Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2020 – 04:01 PM BST

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 (i) symbol.

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

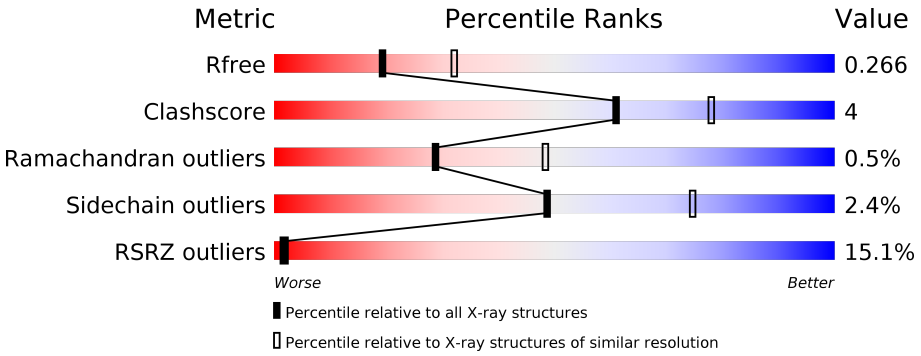
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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	A	1000	15% 86% 13%

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			

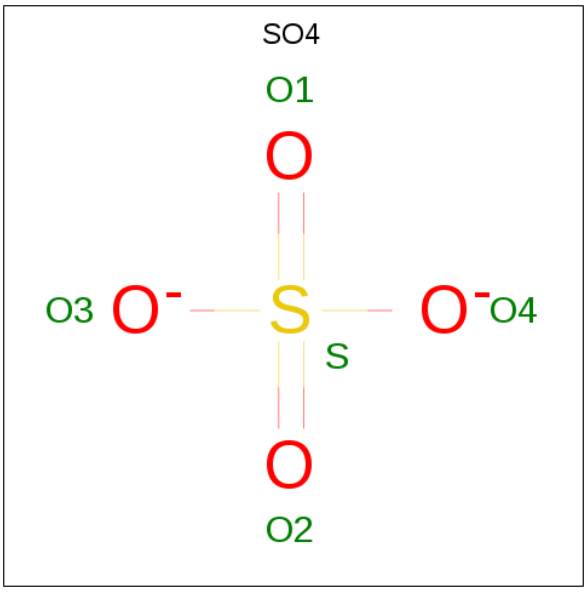
There are 7 discrepancies between the modelled and reference sequences:

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).

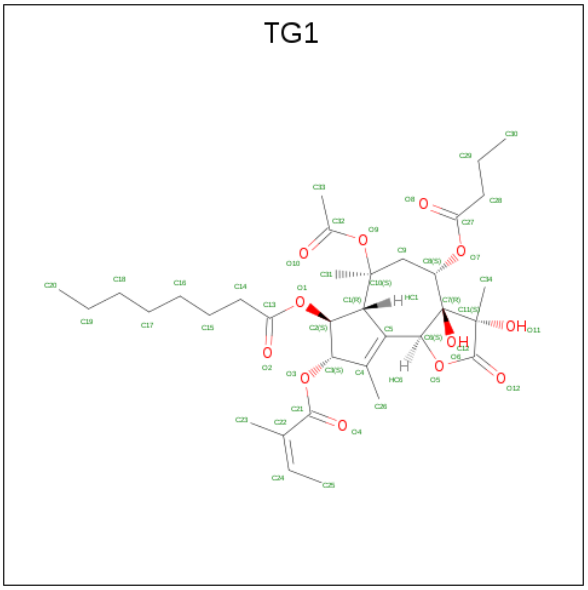
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



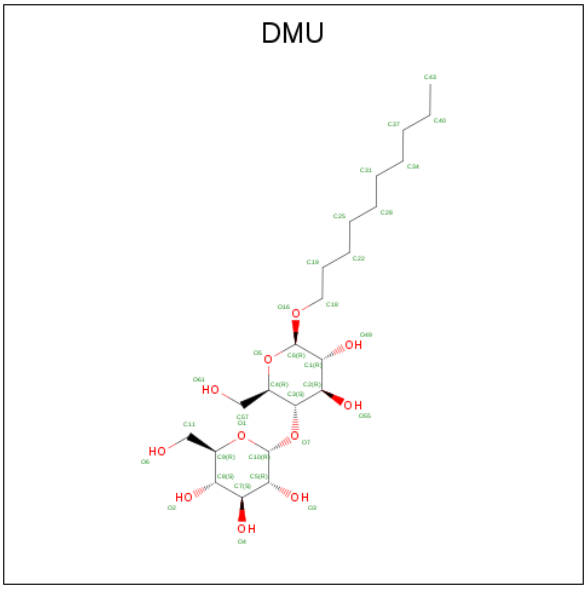
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

- 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: $C_{34}H_{50}O_{12}$).



