



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:49 AM UTC

PDB ID : 3AR7 / pdb_00003ar7
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 ⓘ 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

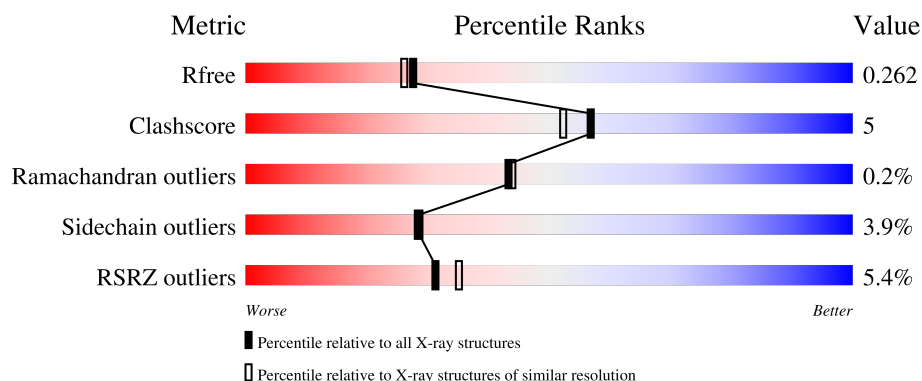
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 $\leq 5\%$. 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	995	5% 87% 12%

2 Entry composition

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
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

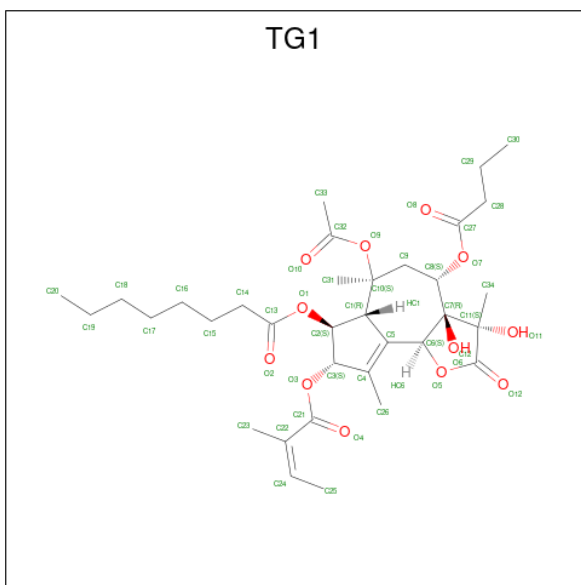
There are 2 discrepancies between the modelled and reference sequences:

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

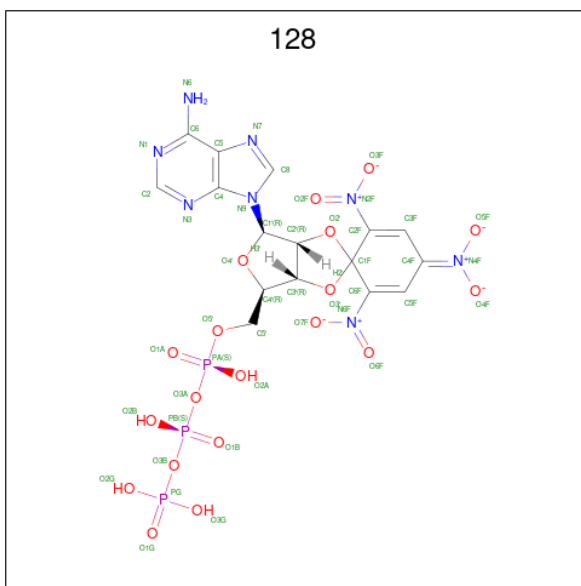
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- 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)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: C₃₄H₅₀O₁₂).



