



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 08:52 AM JST

PDB ID : 5ZMW
Title : Crystal structure of the E309Q mutant of SR Ca²⁺-ATPase in E2(TG)
Authors : Ogawa, H.; Hirata, A.; Tsueda, J.; Toyoshima, C.
Deposited on : 2018-04-06
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

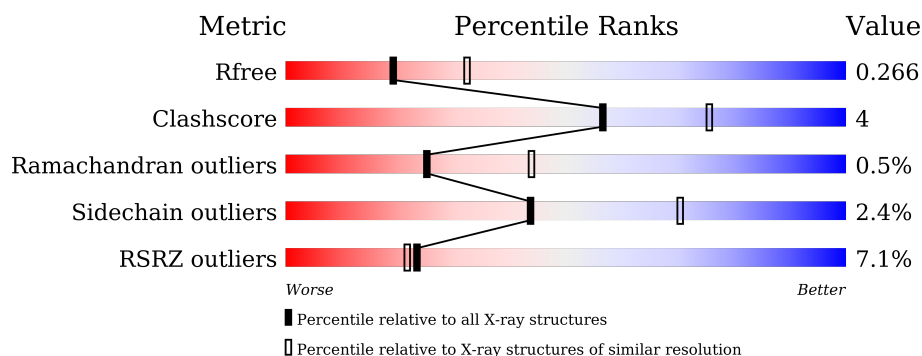
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	1000	<div> <div>7%</div> <div>86%</div> <div>13%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8068 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1000	Total	C	N	O	S	0	1	0
			7714	4901	1295	1460	58			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	SER	-	expression tag	UNP P04191
A	-4	ASP	-	expression tag	UNP P04191
A	-3	ASN	-	expression tag	UNP P04191
A	-2	ALA	-	expression tag	UNP P04191
A	-1	ILE	-	expression tag	UNP P04191
A	0	ALA	-	expression tag	UNP P04191
A	309	GLN	GLU	engineered mutation	UNP P04191

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

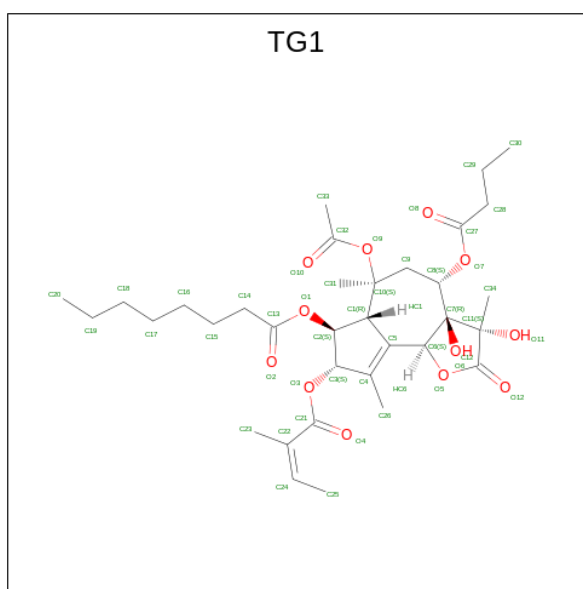
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



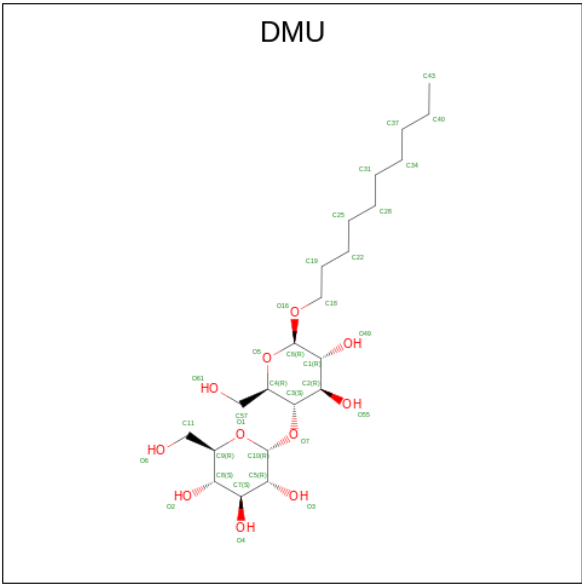
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: C₃₄H₅₀O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 5 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			33	22	11		
5	A	1	Total	C	O	0	0
			33	22	11		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	0
			236	236		

