	64
1	D	166/188 (88%)	165 (99%)	1 (1%)	78	64
All	All	670/752 (89%)	666 (99%)	4 (1%)	78	64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	ASP
1	B	384	ASP
1	C	270	ASP
1	D	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	322	ASN
1	A	393	ASN
1	C	226	ASN
1	C	322	ASN
1	C	398	GLN
1	D	226	ASN
1	D	322	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	ZGL	F	3	2	7,8,9	0.46	0	8,9,11	1.11	1 (12%)
2	ALY	G	4	2	10,11,12	2.24	3 (30%)	7,12,14	0.87	0
2	ALY	F	4	2	10,11,12	2.13	3 (30%)	7,12,14	0.88	0
2	ZGL	G	3	2	7,8,9	0.39	0	8,9,11	0.89	1 (12%)

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	ZGL	F	3	2	-	1/8/8/9	-
2	ALY	G	4	2	-	2/9/10/12	-
2	ALY	F	4	2	-	2/9/10/12	-
2	ZGL	G	3	2	-	1/8/8/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	ALY	OH-CH	5.16	1.34	1.23
2	F	4	ALY	OH-CH	5.09	1.34	1.23
2	G	4	ALY	CH-NZ	-3.53	1.24	1.34
2	F	4	ALY	CH-NZ	-3.44	1.24	1.34
2	G	4	ALY	CB-CA	-2.66	1.49	1.53
2	F	4	ALY	CB-CA	-2.03	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	ZGL	CB-CG-C	-2.61	104.92	112.27
2	G	3	ZGL	CB-CG-C	-2.32	105.75	112.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	4	ALY	OH-CH-NZ-CE
2	G	4	ALY	CH3-CH-NZ-CE
2	F	3	ZGL	O-C-CG-CB
2	G	3	ZGL	O-C-CG-CB
2	F	4	ALY	OH-CH-NZ-CE
2	F	4	ALY	CH3-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	4	ALY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
3	IMD	D	501	-	5,5,5	0.69	0	5,5,5	0.48	0
9	MUB	F	1	2	18,19,20	0.97	1 (5%)	21,26,28	1.40	4 (19%)
5	FMT	B	503	-	2,2,2	0.68	0	1,1,1	0.16	0
3	IMD	B	501	-	5,5,5	0.67	0	5,5,5	0.56	0
5	FMT	A	503	-	2,2,2	0.67	0	1,1,1	0.08	0
3	IMD	A	501	-	5,5,5	0.65	0	5,5,5	0.56	0
6	OXM	B	505	-	5,5,5	2.90	2 (40%)	2,6,6	1.35	0
8	TAR	C	504	-	9,9,9	1.45	1 (11%)	12,12,12	1.84	4 (33%)
7	MPD	C	503	-	7,7,7	0.27	0	9,10,10	0.84	0
9	MUB	G	1	2	18,19,20	1.03	2 (11%)	21,26,28	1.19	3 (14%)
3	IMD	C	501	-	5,5,5	0.68	0	5,5,5	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	D	501	-	-	-	0/1/1/1
9	MUB	F	1	2	-	4/11/32/34	0/1/1/1
3	IMD	B	501	-	-	-	0/1/1/1
3	IMD	A	501	-	-	-	0/1/1/1
3	IMD	C	501	-	-	-	0/1/1/1
8	TAR	C	504	-	-	6/12/12/12	-
9	MUB	G	1	2	-	0/11/32/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	C	503	-	-	2/5/5/5	-
6	OXM	B	505	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	505	OXM	C1-C2	-5.25	1.49	1.55
6	B	505	OXM	C1-N1	3.38	1.43	1.33
9	G	1	MUB	O5-C5	-2.39	1.38	1.44
9	F	1	MUB	O5-C5	-2.25	1.38	1.44
8	C	504	TAR	O2-C2	-2.11	1.38	1.42
9	G	1	MUB	O3-C9	-2.01	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	504	TAR	O11-C1-O1	-2.95	117.39	124.08
8	C	504	TAR	O41-C4-O4	-2.84	117.63	124.08
8	C	504	TAR	O11-C1-C2	2.58	120.49	113.31
9	F	1	MUB	C1-C2-N2	2.43	113.54	110.73
8	C	504	TAR	O41-C4-C3	2.42	120.05	113.31
9	G	1	MUB	C3-C4-C5	2.25	114.37	109.57
9	G	1	MUB	O3-C3-C4	2.11	112.58	107.23
9	F	1	MUB	O7-C7-N2	2.07	125.64	121.98
9	F	1	MUB	O3-C3-C4	2.07	112.50	107.23
9	G	1	MUB	O5-C5-C4	2.04	113.38	109.70
9	F	1	MUB	O5-C1-C2	2.01	111.54	109.52