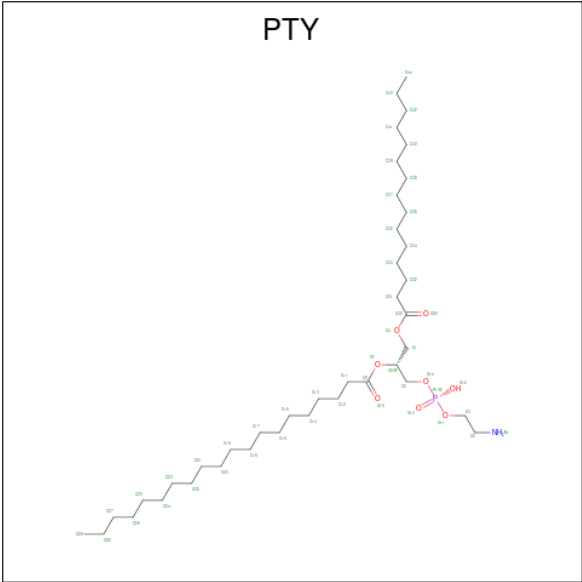
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 4 is SPIRO(2,4,6-TRINITROBENZENE[1,2A]-2O',3O'-METHYLENE-ADENIN E-TRIPHOSPHATE (CCD ID: 128) (formula: $C_{16}H_{16}N_8O_{19}P_3$).



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

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

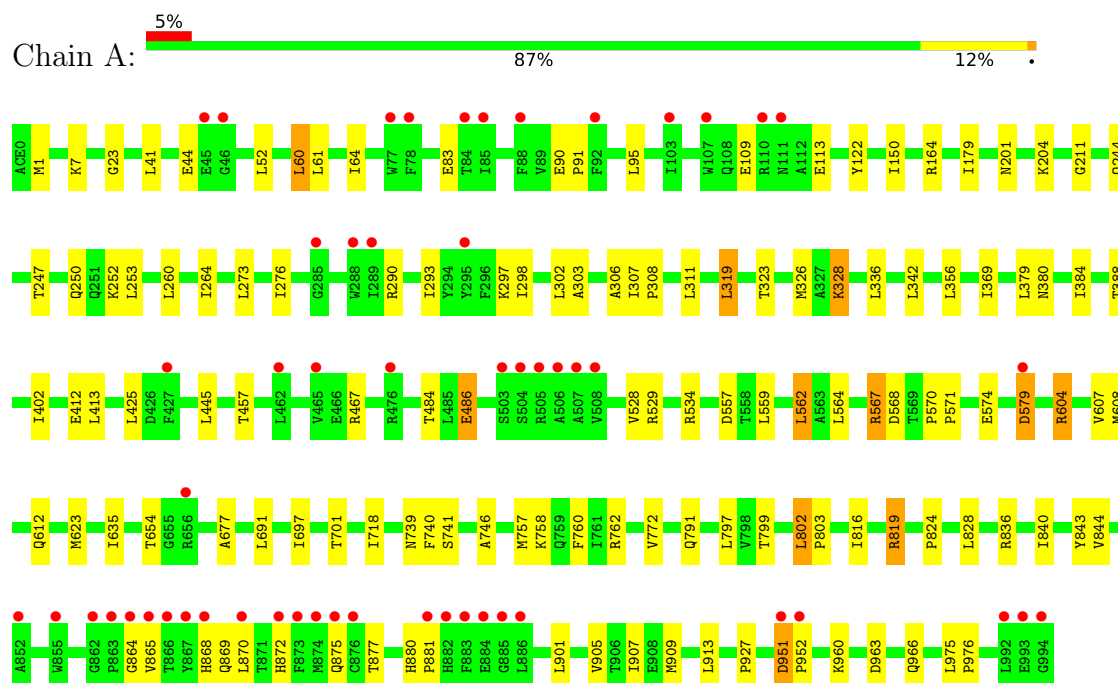
- Molecule 6 is water.

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

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

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 15.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.15) 99.6 (15.00-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/7813	0.80	1/10594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	870	LEU	N-CA-C	-5.10	106.57	112.89

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	72	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	72	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 5.