3 Residue-property plots

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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	260.98Å 86.89Å 60.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.93 – 2.50 15.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.93-2.50) 98.3 (15.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.51Å)	Xtriage
Refinement program	PHENIX (dev_3311: ???)	Depositor
R, R_{free}	0.222 , 0.259 0.225 , 0.266	Depositor DCC
R_{free} test set	1498 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8068	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: DMU, TG1, SO4, 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	0.26	0/7858	0.43	0/10655

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	A	7714	0	7807	71	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	46	0	50	3	0
5	A	66	0	84	1	0
6	A	236	0	0	2	0
All	All	8068	0	7941	71	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 4.

All (71) 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:866:THR:H	1:A:869:GLN:HE21	1.38	0.71
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.74	0.69
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.77	0.66
1:A:302:LEU:HD11	1:A:772:VAL:HG13	1.78	0.65
1:A:567:ARG:NH1	1:A:569:THR:O	2.28	0.65
1:A:210:SER:HB3	1:A:230:THR:HG21	1.77	0.65
1:A:0:ALA:HB3	1:A:225:THR:HG22	1.81	0.61
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.84	0.60
1:A:450:GLU:OE2	1:A:467:ARG:NH2	2.34	0.60
1:A:2:GLU:O	1:A:7:LYS:NZ	2.35	0.59
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.85	0.58
1:A:247:THR:OG1	1:A:340:GLU:OE1	2.22	0.58
1:A:93:VAL:O	1:A:97:ILE:HG12	2.05	0.56
1:A:757:MET:HA	1:A:760:PHE:CE2	2.42	0.55
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.90	0.53
1:A:607:VAL:O	1:A:611:ILE:HG12	2.09	0.53
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.90	0.53
1:A:461:ASN:ND2	6:A:1116:HOH:O	2.42	0.53
1:A:416:ILE:HG12	1:A:513:PHE:HD1	1.75	0.51
1:A:476:ARG:NH2	6:A:1109:HOH:O	2.37	0.51
1:A:13:LEU:HD23	1:A:222:ILE:HD12	1.93	0.51
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.93	0.51
1:A:946:LEU:HD12	1:A:950:VAL:HG21	1.91	0.51
1:A:811:PRO:HG3	1:A:929:VAL:HG12	1.93	0.50
1:A:668:GLU:O	1:A:671:ARG:HG2	2.12	0.49
1:A:108:GLN:HG2	1:A:313:ALA:HB2	1.94	0.49
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.95	0.49
1:A:99:ILE:HG21	5:A:1005:DMU:H25	1.95	0.48
1:A:357:THR:HA	1:A:603:PRO:HA	1.95	0.48
1:A:253:LEU:HD12	4:A:1003:TG1:H301	1.95	0.48
1:A:342:LEU:HD22	1:A:716:ILE:HG12	1.96	0.47
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.15	0.47
1:A:863:PRO:HB3	1:A:886:LEU:HD12	1.97	0.47
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.96	0.46
1:A:834:PHE:HE2	4:A:1003:TG1:HC1	1.80	0.46
1:A:637:ARG:NH1	1:A:643:GLY:O	2.49	0.46
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.97	0.46
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.98	0.46
1:A:59:ASP:OD2	1:A:63:ARG:NH1	2.49	0.46
1:A:834:PHE:CE2	4:A:1003:TG1:HC1	2.52	0.45
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.99	0.45
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:ALA:HA	1:A:992:LEU:HB2	1.99	0.45
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.00	0.45
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.99	0.44
1:A:865:VAL:HG13	1:A:869:GLN:HG3	1.98	0.44
1:A:355:THR:HA	1:A:738:ASP:O	2.17	0.43
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.19	0.43
1:A:388:THR:OG1	1:A:389:TYR:N	2.51	0.43
1:A:369:ILE:HG13	1:A:528:VAL:HG13	2.00	0.43
1:A:880:HIS:N	1:A:881:PRO:HD2	2.34	0.43
1:A:54:ILE:HG22	1:A:106:VAL:HG22	2.01	0.43
1:A:473:SER:O	1:A:477:GLN:HG2	2.19	0.43
1:A:196:ASP:HB3	1:A:199:ALA:HB2	2.01	0.42
1:A:840:ILE:O	1:A:844:VAL:HG23	2.19	0.42
1:A:83:GLU:HB3	1:A:86:THR:HG22	2.01	0.42
1:A:99:ILE:O	1:A:103:ILE:HG12	2.19	0.42
1:A:875:GLN:HB2	1:A:883:PHE:HE2	1.84	0.42
1:A:795:VAL:HA	1:A:799:THR:HB	2.01	0.42
1:A:567:ARG:HH11	1:A:570:PRO:HA	1.83	0.42
1:A:367:PHE:CD1	1:A:379:LEU:HD13	2.54	0.42
1:A:512:MET:HB2	1:A:567:ARG:HB3	2.01	0.42
1:A:913:LEU:HD22	1:A:927:PRO:HB3	2.01	0.41
1:A:975:LEU:N	1:A:976:PRO:HD2	2.35	0.41
1:A:905:VAL:O	1:A:909:MET:HG2	2.20	0.41
1:A:60:LEU:HD23	1:A:63:ARG:HH21	1.84	0.41
1:A:289:ILE:O	1:A:293:ILE:HG13	2.21	0.41
1:A:7:LYS:HB3	1:A:11:GLU:HB2	2.03	0.41
1:A:650:ASP:HB2	1:A:672:ARG:NH1	2.36	0.41
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.90	0.40
1:A:62:VAL:O	1:A:66:LEU:HG	2.22	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	A	999/1000 (100%)	955 (96%)	39 (4%)	5 (0%)	25	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	GLY
1	A	46	GLY
1	A	-1	ILE
1	A	235	ILE
1	A	531	GLY