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

- Molecule 5 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

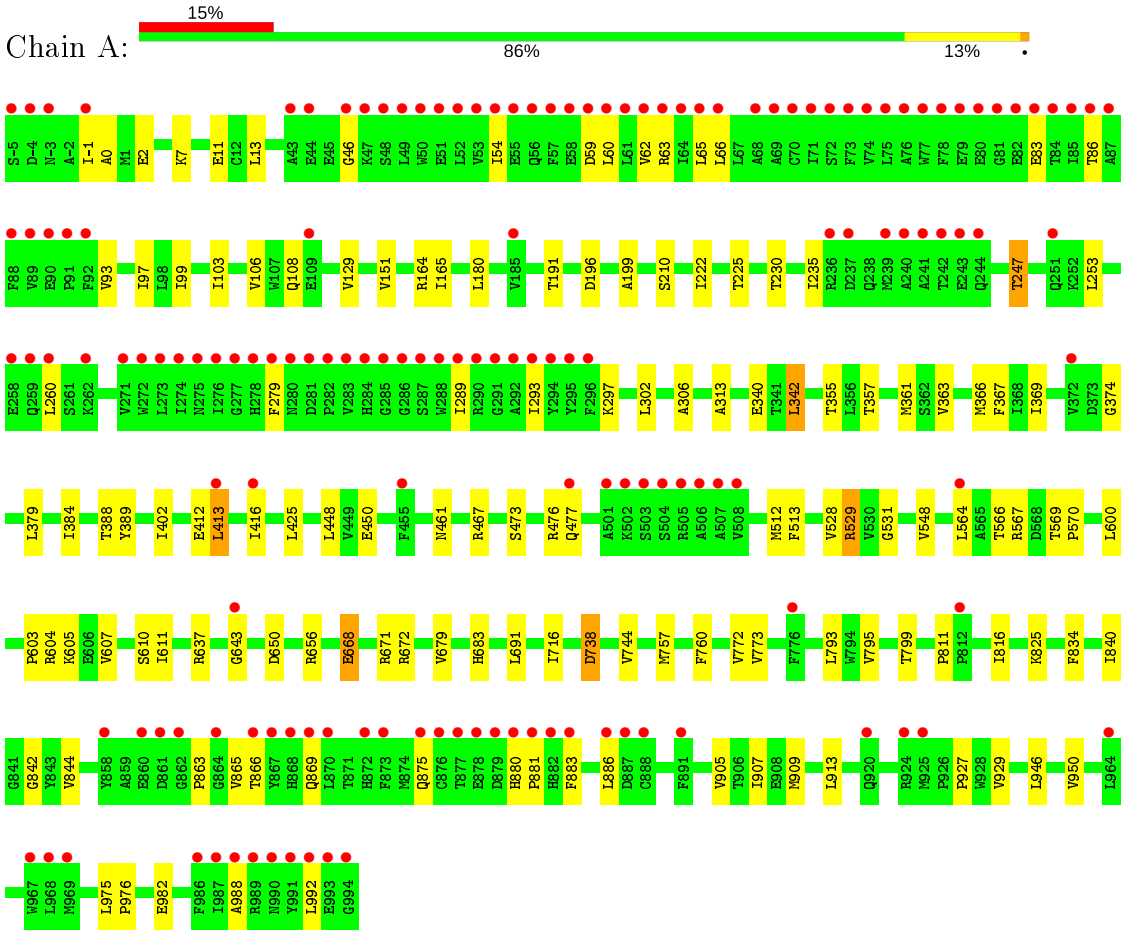
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	236	Total O 236 236	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: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



4 Data and refinement statistics (i)

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 31.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.93-2.50) 98.7 (31.70-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	1488 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 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	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.*

[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: NA, TG1, DMU, SO4

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:412:GLU:OE2	1:A:566:THR:HG21	2.15	0.47
1:A:342:LEU:HD22	1:A:716:ILE:HG12	1.96	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

Continued on next page...

Continued from previous page...

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:473:SER:O	1:A:477:GLN:HG2	2.19	0.43
1:A:54:ILE:HG22	1:A:106:VAL:HG22	2.01	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:875:GLN:HB2	1:A:883:PHE:HE2	1.84	0.42
1:A:99:ILE:O	1:A:103:ILE:HG12	2.19	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:289:ILE:O	1:A:293:ILE:HG13	2.21	0.41
1:A:60:LEU:HD23	1:A:63:ARG:HH21	1.84	0.41
1:A:650:ASP:HB2	1:A:672:ARG:NH1	2.36	0.41
1:A:7:LYS:HB3	1:A:11:GLU:HB2	2.03	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	999/1000 (100%)	955 (96%)	39 (4%)	5 (0%)	29 48

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 (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	845/844 (100%)	825 (98%)	20 (2%)	49 74

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

Continued on next page...

