Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 09:06 PM EDT

PDB ID	:	3AR7
Title	:	Calcium pump crystal structure with bound TNP-ATP and TG in the absence of Ca2+
Authors	:	Toyoshima, C.; Yonekura, S.; Tsueda, J.; Iwasawa, S.
Deposited on	:	2010-11-24
Resolution	:	2.15 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

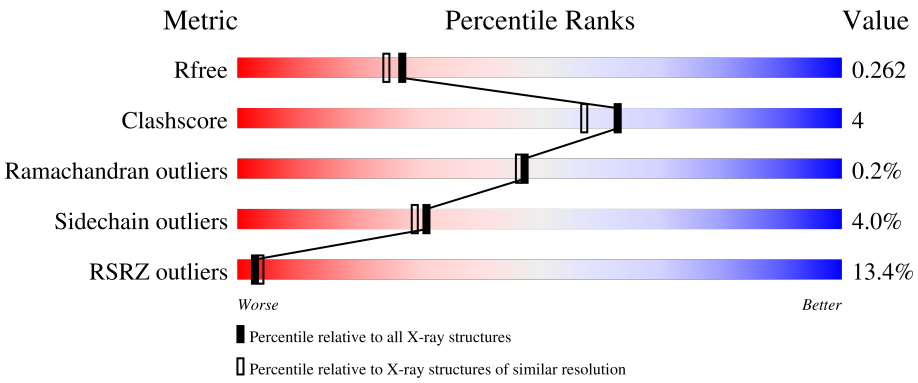
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	995	13% 87% 12% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8005 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
			Total	C	N	O	S			
1	A	995	7674	4878	1287	1452	57	0	0	0

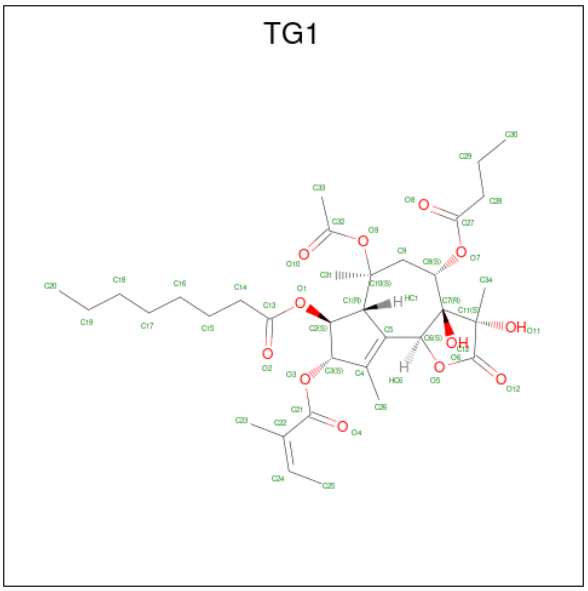
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

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

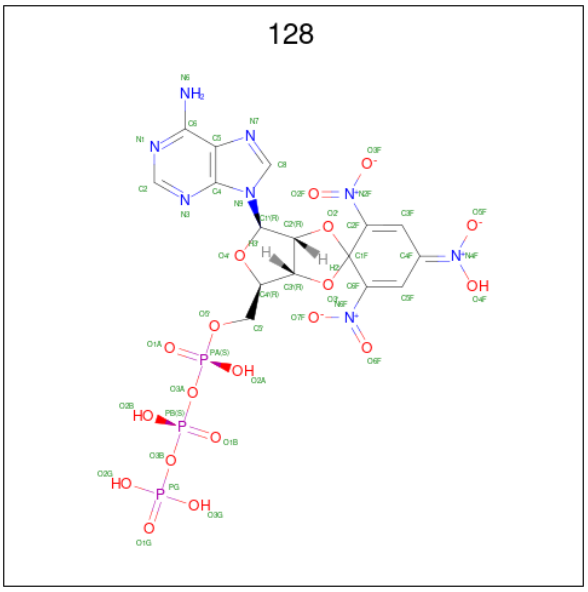
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 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)OX Y]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: $C_{34}H_{50}O_{12}$).



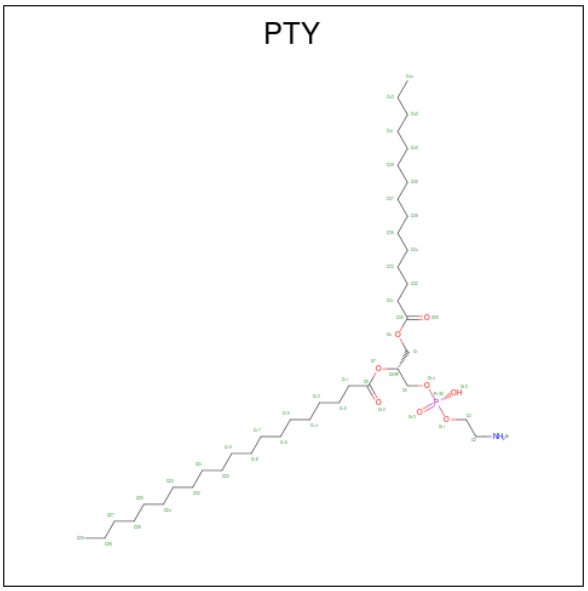
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	46	34	12	0	0

- Molecule 4 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENINE-TRIPHOSPHATE (three-letter code: 128) (formula: $C_{16}H_{17}N_8O_{19}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	46	16	8	19	3	0	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0

- Molecule 6 is water.