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	845/844 (100%)	825 (98%)	20 (2%)	44	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	164	ARG
1	A	180	LEU
1	A	247	THR
1	A	279	PHE
1	A	297	LYS
1	A	342	LEU
1	A	361	MET
1	A	402	ILE
1	A	413	LEU
1	A	529	ARG
1	A	600	LEU
1	A	605	LYS
1	A	656	ARG
1	A	668	GLU
1	A	691	LEU

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Mol	Chain	Res	Type
1	A	738	ASP
1	A	816	ILE
1	A	825	LYS
1	A	982	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	HIS
1	A	284	HIS
1	A	869	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMU	A	1005	-	34,34,34	0.63	0	45,45,45	1.11	4 (8%)
4	TG1	A	1003	-	43,48,48	4.84	13 (30%)	44,72,72	3.74	11 (25%)
5	DMU	A	1004	-	34,34,34	0.59	0	45,45,45	0.97	1 (2%)

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
5	DMU	A	1005	-	-	9/19/59/59	0/2/2/2
4	TG1	A	1003	-	-	14/33/99/99	0/3/3/3
5	DMU	A	1004	-	-	9/19/59/59	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	TG1	C4-C5	28.73	1.58	1.34
4	A	1003	TG1	O12-C12	7.36	1.37	1.20
4	A	1003	TG1	C11-C7	4.61	1.61	1.55
4	A	1003	TG1	O5-C12	4.34	1.42	1.35
4	A	1003	TG1	C1-C5	3.89	1.57	1.51
4	A	1003	TG1	C24-C22	3.53	1.53	1.31
4	A	1003	TG1	C3-C4	3.05	1.54	1.50
4	A	1003	TG1	O7-C8	-2.35	1.42	1.46
4	A	1003	TG1	C9-C8	2.25	1.55	1.52
4	A	1003	TG1	O1-C13	2.11	1.40	1.34
4	A	1003	TG1	O3-C21	2.10	1.39	1.34
4	A	1003	TG1	O9-C10	-2.10	1.44	1.48
4	A	1003	TG1	C31-C10	2.05	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	O12-C12-C11	-16.88	111.31	128.28
4	A	1003	TG1	O5-C12-O12	-11.59	106.26	121.62
4	A	1003	TG1	C10-O9-C32	7.31	138.88	121.53
4	A	1003	TG1	O9-C32-C33	-5.15	101.31	110.68
4	A	1003	TG1	C26-C4-C5	-3.96	119.95	129.82
4	A	1003	TG1	C23-C22-C24	-3.92	107.06	123.20
4	A	1003	TG1	C10-C1-C5	3.63	119.61	115.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	TG1	C11-C7-C6	-3.45	96.39	103.03
4	A	1003	TG1	O3-C21-O4	-3.44	116.76	123.32
4	A	1003	TG1	O9-C32-O10	-2.93	118.22	123.61
4	A	1003	TG1	C23-C22-C21	-2.86	108.94	116.09
5	A	1005	DMU	O5-C4-C57	2.56	112.81	106.44
5	A	1005	DMU	C57-C4-C3	-2.20	106.93	113.33
5	A	1005	DMU	C10-O7-C3	-2.11	112.75	117.96
5	A	1004	DMU	O1-C9-C11	2.09	111.62	106.44
5	A	1005	DMU	C10-O1-C9	2.05	117.71	113.69