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	504	TAR	O1-C1-C2-O2
8	C	504	TAR	O11-C1-C2-O2
8	C	504	TAR	C2-C3-C4-O4
8	C	504	TAR	C2-C3-C4-O41
8	C	504	TAR	O3-C3-C4-O4
8	C	504	TAR	O3-C3-C4-O41
9	F	1	MUB	C4-C5-C6-O6
9	F	1	MUB	O5-C5-C6-O6
9	F	1	MUB	C8-C7-N2-C2

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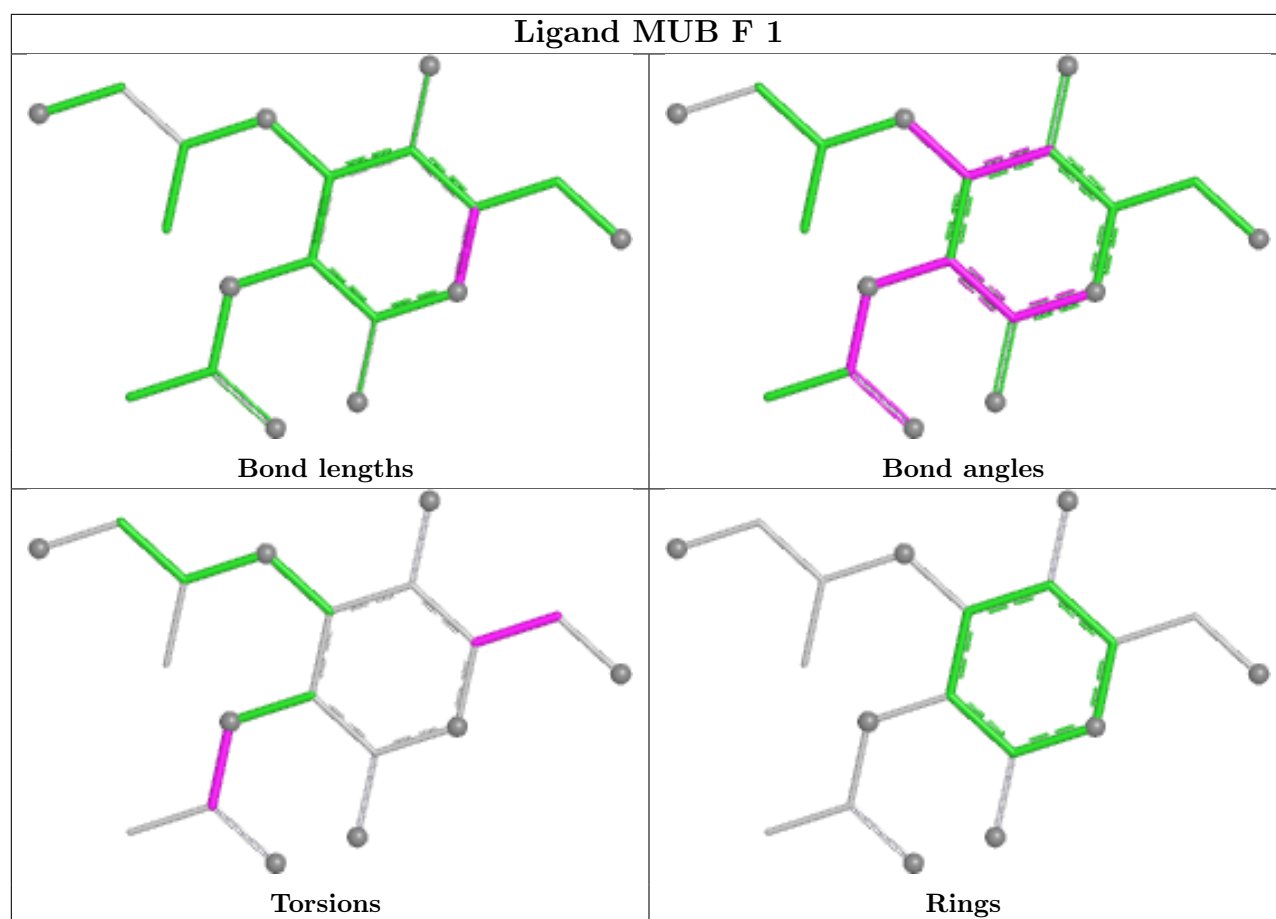
Mol	Chain	Res	Type	Atoms
7	C	503	MPD	O2-C2-C3-C4
7	C	503	MPD	C1-C2-C3-C4
9	F	1	MUB	O7-C7-N2-C2