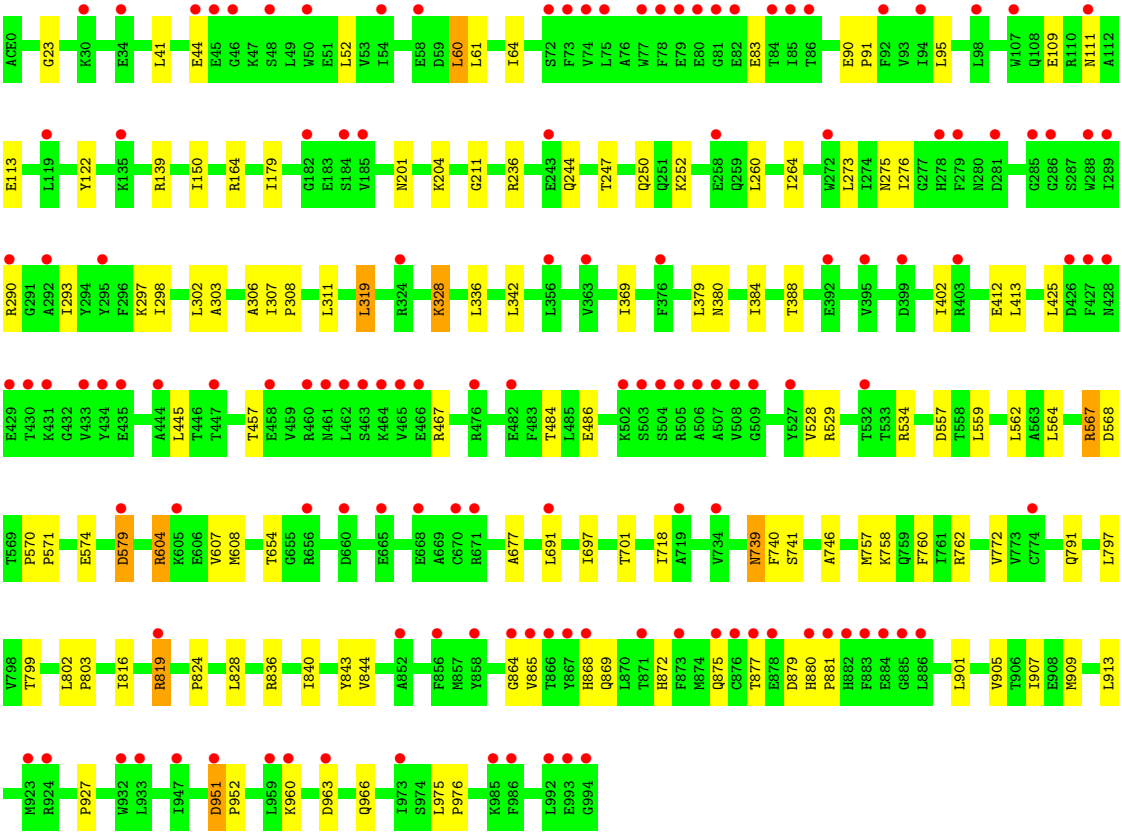
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	181	181	181	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.52Å 71.52Å 586.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.15 14.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.15) 100.0 (14.97-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.16Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.268 0.237 , 0.262	Depositor DCC
R_{free} test set	4303 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	48.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8005	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TG1, ACE, NA, 128, PTY

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	0.35	0/7813	0.51	0/10594

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 (i)

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	7674	0	7765	67	0
2	A	1	0	0	0	0
3	A	46	0	50	2	0
4	A	46	0	13	1	0
5	A	57	0	33	0	0
6	A	181	0	0	4	0
All	All	8005	0	7861	67	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 (67) 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:567:ARG:HD2	1:A:570:PRO:HA	1.65	0.79
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.73	0.70
1:A:758:LYS:O	1:A:762:ARG:HG3	1.92	0.69
1:A:772:VAL:HG21	3:A:1003:TG1:H231	1.74	0.69
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.81	0.62
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.82	0.62
1:A:739:ASN:HD22	1:A:740:PHE:N	1.98	0.60
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.86	0.58
1:A:819:ARG:HH11	1:A:819:ARG:HB3	1.69	0.58
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.05	0.56
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.87	0.56
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.88	0.56
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.89	0.55
1:A:697:ILE:HD11	1:A:824:PRO:HG3	1.87	0.55
1:A:757:MET:HA	1:A:760:PHE:CE2	2.42	0.55
1:A:654:THR:HA	1:A:677:ALA:O	2.08	0.54
1:A:868:HIS:HD2	1:A:881:PRO:HB3	1.73	0.54
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.89	0.54
1:A:880:HIS:HB2	1:A:881:PRO:HD3	1.90	0.53
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.90	0.53
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.89	0.52
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.13	0.52
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.45	0.51
1:A:963:ASP:H	1:A:966:GLN:HE21	1.58	0.50
1:A:562:LEU:HD11	4:A:1002:128:H5F	1.94	0.50
1:A:975:LEU:N	1:A:976:PRO:HD2	2.27	0.49
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.94	0.49
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.78	0.49
1:A:247:THR:H	1:A:250:GLN:NE2	2.11	0.48
1:A:739:ASN:ND2	1:A:741:SER:H	2.11	0.48
1:A:303:ALA:O	1:A:307:ILE:HG12	2.13	0.48
1:A:791:GLN:HB3	1:A:901:LEU:HD13	1.95	0.48
1:A:23:GLY:HA2	1:A:150:ILE:HD13	1.96	0.48
1:A:308:PRO:HB2	1:A:311:LEU:HB2	1.97	0.47
1:A:963:ASP:H	1:A:966:GLN:NE2	2.12	0.47
1:A:179:ILE:HG12	6:A:9040:HOH:O	2.14	0.47
1:A:252:LYS:HD3	1:A:828:LEU:CD1	2.45	0.46
1:A:608:MET:HG3	6:A:9076:HOH:O	2.16	0.46
1:A:869:GLN:HB2	1:A:872:HIS:CG	2.50	0.46
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.97	0.46
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.16	0.45
1:A:567:ARG:CD	1:A:570:PRO:HA	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:LEU:HD22	3:A:1003:TG1:H302	1.97	0.45
1:A:567:ARG:CZ	1:A:571:PRO:HD3	2.47	0.45
1:A:328:LYS:NZ	1:A:328:LYS:HA	2.31	0.45
1:A:298:ILE:O	1:A:302:LEU:HB2	2.16	0.45
1:A:252:LYS:HD3	1:A:828:LEU:HD12	1.99	0.45
1:A:290:ARG:HH22	1:A:875:GLN:HA	1.82	0.45
1:A:486:GLU:H	1:A:486:GLU:CD	2.19	0.44
1:A:868:HIS:CD2	1:A:881:PRO:HB3	2.53	0.44
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.99	0.43
1:A:369:ILE:HG13	1:A:528:VAL:HG13	2.01	0.43
1:A:701:THR:HA	1:A:718:ILE:O	2.19	0.42
1:A:579:ASP:HB2	6:A:9169:HOH:O	2.19	0.42
1:A:122:TYR:O	1:A:211:GLY:HA2	2.20	0.41
1:A:293:ILE:O	1:A:297:LYS:HB2	2.21	0.41
1:A:604:ARG:O	1:A:607:VAL:HG22	2.20	0.41
1:A:273:LEU:O	1:A:276:ILE:HG12	2.21	0.41
1:A:60:LEU:O	1:A:64:ILE:HG12	2.21	0.41
1:A:244:GLN:NE2	6:A:9065:HOH:O	2.54	0.41
1:A:264:ILE:HG23	1:A:302:LEU:HD12	2.02	0.41
1:A:534:ARG:NH2	1:A:568:ASP:HB2	2.35	0.41
1:A:836:ARG:O	1:A:840:ILE:HG12	2.21	0.40
1:A:201:ASN:HA	1:A:204:LYS:HD2	2.03	0.40
1:A:52:LEU:HD11	1:A:109:GLU:HG3	2.02	0.40
1:A:369:ILE:HD13	1:A:379:LEU:HD22	2.03	0.40
1:A:905:VAL:O	1:A:909:MET:HG2	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	993/995 (100%)	963 (97%)	28 (3%)	2 (0%)	47 46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	864	GLY
1	A	951	ASP