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	TG1	C31-C10-O9-C32
4	A	1003	TG1	C22-C21-O3-C3
4	A	1003	TG1	O3-C21-C22-C24
4	A	1003	TG1	O4-C21-C22-C24
4	A	1003	TG1	C21-C22-C24-C25
5	A	1005	DMU	O6-C11-C9-O1
5	A	1005	DMU	O5-C4-C57-O61
4	A	1003	TG1	O4-C21-O3-C3
5	A	1005	DMU	O6-C11-C9-C8
5	A	1005	DMU	C3-C4-C57-O61
5	A	1004	DMU	O5-C6-O16-C18
4	A	1003	TG1	O10-C32-O9-C10
4	A	1003	TG1	C16-C17-C18-C19
5	A	1004	DMU	C22-C25-C28-C31
5	A	1004	DMU	C19-C22-C25-C28
4	A	1003	TG1	O4-C21-C22-C23
5	A	1005	DMU	C18-C19-C22-C25
5	A	1004	DMU	C25-C28-C31-C34
5	A	1004	DMU	C28-C31-C34-C37
5	A	1004	DMU	C31-C34-C37-C40
5	A	1005	DMU	C34-C37-C40-C43
5	A	1005	DMU	C25-C28-C31-C34
5	A	1005	DMU	C31-C34-C37-C40
5	A	1004	DMU	C34-C37-C40-C43
4	A	1003	TG1	C14-C15-C16-C17
5	A	1004	DMU	O6-C11-C9-O1
4	A	1003	TG1	C17-C18-C19-C20
4	A	1003	TG1	O3-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
4	A	1003	TG1	C15-C16-C17-C18
5	A	1004	DMU	C18-C19-C22-C25
4	A	1003	TG1	C1-C10-O9-C32
5	A	1005	DMU	C19-C22-C25-C28

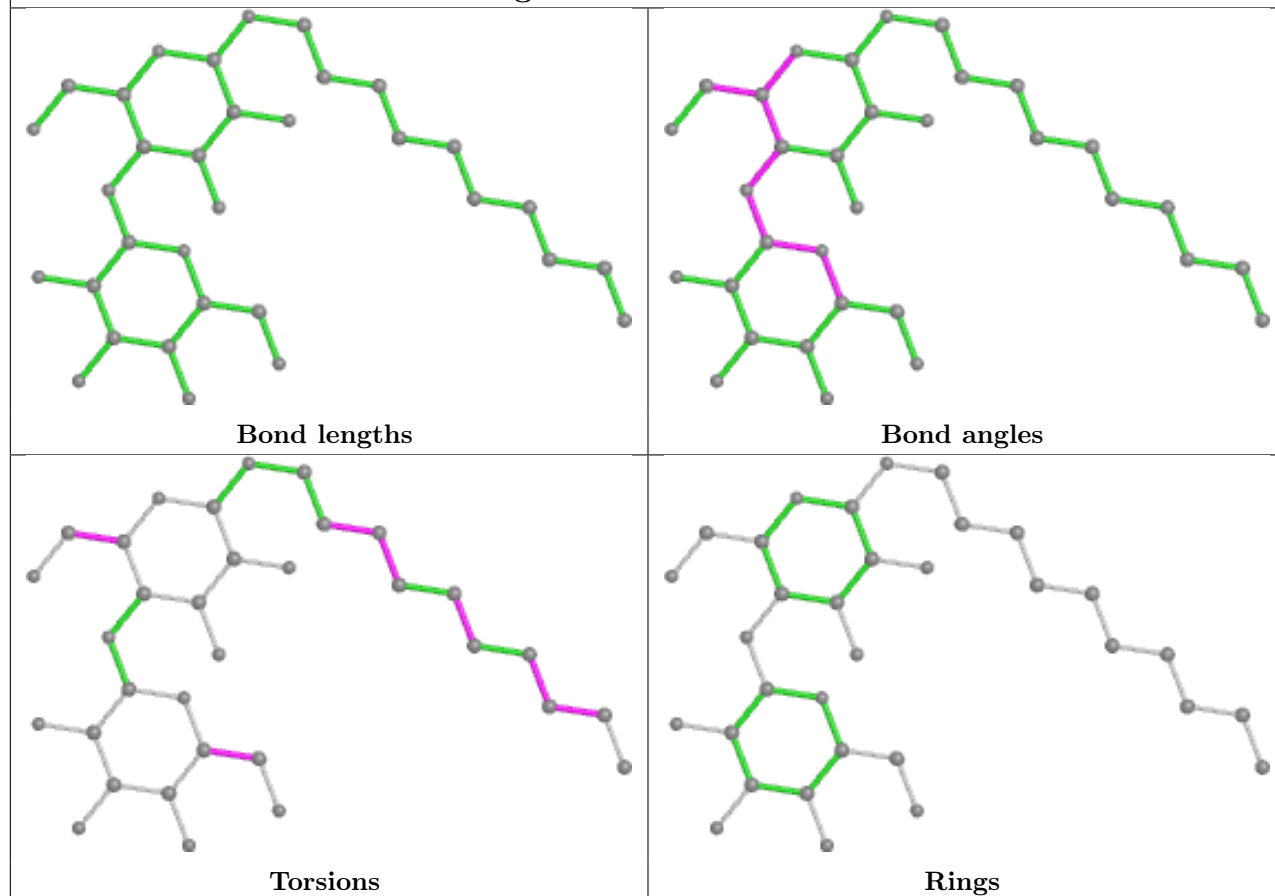
There are no ring outliers.