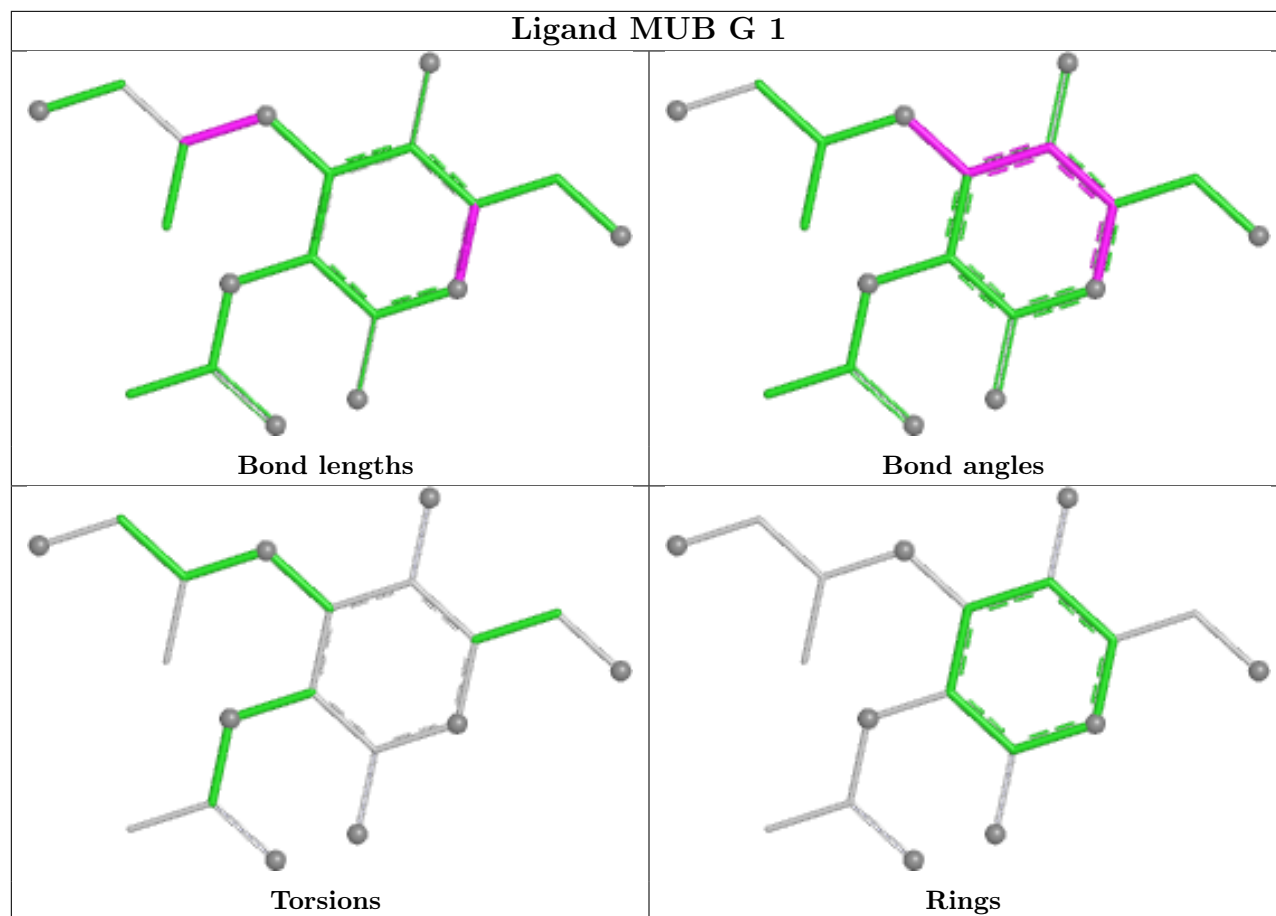
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	FMT	1	0
5	A	503	FMT	1	0
3	A	501	IMD	1	0
7	C	503	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	205/225 (91%)	-0.03	1 (0%) 87 90	14, 19, 32, 50	0
1	B	205/225 (91%)	0.45	4 (1%) 65 73	16, 27, 44, 53	0
1	C	207/225 (92%)	0.08	3 (1%) 73 80	12, 20, 36, 51	1 (0%)
1	D	204/225 (90%)	0.44	6 (2%) 53 62	16, 25, 45, 59	0
2	F	1/5 (20%)	1.68	0 100 100	35, 35, 35, 35	0
2	G	1/5 (20%)	1.14	0 100 100	39, 39, 39, 39	0
All	All	823/910 (90%)	0.24	14 (1%) 69 77	12, 23, 42, 59	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	LEU	3.6
1	B	417	TRP	3.2
1	D	417	TRP	3.1
1	D	332	ALA	2.7
1	C	419	THR	2.5
1	C	221	VAL	2.4
1	B	268	ALA	2.3
1	D	222	ASN	2.3
1	A	222	ASN	2.2
1	C	222	ASN	2.2
1	B	332	ALA	2.1
1	D	415	ALA	2.1
1	D	334	PHE	2.0
1	B	273	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	ALY	F	4	12/13	0.94	0.09	18,23,41,44	0
2	ZGL	F	3	9/10	0.94	0.09	19,26,33,35	0
2	DAL	F	5	5/6	0.94	0.09	26,27,29,30	0
2	DAL	G	5	5/6	0.94	0.09	27,28,31,34	0
2	ALY	G	4	12/13	0.95	0.10	19,25,48,55	0
2	ZGL	G	3	9/10	0.95	0.08	17,25,36,37	0