All (72) 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:1:MET:HE2	1:A:7:LYS:HG3	1.78	0.65
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:623:MET:HE1	1:A:635:ILE:HG22	1.86	0.57
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:529:ARG:HH22	1:A:568:ASP:CG	2.13	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: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:486:GLU:H	1:A:486:GLU:CD	2.19	0.49
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:323:THR:HA	1:A:326:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:868:HIS:CD2	1:A:881:PRO:HB3	2.53	0.44
1:A:356:LEU:HD23	1:A:623:MET:HE2	2.00	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:739:ASN:HD22	1:A:739:ASN:C	2.26	0.42
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

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	993/995 (100%)	963 (97%)	28 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

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

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	840/840 (100%)	807 (96%)	33 (4%)	28	28

All (33) 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	113	GLU
1	A	164	ARG
1	A	253	LEU
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

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Mol	Chain	Res	Type
1	A	445	LEU
1	A	457	THR
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	562	LEU
1	A	567	ARG
1	A	574	GLU
1	A	579	ASP
1	A	604	ARG
1	A	612	GLN
1	A	691	LEU
1	A	797	LEU
1	A	802	LEU
1	A	816	ILE
1	A	819	ARG
1	A	877	THR
1	A	960	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	244	GLN
1	A	250	GLN
1	A	278	HIS
1	A	359	ASN
1	A	398	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	911	ASN
1	A	914	ASN
1	A	919	ASN
1	A	966	GLN
1	A	990	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
5	PTY	A	1012	-	18,18,49	1.50	2 (11%)	21,23,54	1.34	1 (4%)
5	PTY	A	1011	-	18,18,49	1.47	2 (11%)	21,23,54	1.45	3 (14%)
5	PTY	A	1013	-	18,18,49	1.48	2 (11%)	21,23,54	1.48	3 (14%)
4	128	A	1002	-	42,50,50	2.19	11 (26%)	55,80,80	2.88	17 (30%)
3	TG1	A	1003	-	44,48,48	2.89	8 (18%)	47,72,72	3.44	13 (27%)