2 monomers are involved in 4 short contacts:

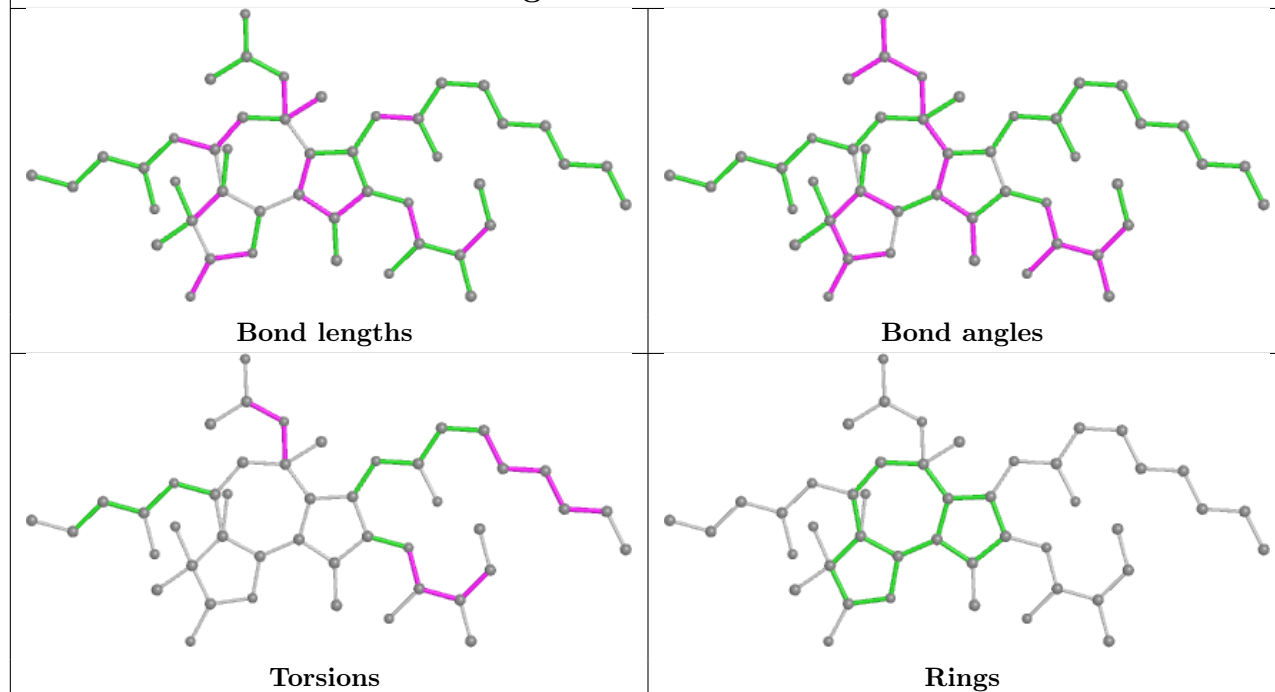
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1005	DMU	1	0
4	A	1003	TG1	3	0