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	840/840 (100%)	806 (96%)	34 (4%)	31 29

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	44	GLU
1	A	60	LEU
1	A	83	GLU
1	A	95	LEU
1	A	111	ASN
1	A	113	GLU
1	A	139	ARG
1	A	164	ARG
1	A	236	ARG
1	A	275	ASN
1	A	319	LEU
1	A	328	LYS
1	A	380	ASN
1	A	384	ILE
1	A	388	THR
1	A	402	ILE
1	A	425	LEU
1	A	445	LEU
1	A	457	THR
1	A	467	ARG
1	A	484	THR
1	A	567	ARG

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Mol	Chain	Res	Type
1	A	574	GLU
1	A	579	ASP
1	A	604	ARG
1	A	691	LEU
1	A	739	ASN
1	A	797	LEU
1	A	816	ILE
1	A	819	ARG
1	A	877	THR
1	A	879	ASP
1	A	960	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	244	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN
1	A	510	ASN
1	A	739	ASN
1	A	868	HIS
1	A	872	HIS
1	A	875	GLN
1	A	919	ASN
1	A	966	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	128	A	1002	-	33,50,50	2.12	7 (21%)	36,80,80	2.87	11 (30%)
5	PTY	A	1011	-	18,18,49	1.44	2 (11%)	21,23,54	1.40	3 (14%)
5	PTY	A	1013	-	18,18,49	1.45	2 (11%)	21,23,54	1.43	3 (14%)
3	TG1	A	1003	-	43,48,48	2.83	8 (18%)	44,72,72	3.52	12 (27%)
5	PTY	A	1012	-	18,18,49	1.48	2 (11%)	21,23,54	1.31	1 (4%)

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	128	A	1002	-	-	1/22/80/80	0/5/5/5
5	PTY	A	1011	-	-	7/20/20/53	-
5	PTY	A	1013	-	-	10/20/20/53	-
3	TG1	A	1003	-	-	11/33/99/99	0/3/3/3
5	PTY	A	1012	-	-	8/20/20/53	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	TG1	O4-C21	10.91	1.44	1.21
3	A	1003	TG1	O12-C12	9.75	1.43	1.20
4	A	1002	128	O2'-C1F	7.01	1.51	1.41
4	A	1002	128	O3'-C1F	6.31	1.50	1.41
3	A	1003	TG1	O5-C12	5.55	1.43	1.35
5	A	1012	PTY	O7-C8	5.10	1.46	1.35
5	A	1013	PTY	O7-C8	4.95	1.46	1.35
5	A	1011	PTY	O7-C8	4.89	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	TG1	O9-C32	4.73	1.46	1.35
3	A	1003	TG1	O1-C13	4.41	1.46	1.34
3	A	1003	TG1	O7-C27	4.23	1.46	1.34
3	A	1003	TG1	O3-C21	3.84	1.43	1.34
4	A	1002	128	C5F-C6F	3.51	1.47	1.37
4	A	1002	128	C3'-C4'	-2.97	1.44	1.52
4	A	1002	128	C2-N3	2.80	1.36	1.32
3	A	1003	TG1	O9-C10	-2.75	1.43	1.48
5	A	1012	PTY	O4-C30	2.61	1.46	1.33
5	A	1011	PTY	O4-C30	2.61	1.46	1.33
5	A	1013	PTY	O4-C30	2.59	1.46	1.33
4	A	1002	128	C2-N1	2.42	1.38	1.33
4	A	1002	128	C4-N3	2.34	1.38	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1003	TG1	O12-C12-C11	-17.17	111.03	128.28
4	A	1002	128	O3'-C1F-C6F	-9.75	97.13	110.47
3	A	1003	TG1	O5-C12-O12	-8.53	110.32	121.62
3	A	1003	TG1	O3-C21-O4	-7.04	109.90	123.32
4	A	1002	128	O2'-C1F-C2F	-6.49	101.59	110.47
4	A	1002	128	O2'-C2'-C3'	6.33	113.69	103.58
3	A	1003	TG1	O4-C21-C22	-5.25	108.71	125.21
5	A	1013	PTY	O7-C8-C11	4.63	119.61	111.09
4	A	1002	128	O4'-C1'-C2'	-4.53	98.72	106.59
5	A	1011	PTY	O7-C8-C11	4.49	119.35	111.09
4	A	1002	128	N3-C2-N1	-4.33	121.91	128.68
5	A	1012	PTY	O7-C8-C11	4.18	118.78	111.09
3	A	1003	TG1	O1-C13-C14	3.90	119.90	111.50
4	A	1002	128	O3'-C1F-C2F	3.85	115.74	110.47
3	A	1003	TG1	O9-C32-C33	3.71	117.44	110.68
3	A	1003	TG1	O7-C27-C28	3.68	119.43	111.50
4	A	1002	128	PB-O3B-PG	-3.29	121.55	132.83
4	A	1002	128	PA-O3A-PB	-3.18	121.92	132.83
4	A	1002	128	O2'-C1F-C6F	2.97	114.52	110.47
4	A	1002	128	O5'-C5'-C4'	2.68	118.23	108.99
3	A	1003	TG1	C8-O7-C27	-2.61	113.01	117.92
3	A	1003	TG1	O7-C8-C9	2.57	111.22	106.63
5	A	1013	PTY	C6-O7-C8	-2.54	113.16	117.90
3	A	1003	TG1	C10-O9-C32	2.52	127.50	121.53
3	A	1003	TG1	C2-O1-C13	-2.37	113.58	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1011	PTY	C6-O7-C8	-2.33	113.56	117.90
4	A	1002	128	C2'-C3'-C4'	2.22	108.99	103.72
5	A	1011	PTY	O7-C8-O10	-2.18	118.62	122.96
5	A	1013	PTY	O7-C8-O10	-2.17	118.64	122.96
3	A	1003	TG1	C3-O3-C21	-2.14	112.52	117.07

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	TG1	C31-C10-O9-C32
5	A	1012	PTY	C5-O14-P1-O12
5	A	1013	PTY	N1-C2-C3-O11
5	A	1011	PTY	C11-C8-O7-C6
5	A	1013	PTY	C11-C8-O7-C6
5	A	1011	PTY	O10-C8-O7-C6
5	A	1012	PTY	C11-C8-O7-C6
5	A	1013	PTY	O10-C8-O7-C6
5	A	1011	PTY	C31-C30-O4-C1
5	A	1012	PTY	C31-C30-O4-C1
5	A	1013	PTY	C31-C30-O4-C1
3	A	1003	TG1	O4-C21-O3-C3
5	A	1012	PTY	O30-C30-O4-C1
5	A	1011	PTY	O30-C30-O4-C1
5	A	1013	PTY	O30-C30-O4-C1
5	A	1012	PTY	O10-C8-O7-C6
5	A	1012	PTY	C5-O14-P1-O11
3	A	1003	TG1	C14-C15-C16-C17
3	A	1003	TG1	C13-C14-C15-C16
3	A	1003	TG1	O4-C21-C22-C23
3	A	1003	TG1	C16-C17-C18-C19
5	A	1013	PTY	O14-C5-C6-O7
5	A	1013	PTY	O4-C1-C6-C5
3	A	1003	TG1	O4-C21-C22-C24
5	A	1013	PTY	O14-C5-C6-C1
5	A	1013	PTY	O4-C1-C6-O7
4	A	1002	128	PB-O3A-PA-O1A
5	A	1011	PTY	C3-O11-P1-O14
5	A	1012	PTY	C3-O11-P1-O14
5	A	1013	PTY	C3-O11-P1-O14
5	A	1012	PTY	C6-C5-O14-P1
5	A	1011	PTY	O4-C1-C6-O7