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	PTY	A	1012	-	-	7/20/20/53	-
5	PTY	A	1011	-	-	5/20/20/53	-
5	PTY	A	1013	-	-	9/20/20/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	128	A	1002	-	-	1/26/80/80	0/5/5/5
3	TG1	A	1003	-	-	11/33/99/99	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	TG1	O4-C21	11.24	1.44	1.21
3	A	1003	TG1	O12-C12	10.22	1.43	1.20
4	A	1002	128	O2'-C1F	6.56	1.51	1.41
4	A	1002	128	O3'-C1F	5.89	1.50	1.41
3	A	1003	TG1	O5-C12	5.73	1.43	1.35
5	A	1012	PTY	O7-C8	5.21	1.46	1.35
4	A	1002	128	C1'-N9	5.06	1.60	1.46
5	A	1013	PTY	O7-C8	5.06	1.46	1.35
3	A	1003	TG1	O9-C32	5.03	1.46	1.35
5	A	1011	PTY	O7-C8	5.00	1.46	1.35
3	A	1003	TG1	O1-C13	4.41	1.46	1.34
3	A	1003	TG1	O7-C27	4.24	1.46	1.34
3	A	1003	TG1	O3-C21	3.98	1.43	1.34
4	A	1002	128	C5F-C6F	3.66	1.47	1.37
4	A	1002	128	C5-N7	-3.15	1.33	1.39
4	A	1002	128	C3'-C4'	-3.10	1.44	1.52
4	A	1002	128	PB-O3B	2.83	1.62	1.59
3	A	1003	TG1	O9-C10	-2.82	1.43	1.48
5	A	1012	PTY	O4-C30	2.68	1.46	1.33
5	A	1011	PTY	O4-C30	2.68	1.46	1.33
5	A	1013	PTY	O4-C30	2.66	1.46	1.33
4	A	1002	128	O7F-N6F	-2.57	1.18	1.35
4	A	1002	128	C2-N1	2.52	1.38	1.33
4	A	1002	128	C4-N3	2.39	1.38	1.34
4	A	1002	128	C6-N1	2.05	1.41	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	TG1	O12-C12-C11	-17.06	111.03	128.28
4	A	1002	128	O3'-C1F-C6F	-9.75	97.13	110.47
3	A	1003	TG1	O5-C12-O12	-8.72	110.32	121.60
3	A	1003	TG1	O3-C21-O4	-7.24	109.90	123.40
4	A	1002	128	C5-C4-N3	-6.81	117.34	126.72
4	A	1002	128	O2'-C1F-C2F	-6.49	101.59	110.47
4	A	1002	128	O2'-C2'-C3'	6.31	113.69	103.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	128	C4'-O4'-C1'	5.68	122.00	109.47
4	A	1002	128	N3-C4-N9	5.53	136.57	127.17
3	A	1003	TG1	O4-C21-C22	-5.22	108.71	125.28
5	A	1013	PTY	O7-C8-C11	4.78	119.61	111.09
4	A	1002	128	C2-N3-C4	4.64	123.17	111.83
5	A	1011	PTY	O7-C8-C11	4.63	119.35	111.09
4	A	1002	128	O4'-C1'-C2'	-4.57	98.72	106.59
4	A	1002	128	N3-C2-N1	-4.41	121.91	128.58
5	A	1012	PTY	O7-C8-C11	4.32	118.78	111.09
4	A	1002	128	C1F-O2'-C2'	-4.06	98.59	107.85
3	A	1003	TG1	O9-C32-C33	3.99	117.44	110.67
3	A	1003	TG1	O1-C13-C14	3.89	119.90	111.48
4	A	1002	128	O3'-C1F-C2F	3.85	115.74	110.47
3	A	1003	TG1	O7-C27-C28	3.67	119.43	111.48
4	A	1002	128	O2'-C1F-C6F	2.97	114.52	110.47
3	A	1003	TG1	C8-O7-C27	-2.75	113.01	118.03
4	A	1002	128	O5'-C5'-C4'	2.71	118.23	108.99
5	A	1013	PTY	C6-O7-C8	-2.66	113.16	117.85
3	A	1003	TG1	C10-O9-C32	2.62	127.50	121.36
3	A	1003	TG1	O7-C8-C9	2.57	111.22	106.63
3	A	1003	TG1	C2-O1-C13	-2.46	113.58	117.59
5	A	1011	PTY	C6-O7-C8	-2.43	113.56	117.85
5	A	1011	PTY	O7-C8-O10	-2.26	118.62	122.99
5	A	1013	PTY	O7-C8-O10	-2.25	118.64	122.99
4	A	1002	128	N9-C8-N7	-2.25	110.75	113.94
4	A	1002	128	C2'-C3'-C4'	2.25	108.99	103.78
3	A	1003	TG1	C3-O3-C21	-2.13	112.52	116.96
4	A	1002	128	C6-C5-C4	2.11	120.06	117.18
4	A	1002	128	C2'-C1'-N9	-2.01	110.45	113.75
3	A	1003	TG1	O9-C32-O10	-2.00	120.12	123.61

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	TG1	C31-C10-O9-C32
5	A	1011	PTY	C11-C8-O7-C6
5	A	1012	PTY	C5-O14-P1-O11
5	A	1012	PTY	C5-O14-P1-O12
5	A	1013	PTY	N1-C2-C3-O11
5	A	1013	PTY	C11-C8-O7-C6
5	A	1011	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
5	A	1013	PTY	O10-C8-O7-C6
5	A	1012	PTY	C11-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
3	A	1003	TG1	C14-C15-C16-C17
3	A	1003	TG1	C13-C14-C15-C16
3	A	1003	TG1	O4-C21-C22-C23
5	A	1013	PTY	O14-C5-C6-O7
3	A	1003	TG1	C16-C17-C18-C19
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	O4-C1-C6-O7
5	A	1012	PTY	C6-C5-O14-P1
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