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
9	MUB	G	1	19/20	0.74	0.16	39,54,60,61	0
9	MUB	F	1	19/20	0.78	0.15	31,40,46,47	0
3	IMD	D	501	5/5	0.82	0.14	44,45,47,48	0
7	MPD	C	503	8/8	0.83	0.18	32,37,48,52	0
3	IMD	B	501	5/5	0.85	0.12	36,37,40,42	0
3	IMD	C	501	5/5	0.86	0.13	36,36,39,40	0
6	OXM	B	505	6/6	0.87	0.11	28,39,51,53	0
8	TAR	C	504	10/10	0.88	0.14	18,32,37,41	10
3	IMD	A	501	5/5	0.90	0.11	29,33,35,37	0
5	FMT	B	503	3/3	0.92	0.11	38,38,40,44	0
5	FMT	A	503	3/3	0.93	0.16	36,36,41,44	0
4	NA	B	504	1/1	0.95	0.08	33,33,33,33	0
4	NA	C	502	1/1	0.97	0.05	24,24,24,24	0
4	NA	A	504	1/1	0.97	0.08	27,27,27,27	0
4	NA	D	503	1/1	0.98	0.05	22,22,22,22	0
4	NA	B	502	1/1	0.98	0.04	25,25,25,25	0

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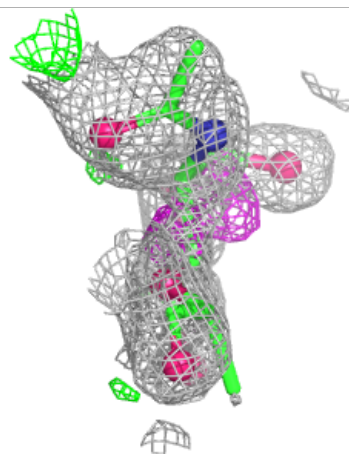
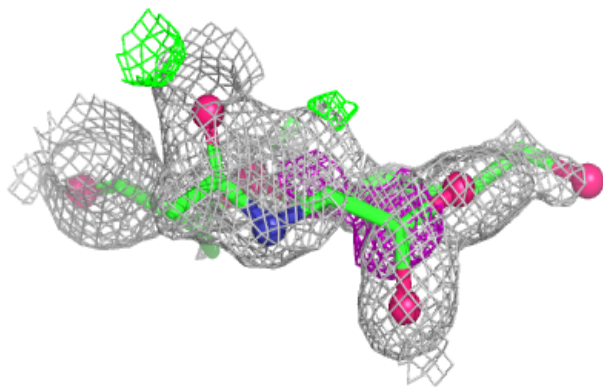
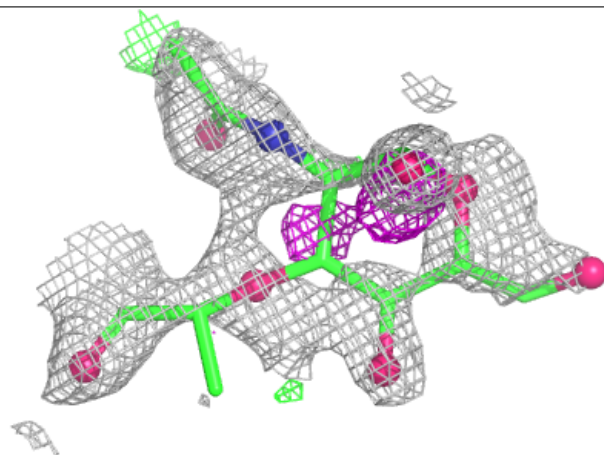
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	502	1/1	0.99	0.04	29,29,29,29	0
4	NA	A	502	1/1	0.99	0.02	22,22,22,22	0
4	NA	C	505	1/1	0.99	0.07	19,19,19,19	0

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.

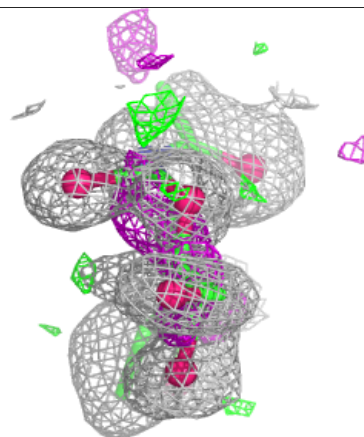
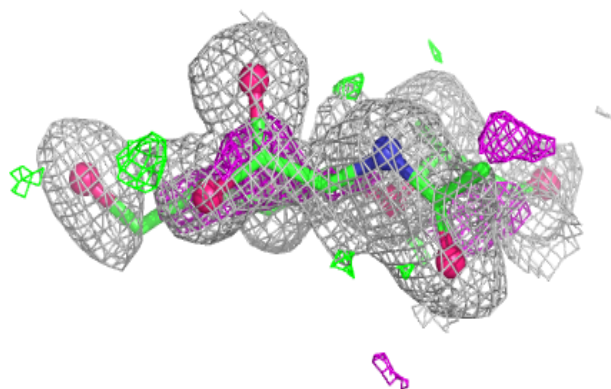
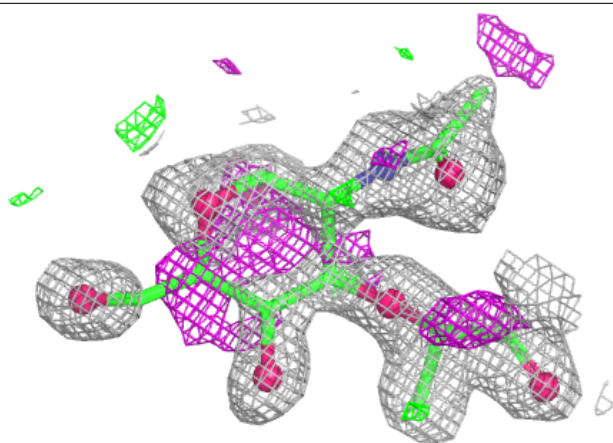
Electron density around MUB G 1:

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 MUB F 1:

$2mF_o - DF_c$ (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.