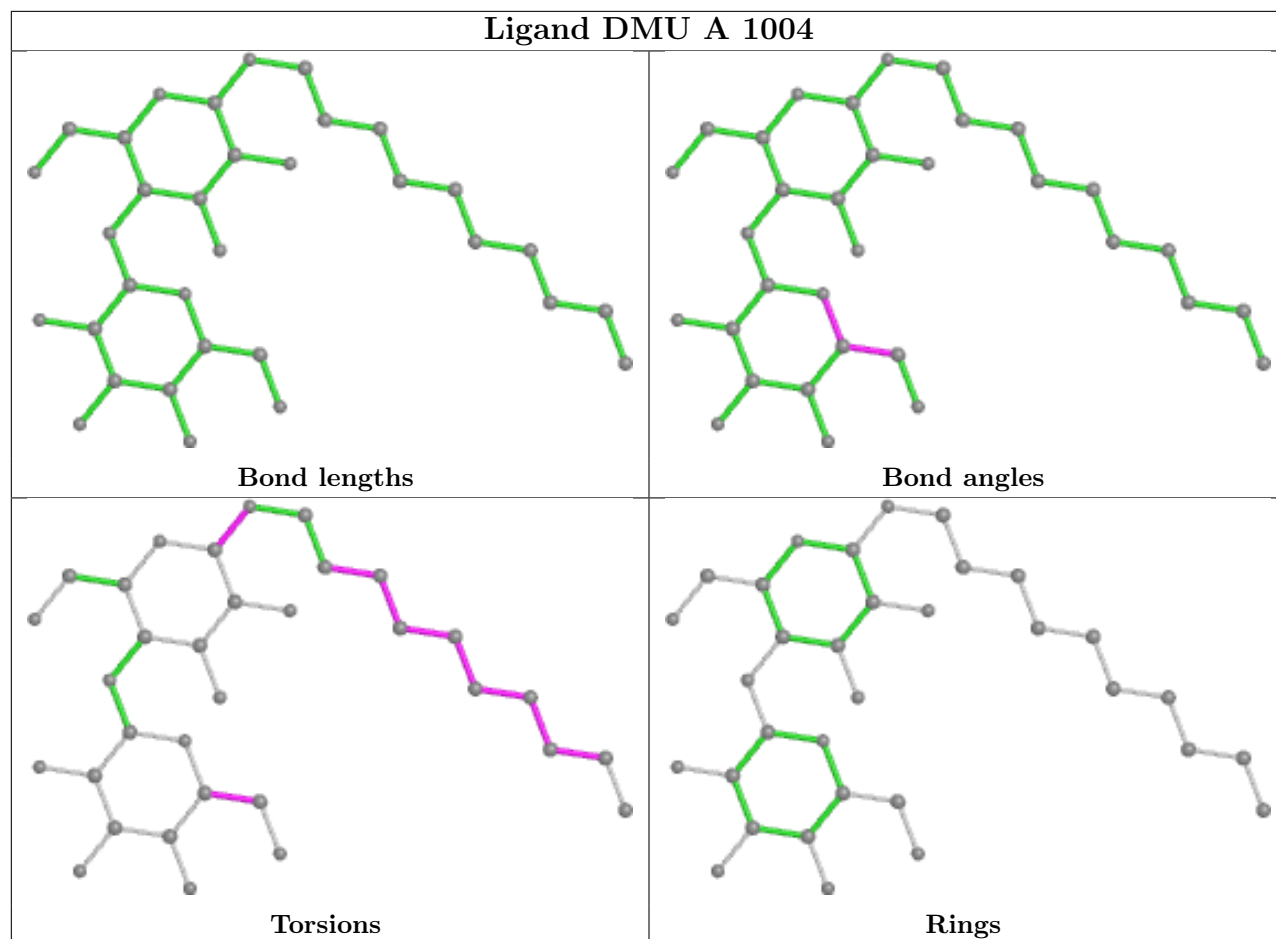
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 DMU A 1005