Continued from previous page...

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

Some 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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
4	TG1	A	1003	-	43,48,48	4.84	13 (30%)	44,72,72	3.74	11 (25%)
5	DMU	A	1005	-	34,34,34	0.63	0	45,45,45	1.11	4 (8%)
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
4	TG1	A	1003	-	-	14/33/99/99	0/3/3/3
5	DMU	A	1005	-	-	9/19/59/59	0/2/2/2
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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

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

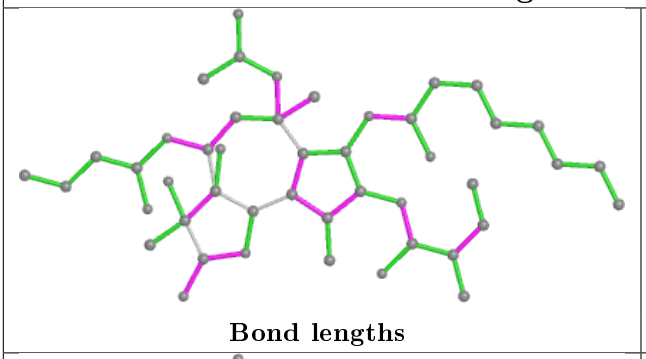
There are no ring outliers.

2 monomers are involved in 4 short contacts:

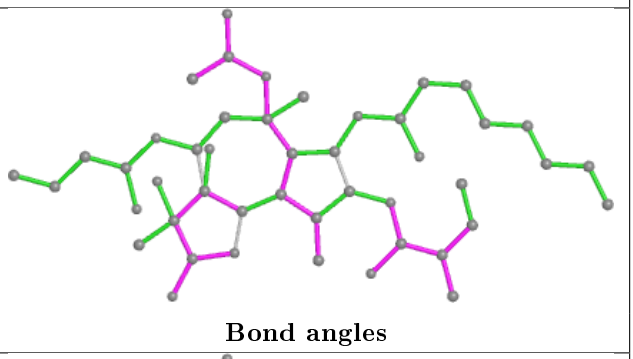
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	TG1	3	0
5	A	1005	DMU	1	0

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.