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Mol	Chain	Res	Type	Atoms
3	A	1003	TG1	O7-C27-C28-C29
3	A	1003	TG1	O1-C13-C14-C15
3	A	1003	TG1	O2-C13-C14-C15
3	A	1003	TG1	O8-C27-C28-C29
5	A	1011	PTY	C2-C3-O11-P1

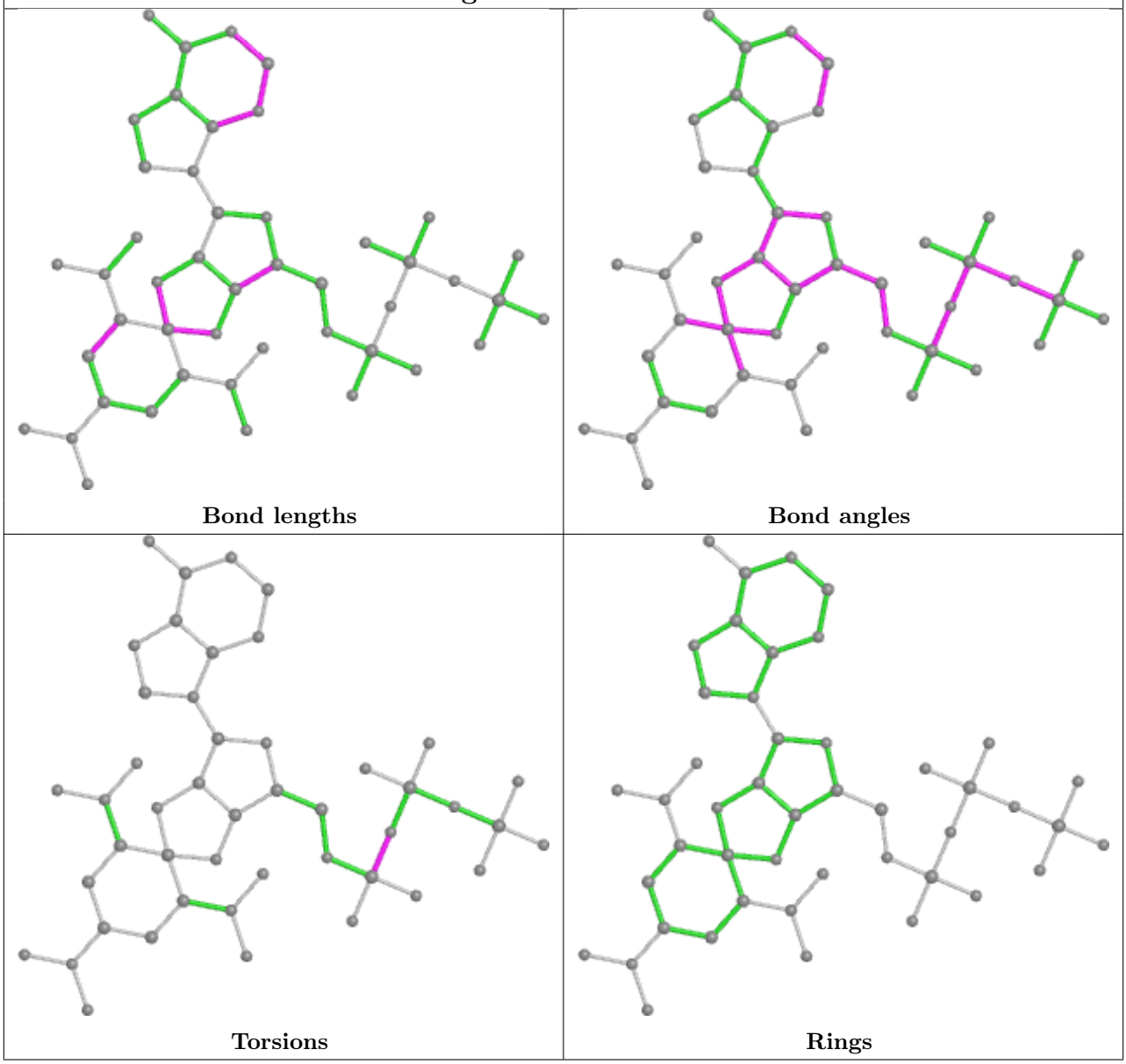
There are no ring outliers.

2 monomers are involved in 3 short contacts:

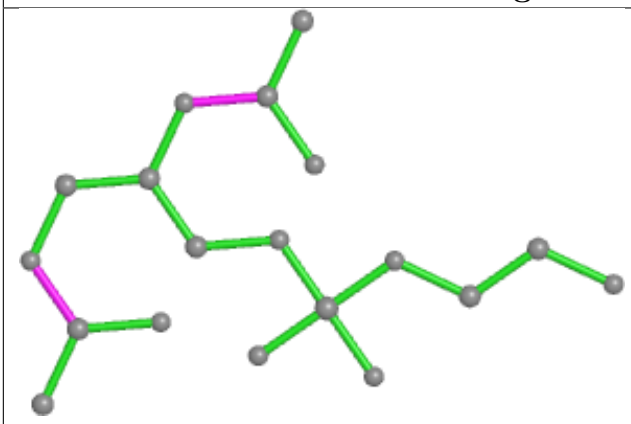
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	128	1	0
3	A	1003	TG1	2	0

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 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.