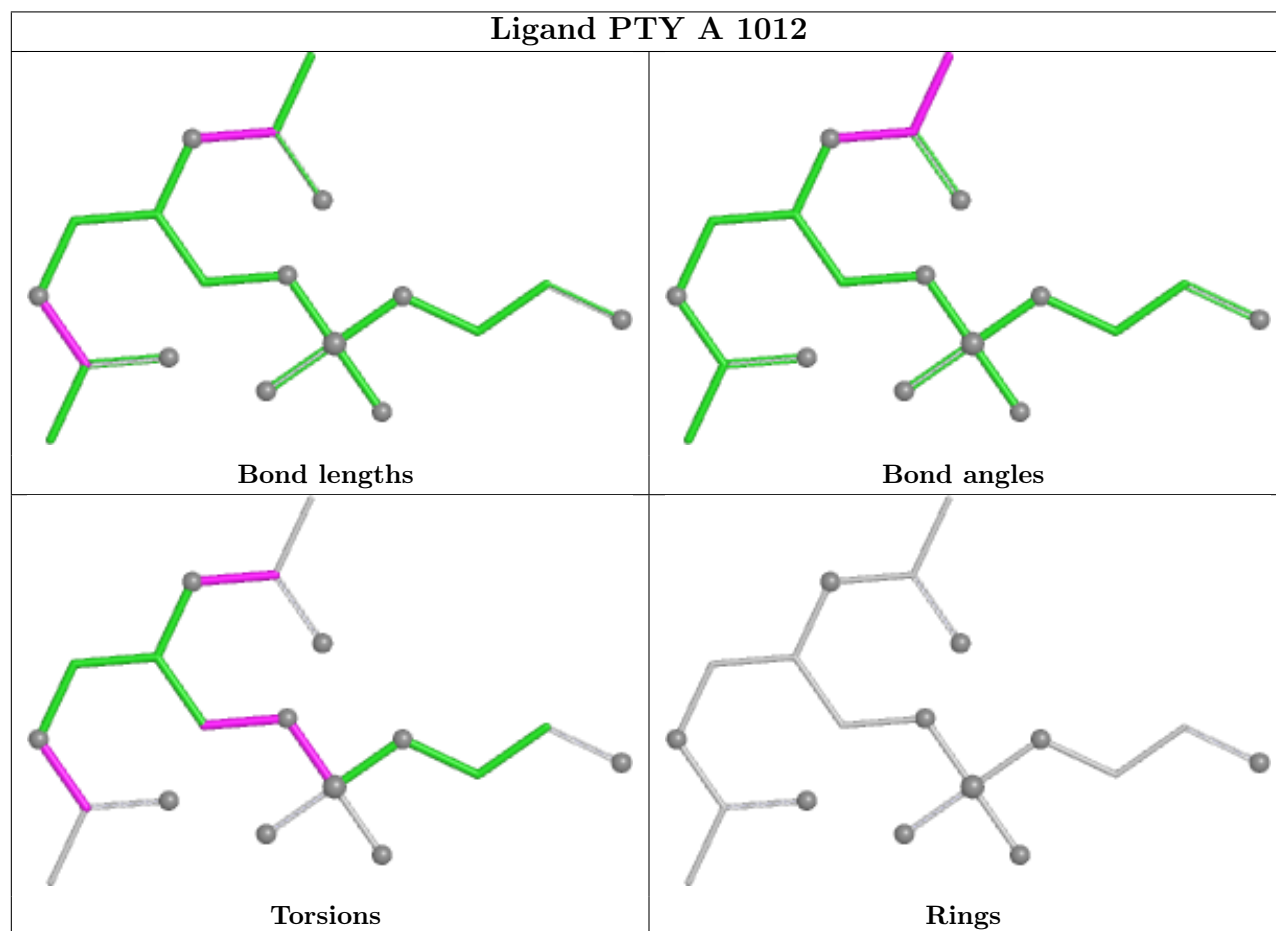
There are no ring outliers.