Ligand TG1 A 1003





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	1000/1000 (100%)	0.10	71 (7%)	23 22	18, 56, 181, 308	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	864	GLY	6.0
1	A	49	LEU	6.0
1	A	883	PHE	5.5
1	A	62	VAL	5.3
1	A	876	CYS	4.7
1	A	71	ILE	4.6
1	A	868	HIS	4.5
1	A	877	THR	4.2
1	A	74	VAL	4.2
1	A	282	PRO	4.0
1	A	292	ALA	3.6
1	A	289	ILE	3.5
1	A	293	ILE	3.5
1	A	77	TRP	3.5
1	A	508	VAL	3.5
1	A	87	ALA	3.4
1	A	60	LEU	3.3
1	A	276	ILE	3.3
1	A	81	GLY	3.3
1	A	951	ASP	3.2
1	A	278	HIS	3.1
1	A	85	ILE	3.1
1	A	279	PHE	3.1
1	A	73	PHE	3.0
1	A	84	THR	3.0
1	A	89	VAL	3.0
1	A	69	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	2.9
1	A	-5	SER	2.9
1	A	277	GLY	2.9
1	A	880	HIS	2.9
1	A	70	CYS	2.9
1	A	891	PHE	2.9
1	A	886	LEU	2.8
1	A	53	VAL	2.8
1	A	64	ILE	2.8
1	A	48	SER	2.8
1	A	867	TYR	2.8
1	A	66	LEU	2.7
1	A	888	CYS	2.7
1	A	52	LEU	2.7
1	A	75	LEU	2.7
1	A	241	ALA	2.7
1	A	65	LEU	2.6
1	A	873	PHE	2.6
1	A	44	GLU	2.6
1	A	61	LEU	2.6
1	A	863	PRO	2.6
1	A	88	PHE	2.6
1	A	46	GLY	2.5
1	A	47	LYS	2.5
1	A	288	TRP	2.5
1	A	973	ILE	2.4
1	A	858	TYR	2.4
1	A	866	THR	2.4
1	A	870	LEU	2.3
1	A	-1	ILE	2.3
1	A	58	GLU	2.3
1	A	291	GLY	2.3
1	A	403	ARG	2.3
1	A	-2	ALA	2.3
1	A	885	GLY	2.2
1	A	57	PHE	2.2
1	A	881	PRO	2.2
1	A	274	ILE	2.2
1	A	76	ALA	2.2
1	A	286	GLY	2.1
1	A	82	GLU	2.1
1	A	260	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	2.0
1	A	860	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

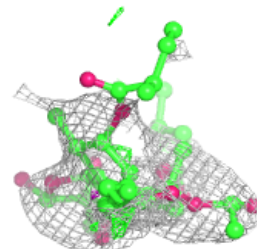
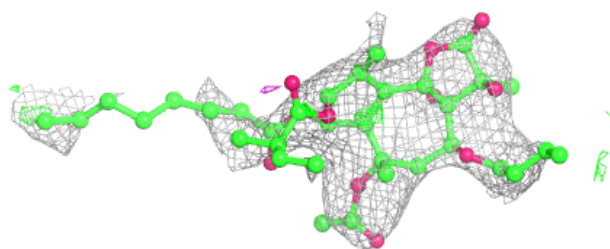
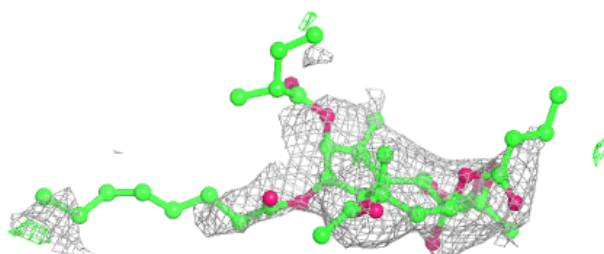
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	1002	5/5	0.77	0.20	136,138,140,143	0
4	TG1	A	1003	46/46	0.82	0.18	91,114,138,144	0
5	DMU	A	1004	33/33	0.82	0.13	50,91,111,120	0
5	DMU	A	1005	33/33	0.84	0.12	36,80,105,116	0
2	NA	A	1001	1/1	0.98	0.03	42,42,42,42	0