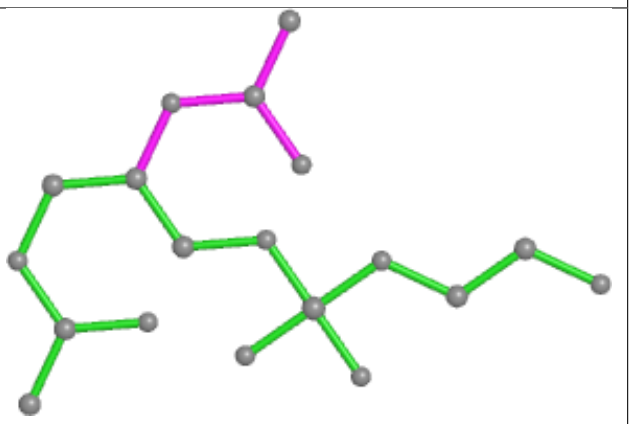
Ligand 128 A 1002



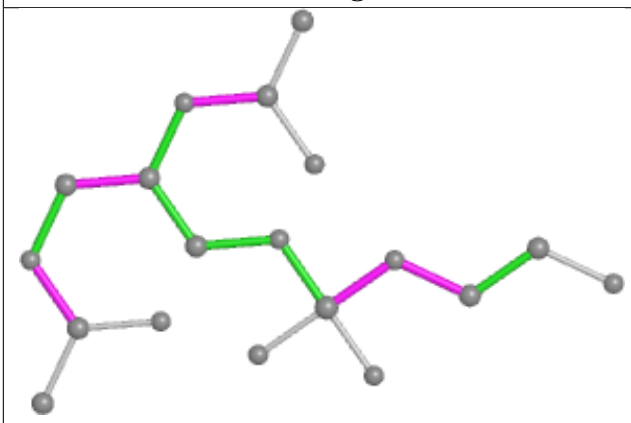
Ligand PTY A 1011



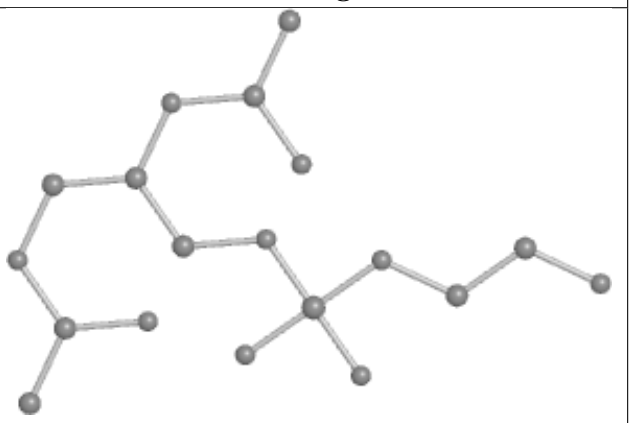
Bond lengths



Bond angles

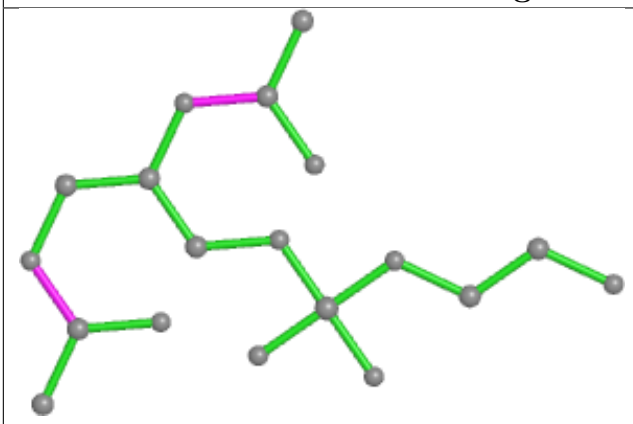


Torsions

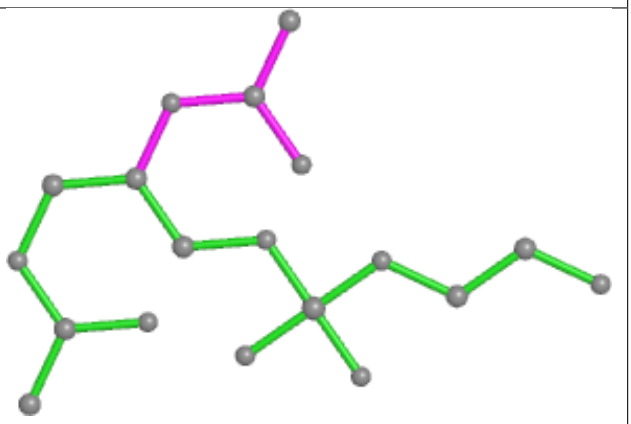


Rings

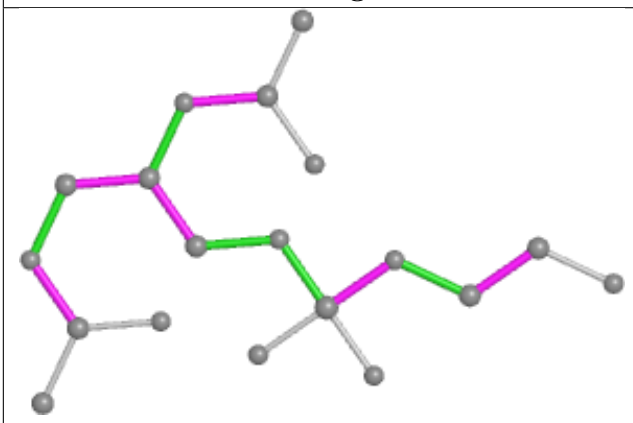
Ligand PTY A 1013



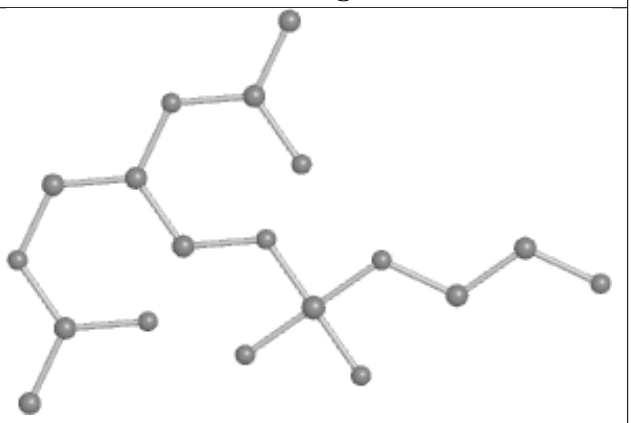
Bond lengths



Bond angles

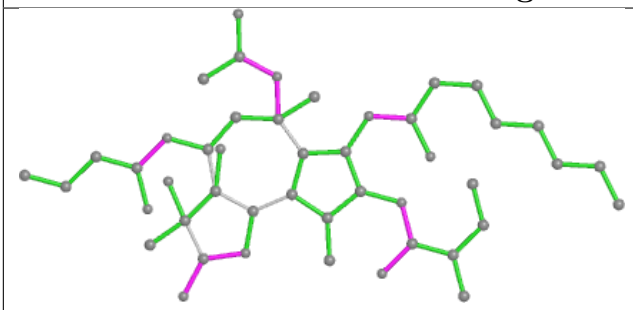


Torsions

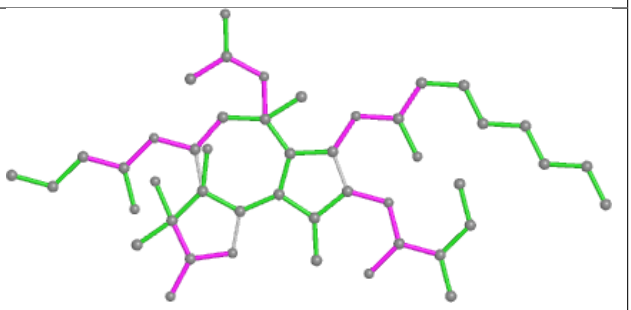


Rings

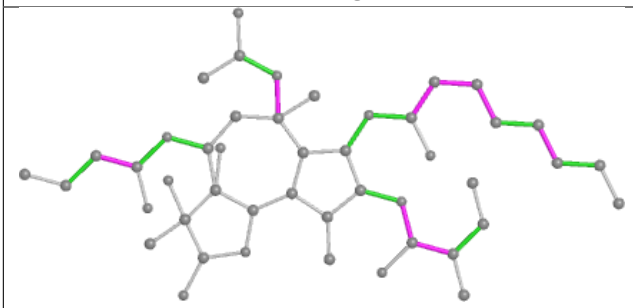
Ligand TG1 A 1003



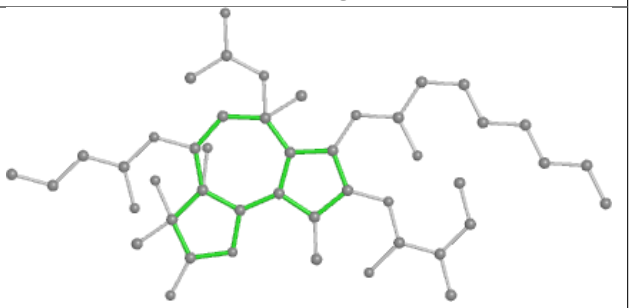
Bond lengths



Bond angles

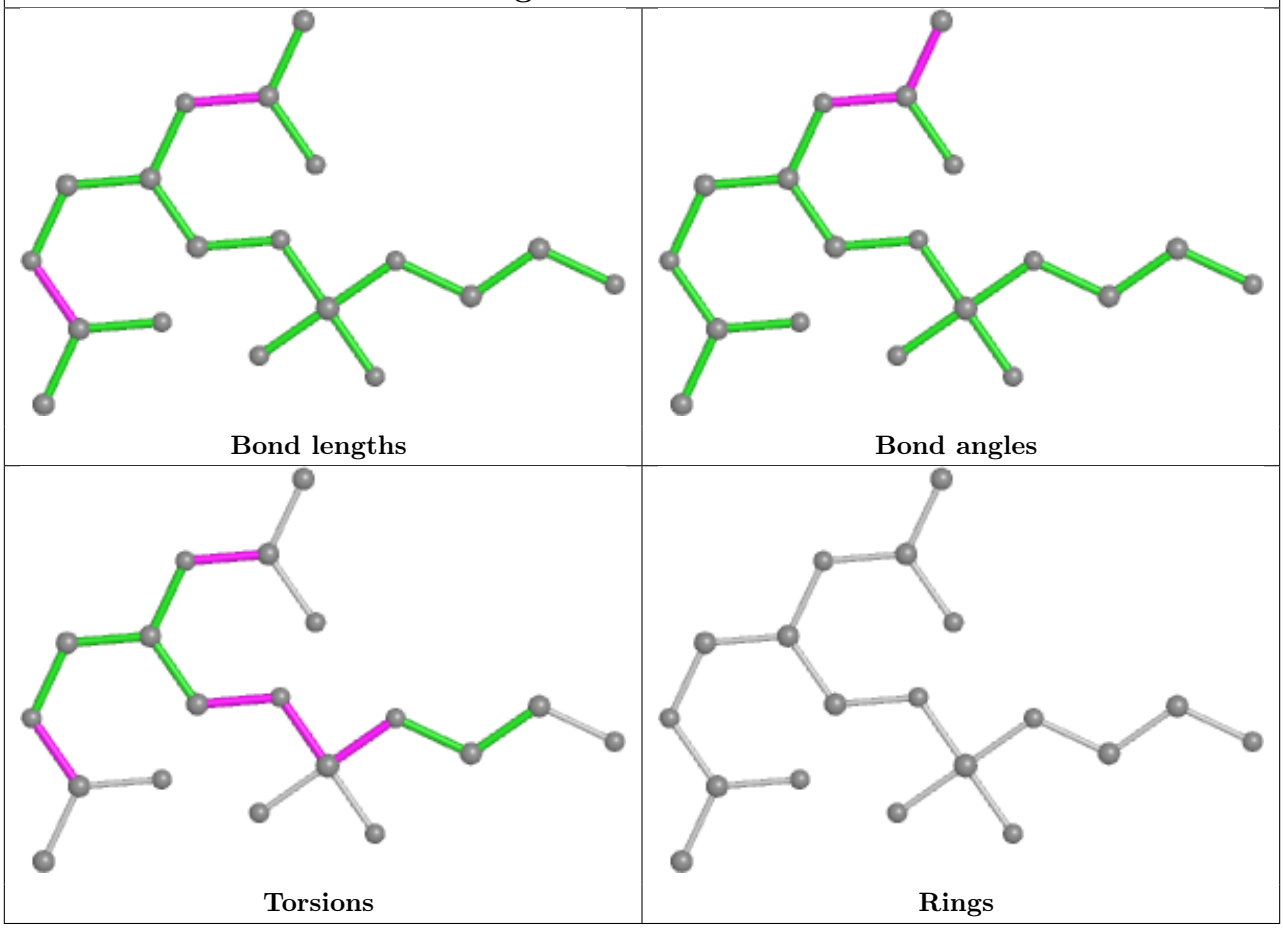


Torsions



Rings

Ligand PTY A 1012



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	994/995 (99%)	0.79	133 (13%)	3	4	36, 63, 120, 160	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	885	GLY	16.2
1	A	883	PHE	14.7
1	A	886	LEU	14.4
1	A	508	VAL	12.4
1	A	507	ALA	11.3
1	A	85	ILE	10.8
1	A	994	GLY	9.0
1	A	503	SER	7.5
1	A	505	ARG	7.5
1	A	504	SER	7.5
1	A	868	HIS	7.3
1	A	506	ALA	7.3
1	A	867	TYR	7.1
1	A	873	PHE	7.1
1	A	866	THR	6.9
1	A	84	THR	6.8
1	A	993	GLU	6.3
1	A	992	LEU	6.1
1	A	46	GLY	5.9
1	A	82	GLU	5.9
1	A	884	GLU	5.9
1	A	881	PRO	5.8
1	A	285	GLY	5.7