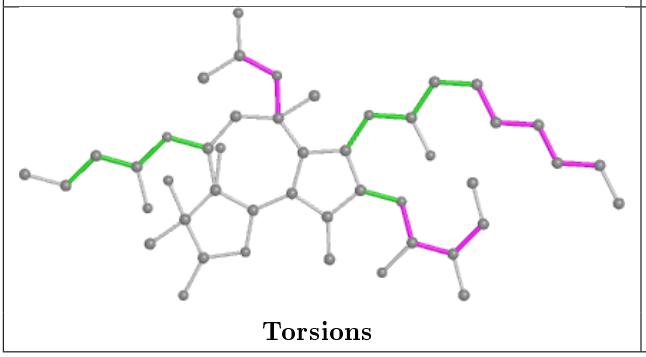
Ligand TG1 A 1003



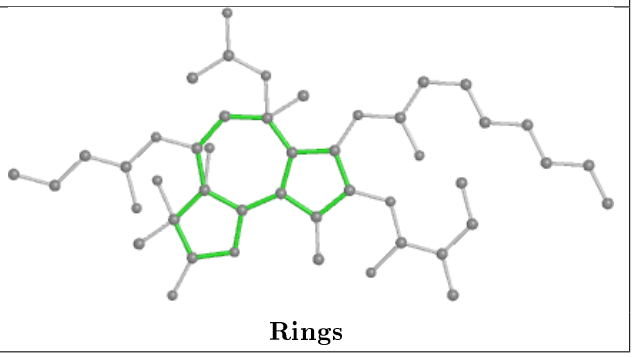
Bond lengths



Bond angles

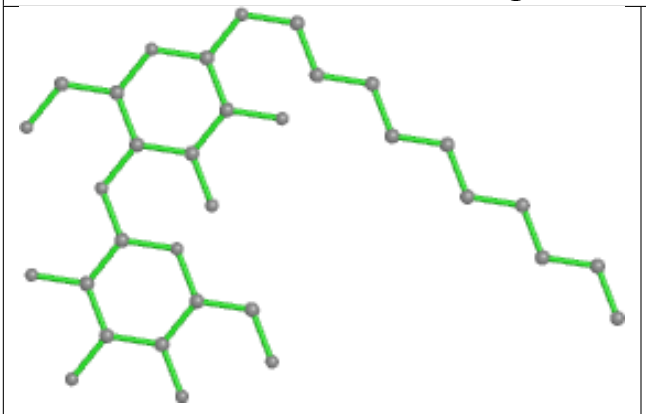


Torsions

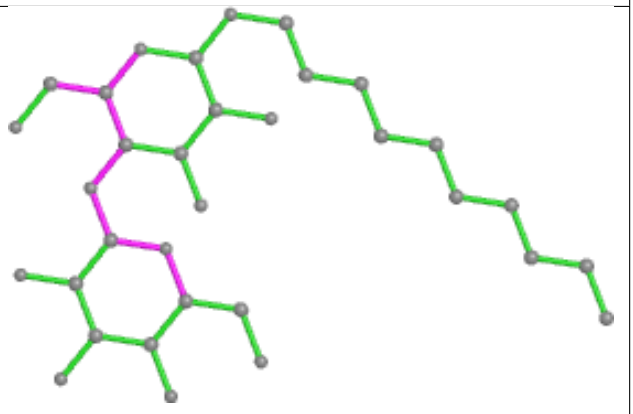


Rings

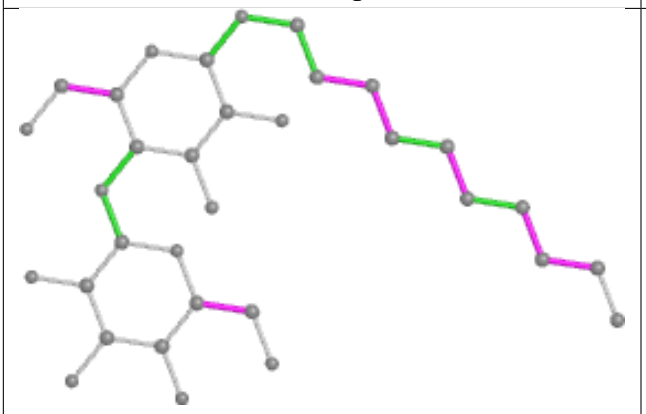
Ligand DMU A 1005



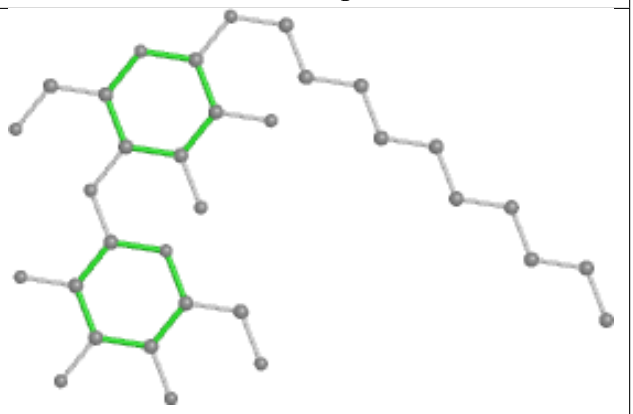
Bond lengths



Bond angles

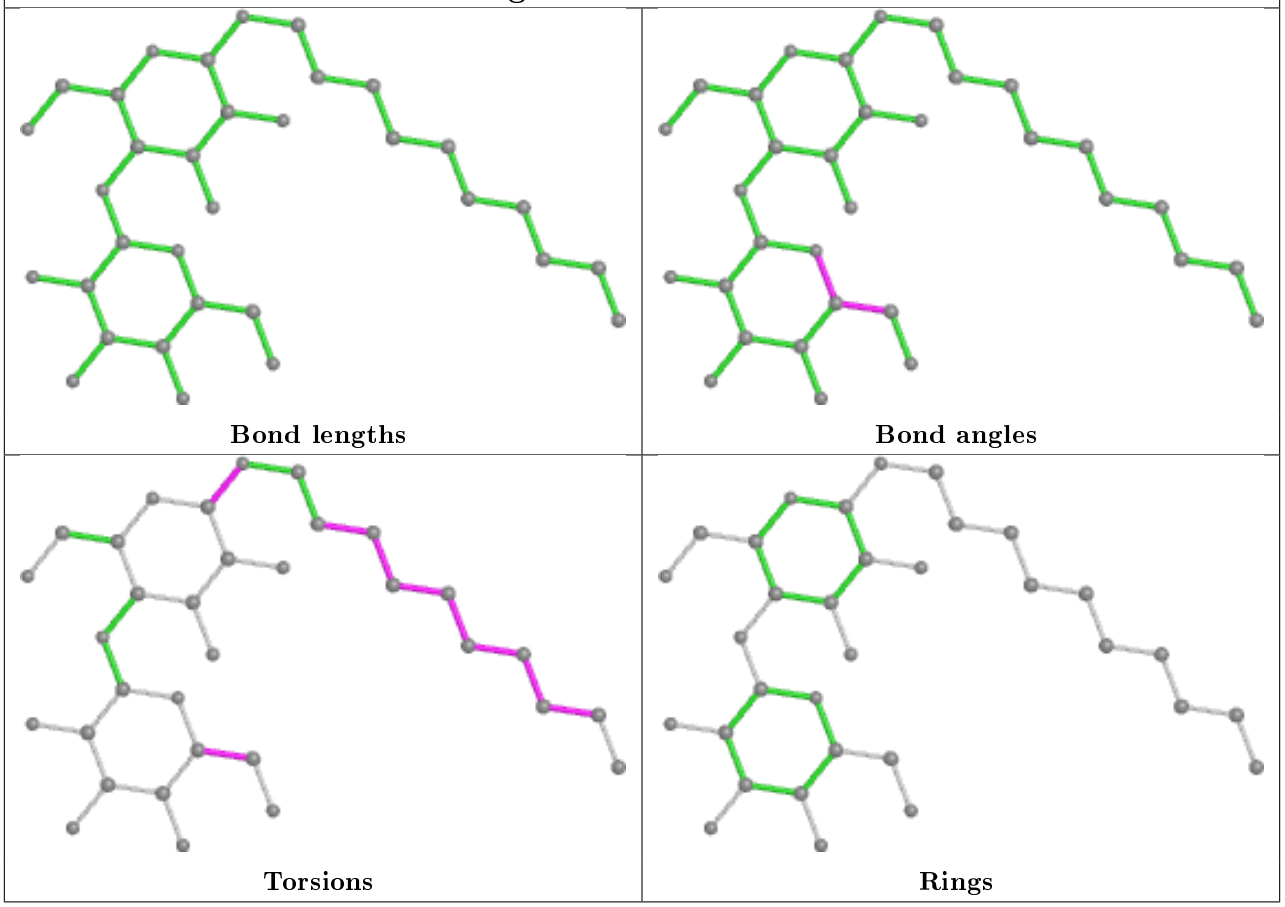


Torsions



Rings

Ligand DMU A 1004



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	1000/1000 (100%)	0.90	151 (15%)	2	1	18, 56, 181, 308	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	PHE	18.8
1	A	73	PHE	18.5
1	A	864	GLY	16.5
1	A	994	GLY	15.7
1	A	280	ASN	15.2
1	A	883	PHE	14.4
1	A	76	ALA	14.4
1	A	286	GLY	13.8
1	A	89	VAL	13.5
1	A	77	TRP	13.3
1	A	75	LEU	12.4
1	A	279	PHE	11.7
1	A	87	ALA	11.7
1	A	62	VAL	11.0
1	A	86	THR	10.5
1	A	49	LEU	10.5
1	A	284	HIS	10.4
1	A	282	PRO	10.2
1	A	288	TRP	9.8
1	A	61	LEU	9.7
1	A	285	GLY	9.7
1	A	70	CYS	8.8
1	A	71	ILE	8.7
1	A	48	SER	8.6
1	A	289	ILE	8.6
1	A	79	GLU	8.5