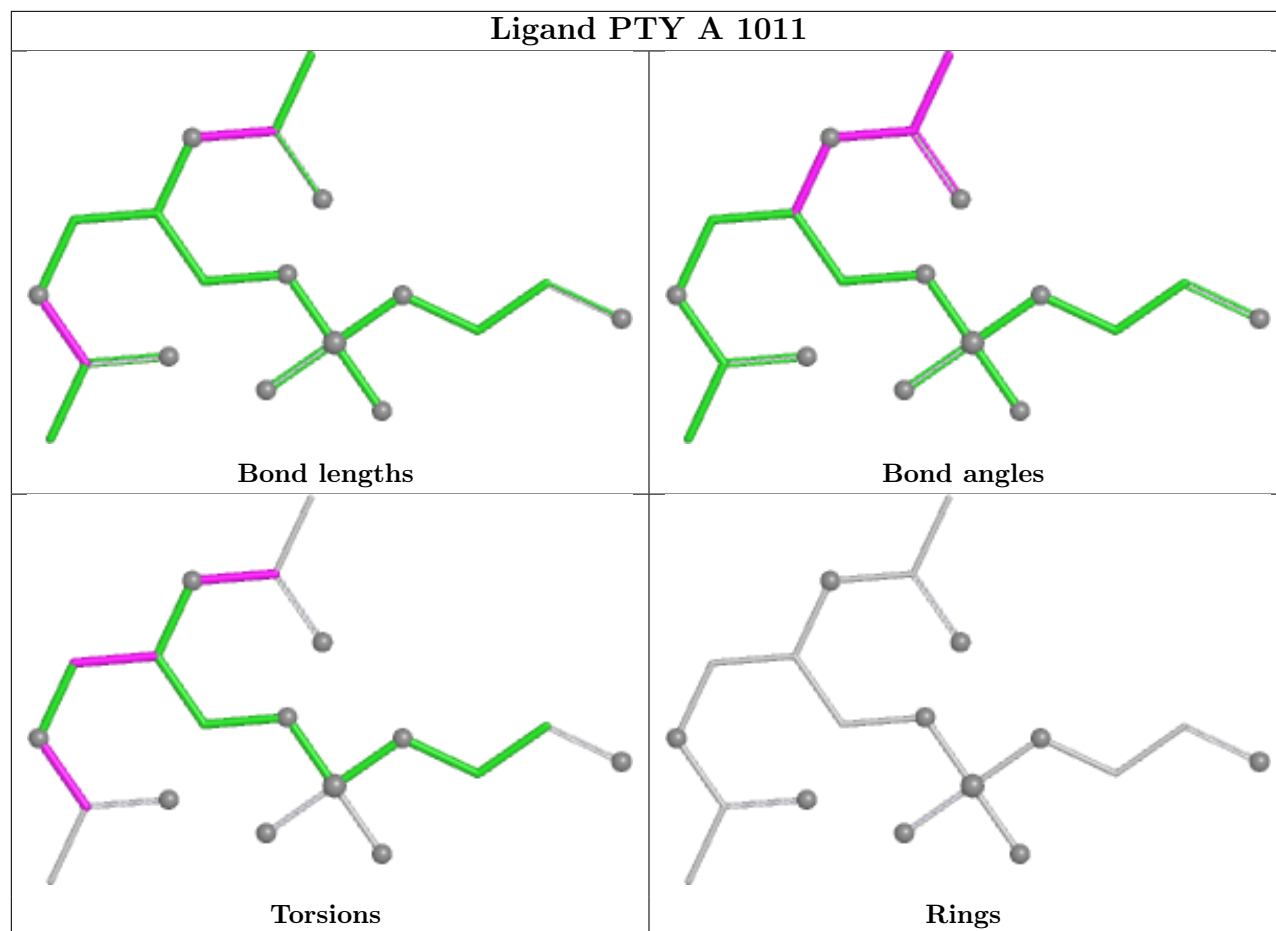
2 monomers are involved in 3 short contacts:

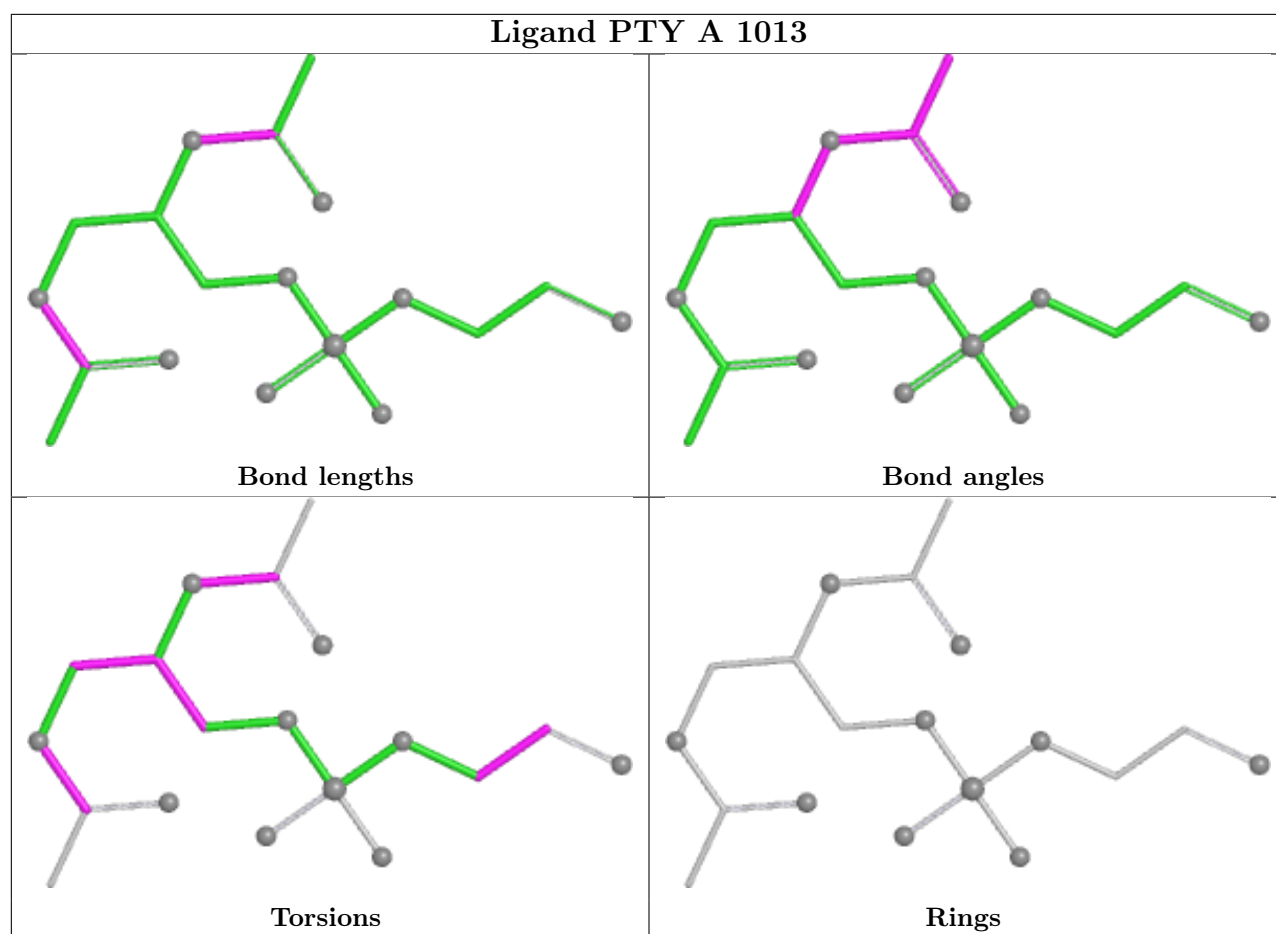
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	128	1	0
3	A	1003	TG1	2	0

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 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