1	A	77	TRP	5.7
1	A	433	VAL	5.4
1	A	45	GLU	5.4
1	A	80	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	107	TRP	5.0
1	A	92	PHE	5.0
1	A	427	PHE	5.0
1	A	951	ASP	4.8
1	A	878	GLU	4.8
1	A	78	PHE	4.7
1	A	111	ASN	4.3
1	A	461	ASN	4.3
1	A	429	GLU	4.3
1	A	289	ILE	4.2
1	A	502	LYS	4.1
1	A	875	GLN	4.1
1	A	81	GLY	4.0
1	A	877	THR	3.9
1	A	865	VAL	3.9
1	A	656	ARG	3.8
1	A	50	TRP	3.7
1	A	428	ASN	3.7
1	A	932	TRP	3.6
1	A	871	THR	3.6
1	A	278	HIS	3.6
1	A	54	ILE	3.6
1	A	947	ILE	3.6
1	A	532	THR	3.5
1	A	876	CYS	3.4
1	A	324	ARG	3.3
1	A	44	GLU	3.3
1	A	460	ARG	3.3
1	A	94	ILE	3.3
1	A	431	LYS	3.2
1	A	973	ILE	3.2
1	A	73	PHE	3.2
1	A	960	LYS	3.2
1	A	403	ARG	3.1
1	A	864	GLY	3.1
1	A	880	HIS	3.1
1	A	184	SER	3.1
1	A	426	ASP	3.1
1	A	670	CYS	3.1
1	A	466	GLU	3.1
1	A	933	LEU	3.0
1	A	272	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	462	LEU	2.9
1	A	959	LEU	2.9
1	A	963	ASP	2.8
1	A	856	PHE	2.8
1	A	290	ARG	2.8
1	A	852	ALA	2.8
1	A	79	GLU	2.8
1	A	924	ARG	2.7
1	A	279	PHE	2.7
1	A	476	ARG	2.6
1	A	463	SER	2.6
1	A	579	ASP	2.6
1	A	819	ARG	2.6
1	A	858	TYR	2.6
1	A	882	HIS	2.5
1	A	458	GLU	2.5
1	A	34	GLU	2.5
1	A	430	THR	2.5
1	A	434	TYR	2.5
1	A	185	VAL	2.5
1	A	671	ARG	2.5
1	A	75	LEU	2.5
1	A	665	GLU	2.5
1	A	376	PHE	2.5
1	A	86	THR	2.4
1	A	74	VAL	2.4
1	A	58	GLU	2.4
1	A	135	LYS	2.4
1	A	286	GLY	2.4