1	A	281	ASP	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	GLU	8.5
1	A	84	THR	8.4
1	A	886	LEU	8.1
1	A	283	VAL	8.1
1	A	292	ALA	7.9
1	A	241	ALA	7.8
1	A	287	SER	7.6
1	A	57	PHE	7.6
1	A	278	HIS	7.5
1	A	44	GLU	7.5
1	A	506	ALA	7.5
1	A	56	GLN	7.4
1	A	60	LEU	7.4
1	A	293	ILE	7.4
1	A	876	CYS	7.2
1	A	-5	SER	7.1
1	A	277	GLY	6.9
1	A	85	ILE	6.7
1	A	78	PHE	6.7
1	A	58	GLU	6.5
1	A	291	GLY	6.5
1	A	74	VAL	6.5
1	A	63	ARG	6.5
1	A	82	GLU	6.4
1	A	866	THR	6.3
1	A	240	ALA	6.3
1	A	53	VAL	6.2
1	A	993	GLU	6.2
1	A	868	HIS	6.0
1	A	64	ILE	6.0
1	A	924	ARG	5.9
1	A	276	ILE	5.8
1	A	273	LEU	5.7
1	A	72	SER	5.7
1	A	290	ARG	5.6
1	A	990	ASN	5.6
1	A	986	PHE	5.5
1	A	66	LEU	5.5
1	A	54	ILE	5.4
1	A	83	GLU	5.3
1	A	90	GLU	5.3
1	A	888	CYS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	5.1
1	A	65	LEU	5.0
1	A	239	MET	5.0
1	A	50	TRP	5.0
1	A	869	GLN	5.0
1	A	505	ARG	5.0
1	A	46	GLY	4.9
1	A	877	THR	4.8
1	A	875	GLN	4.7
1	A	507	ALA	4.5
1	A	237	ASP	4.5
1	A	992	LEU	4.5
1	A	244	GLN	4.4
1	A	882	HIS	4.3
1	A	987	ILE	4.2
1	A	891	PHE	4.2
1	A	91	PRO	4.1
1	A	989	ARG	4.1
1	A	-4	ASP	4.0
1	A	-3	ASN	3.9
1	A	991	TYR	3.9