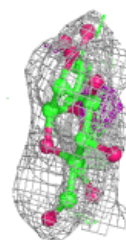
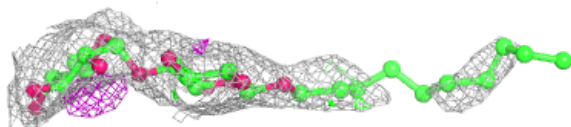
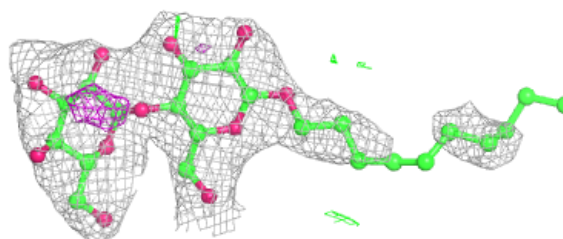
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

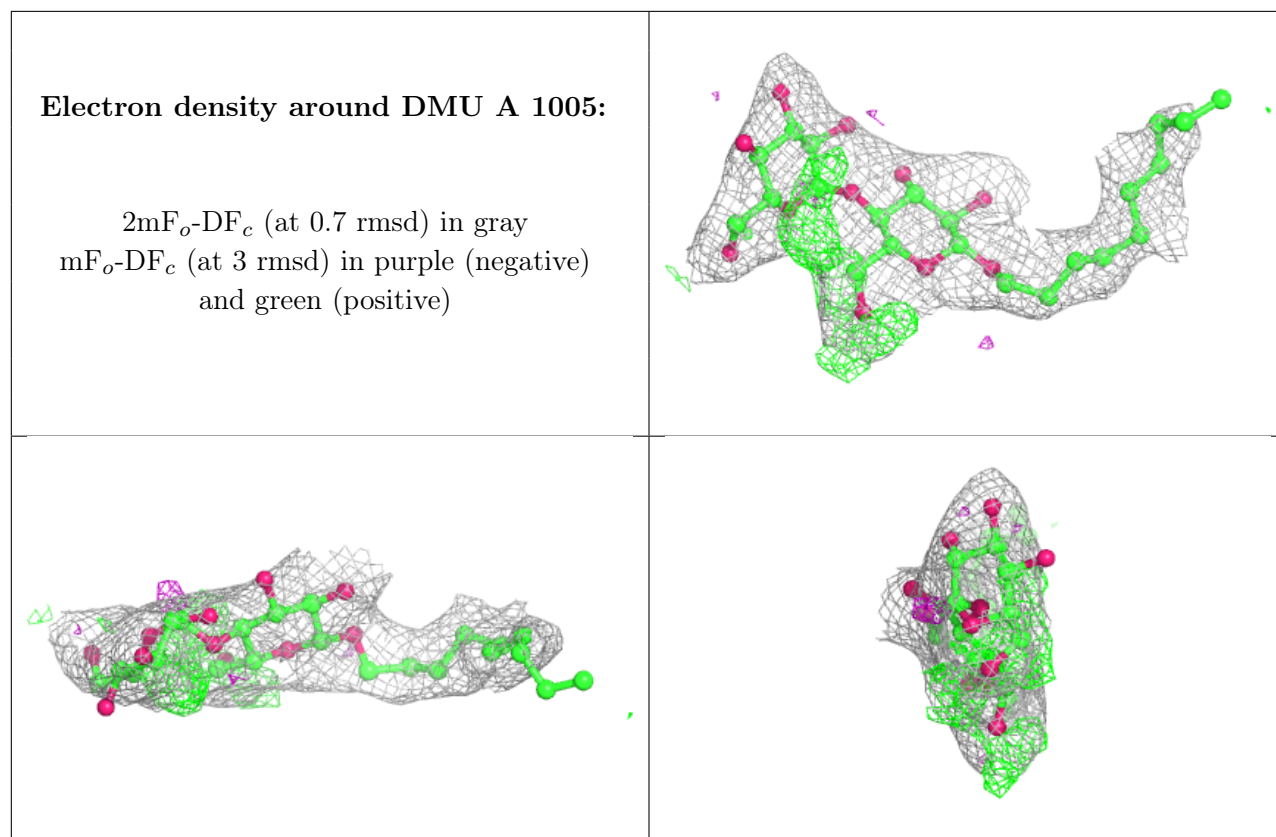
Electron density around TG1 A 1003:

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

**Electron density around DMU A 1004:**

$2mF_o-DF_c$ (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.