1	A	691	LEU	2.4
1	A	509	GLY	2.4
1	A	986	PHE	2.4
1	A	243	GLU	2.3
1	A	668	GLU	2.3
1	A	985	LYS	2.3
1	A	48	SER	2.3
1	A	295	TYR	2.3
1	A	30	LYS	2.3
1	A	288	TRP	2.3
1	A	356	LEU	2.2
1	A	605	LYS	2.2
1	A	119	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	ALA	2.2
1	A	435	GLU	2.2
1	A	464	LYS	2.2
1	A	392	GLU	2.2
1	A	719	ALA	2.2
1	A	734	VAL	2.2
1	A	447	THR	2.2
1	A	482	GLU	2.1
1	A	363	VAL	2.1
1	A	923	MET	2.1
1	A	72	SER	2.1
1	A	281	ASP	2.1
1	A	182	GLY	2.1
1	A	774	CYS	2.1
1	A	465	VAL	2.0
1	A	258	GLU	2.0
1	A	399	ASP	2.0
1	A	444	ALA	2.0
1	A	395	VAL	2.0
1	A	660	ASP	2.0
1	A	527	TYR	2.0
1	A	98	LEU	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(Å^2)	Q<0.9
5	PTY	A	1011	19/50	0.68	0.30	125,128,130,130	0

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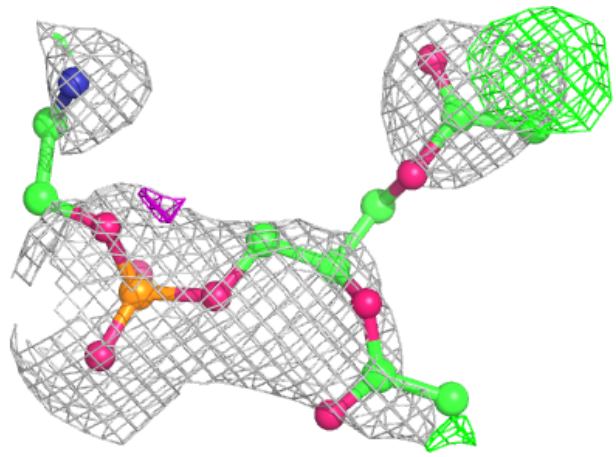
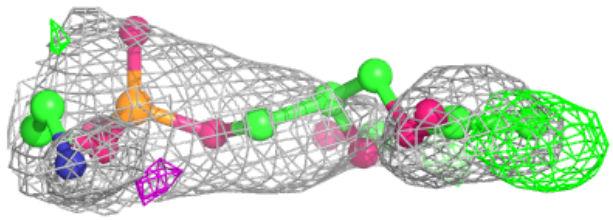
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PTY	A	1013	19/50	0.76	0.27	114,119,122,123	0
5	PTY	A	1012	19/50	0.83	0.32	104,105,105,105	0
4	128	A	1002	46/46	0.88	0.15	56,89,105,108	0
3	TG1	A	1003	46/46	0.89	0.17	64,70,78,78	0
2	NA	A	1000	1/1	0.92	0.06	54,54,54,54	0

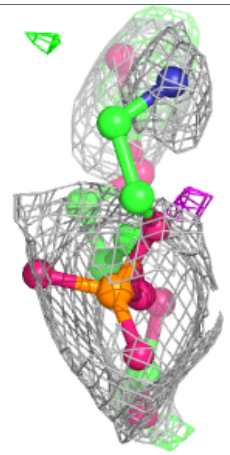
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTY A 1011:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