1	A	860	GLU	3.8
1	A	47	LYS	3.7
1	A	873	PHE	3.7
1	A	242	THR	3.7
1	A	503	SER	3.7
1	A	274	ILE	3.7
1	A	880	HIS	3.6
1	A	295	TYR	3.6
1	A	294	TYR	3.3
1	A	867	TYR	3.3
1	A	887	ASP	3.3
1	A	879	ASP	3.3
1	A	92	PHE	3.2
1	A	55	GLU	3.2
1	A	236	ARG	3.1
1	A	262	LYS	3.1
1	A	502	LYS	3.1
1	A	988	ALA	3.1
1	A	296	PHE	3.1
1	A	-1	ILE	3.0
1	A	243	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	3.0
1	A	968	LEU	3.0
1	A	109	GLU	3.0
1	A	271	VAL	3.0
1	A	858	TYR	2.9
1	A	501	ALA	2.9
1	A	881	PRO	2.8
1	A	964	LEU	2.8
1	A	508	VAL	2.8
1	A	259	GLN	2.8
1	A	258	GLU	2.7
1	A	969	MET	2.7
1	A	68	ALA	2.7
1	A	51	GLU	2.7
1	A	504	SER	2.7
1	A	455	PHE	2.6
1	A	862	GLY	2.6
1	A	643	GLY	2.5
1	A	69	ALA	2.5
1	A	861	ASP	2.5
1	A	372	VAL	2.5
1	A	59	ASP	2.4
1	A	878	GLU	2.4
1	A	52	LEU	2.4
1	A	272	TRP	2.4
1	A	43	ALA	2.3
1	A	870	LEU	2.3
1	A	251	GLN	2.3
1	A	925	MET	2.3
1	A	416	ILE	2.3
1	A	564	LEU	2.2
1	A	275	ASN	2.2
1	A	812	PRO	2.2
1	A	185	VAL	2.1
1	A	920	GLN	2.1
1	A	477	GLN	2.1
1	A	413	LEU	2.1
1	A	967	TRP	2.1
1	A	872	HIS	2.0
1	A	776	PHE	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)