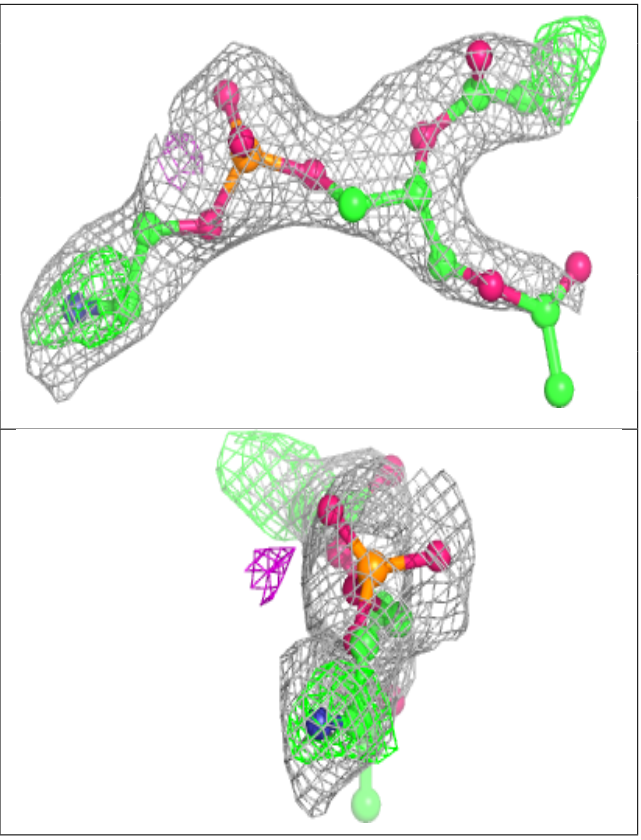






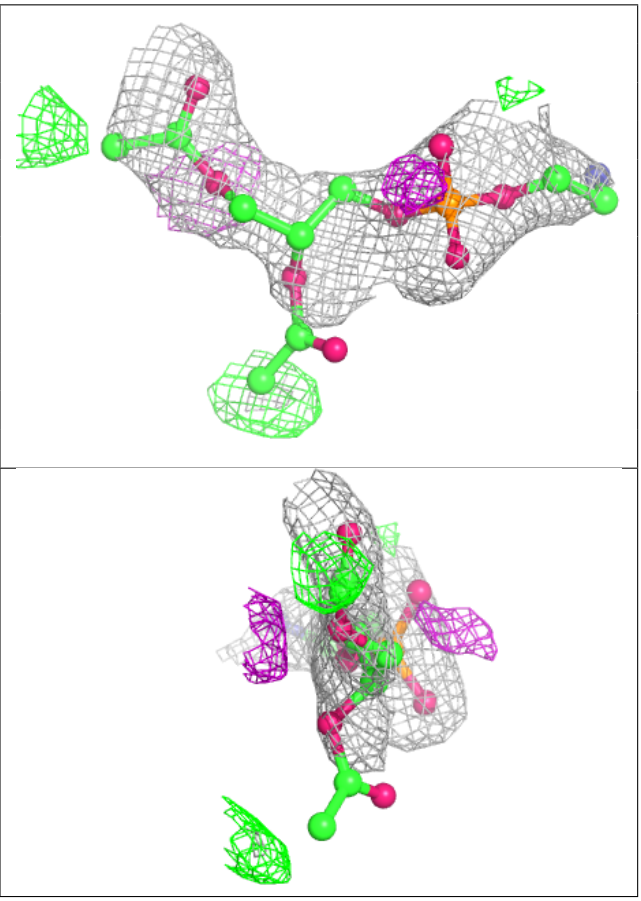
Electron density around PTY A 1013:

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



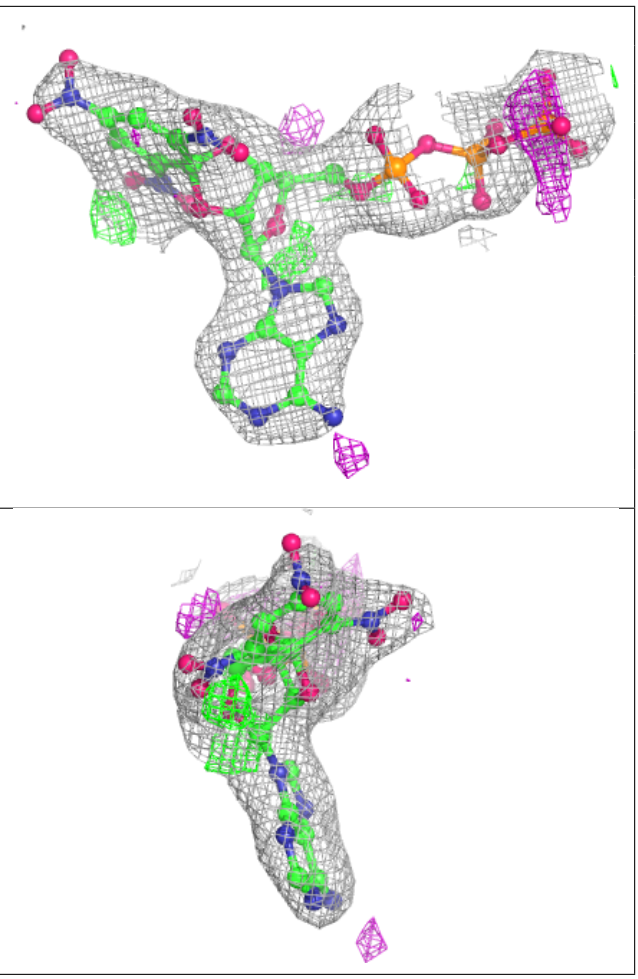
Electron density around PTY A 1012:

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



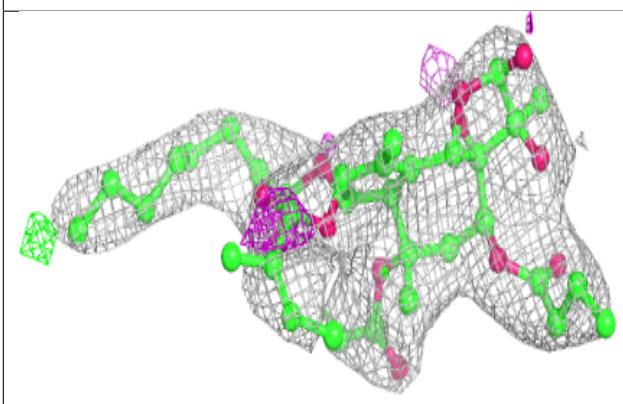
Electron density around 128 A 1002:

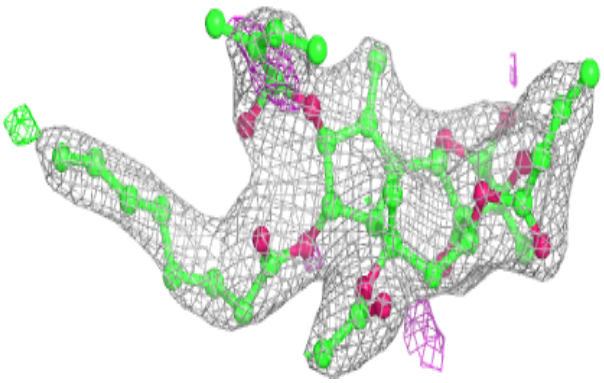
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

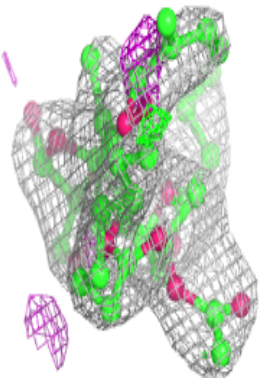


Electron density around TG1 A 1003:

$2mF_o$-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 (i)

There are no such residues in this entry.