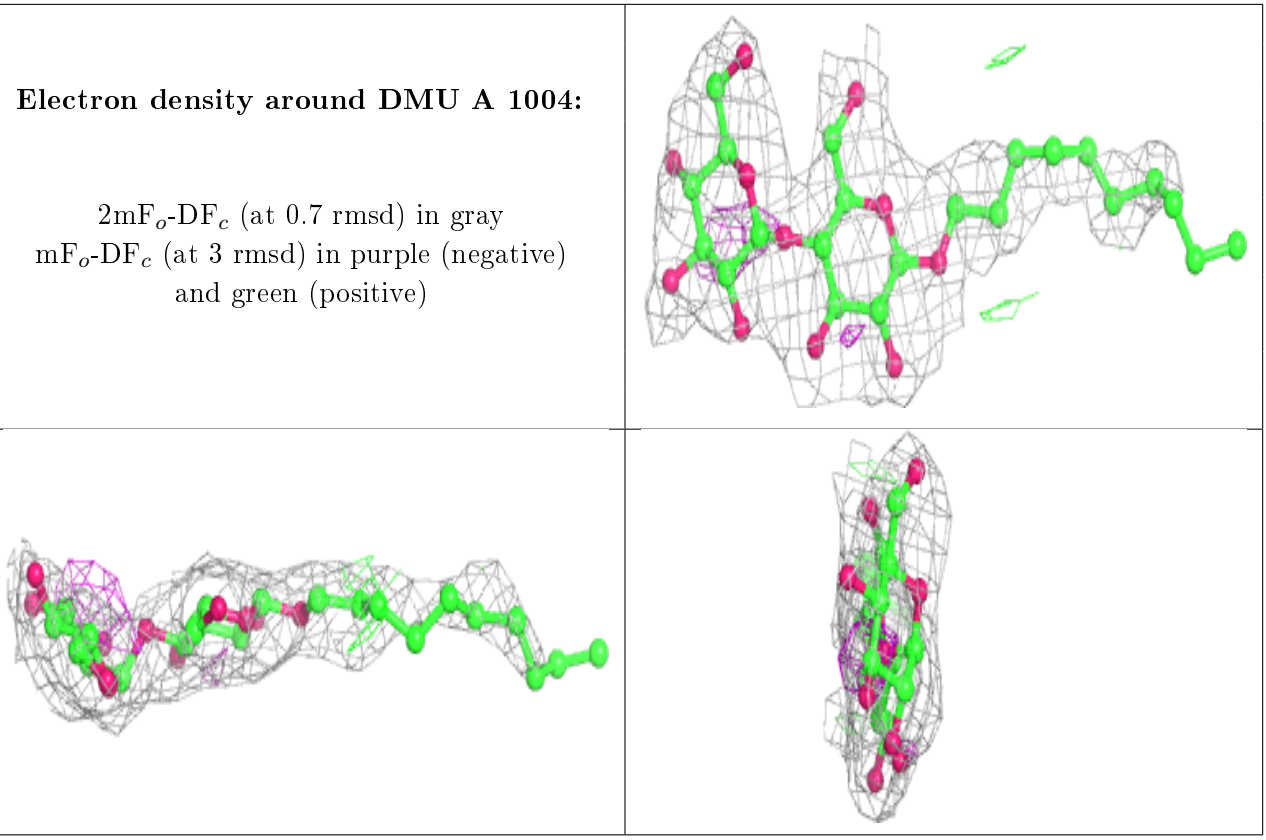
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	A	1002	5/5	0.82	0.26	136,138,140,143	0
5	DMU	A	1004	33/33	0.83	0.22	50,91,111,120	0
5	DMU	A	1005	33/33	0.87	0.22	36,80,105,116	0
4	TG1	A	1003	46/46	0.87	0.36	91,114,138,144	0
2	NA	A	1001	1/1	0.94	0.12	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.

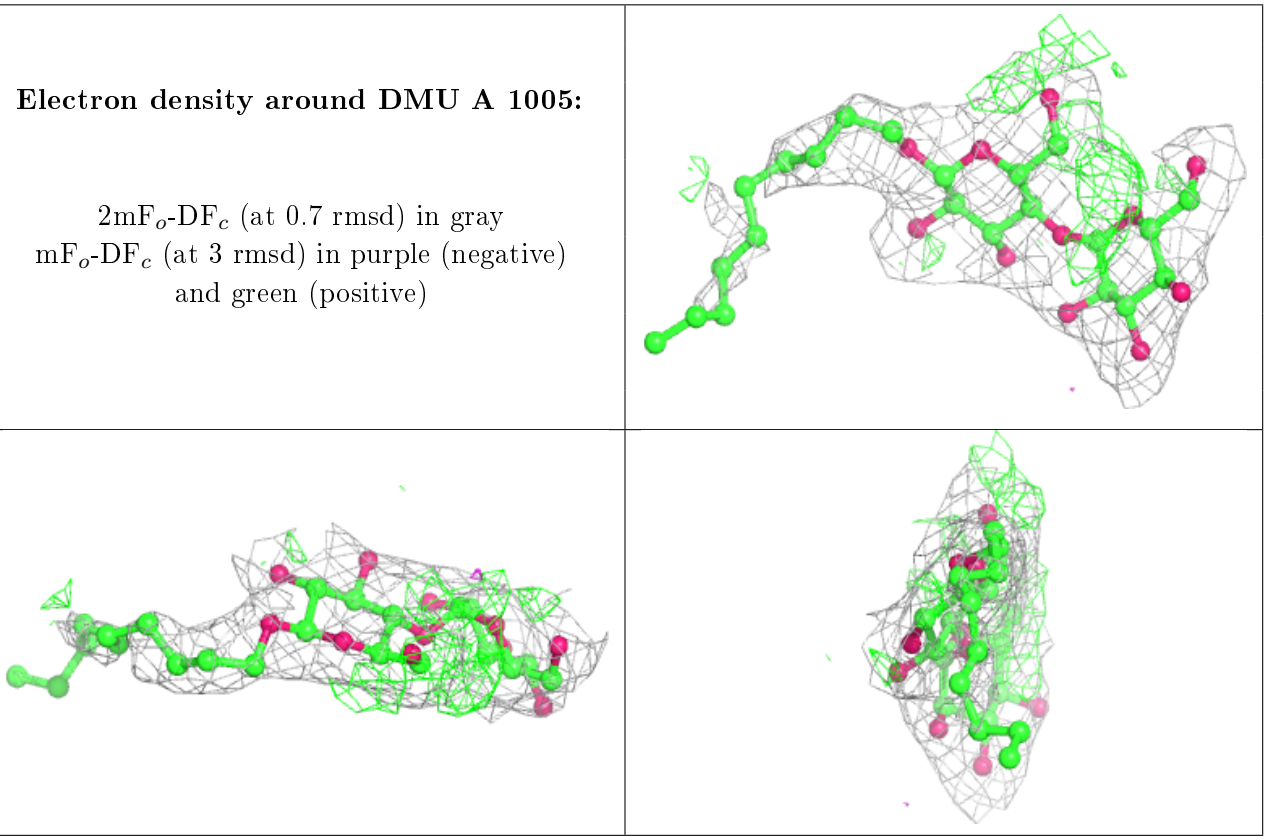
Electron density around DMU A 1004:

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



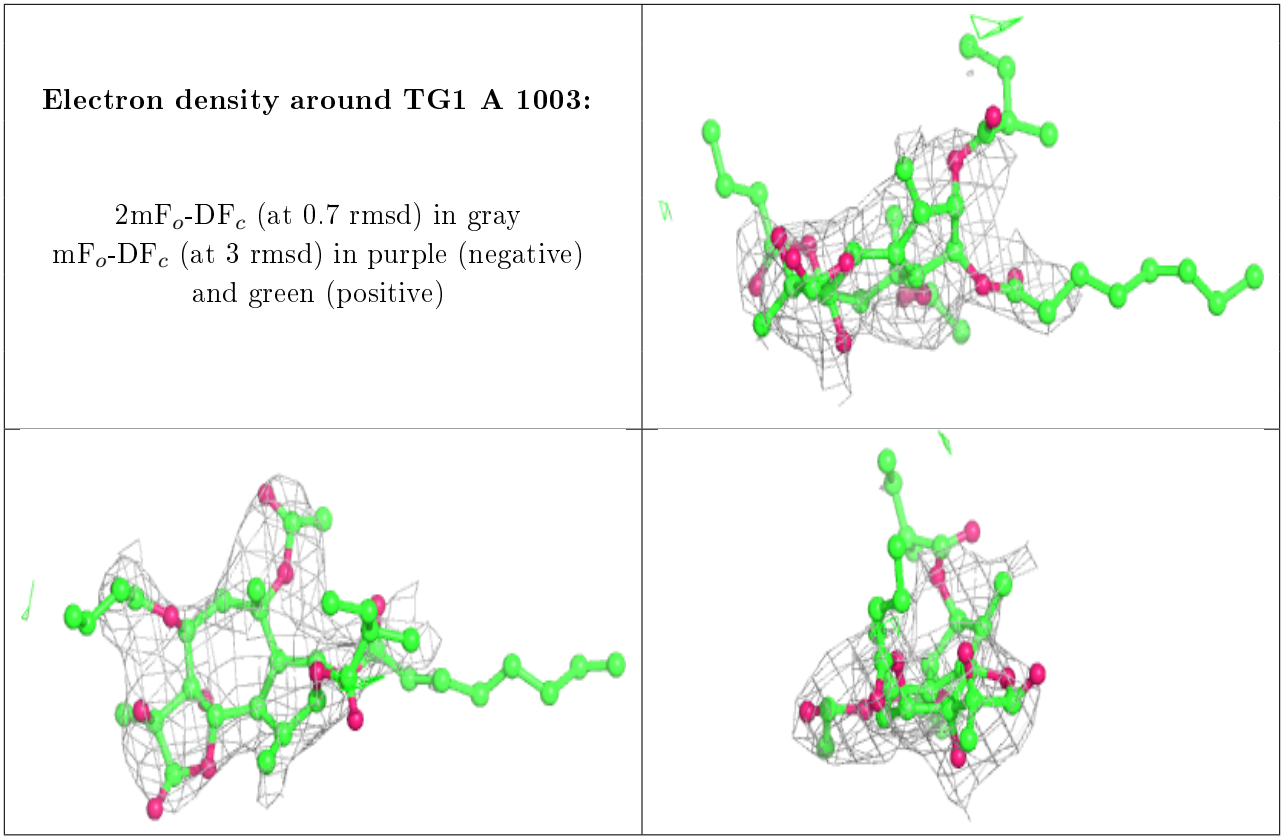
Electron density around DMU A 1005:

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



Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.