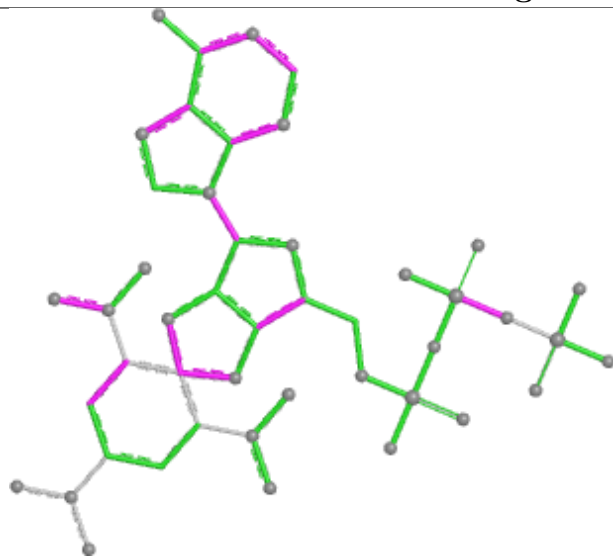
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



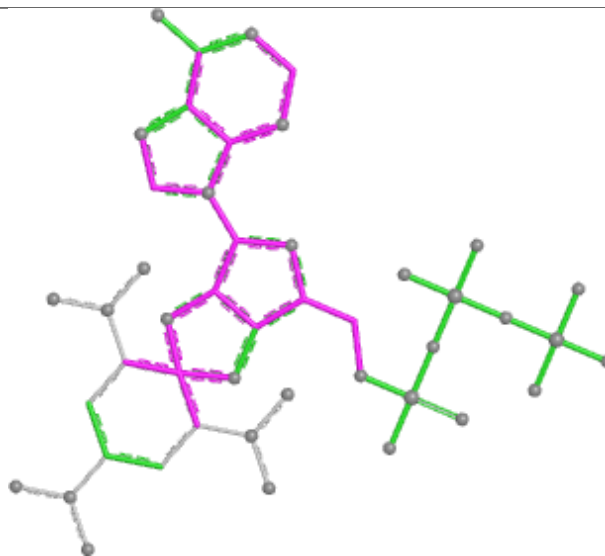




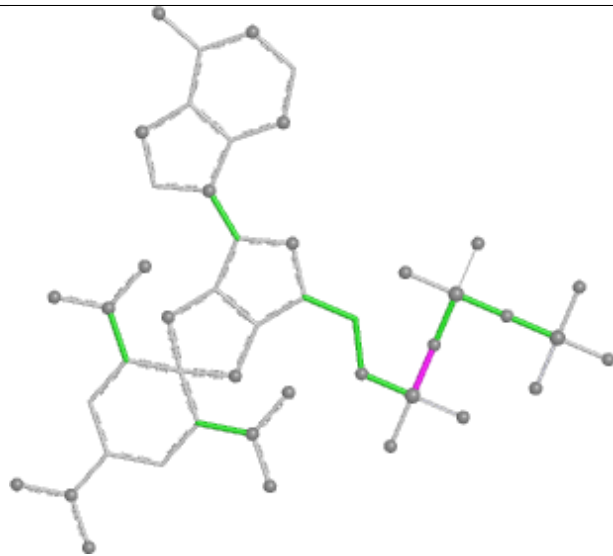
Ligand 128 A 1002



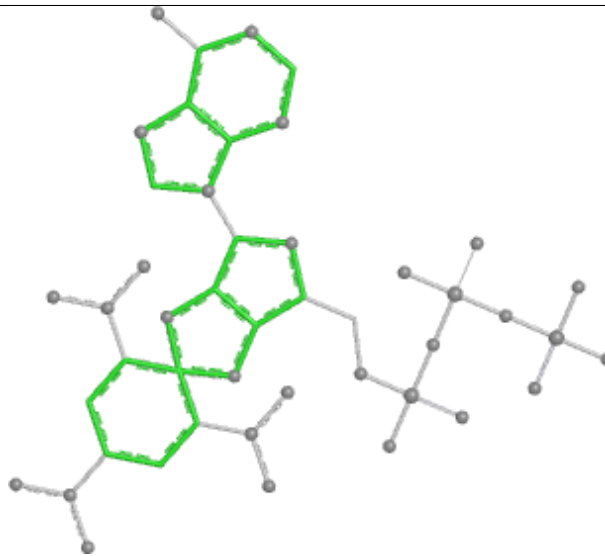
Bond lengths



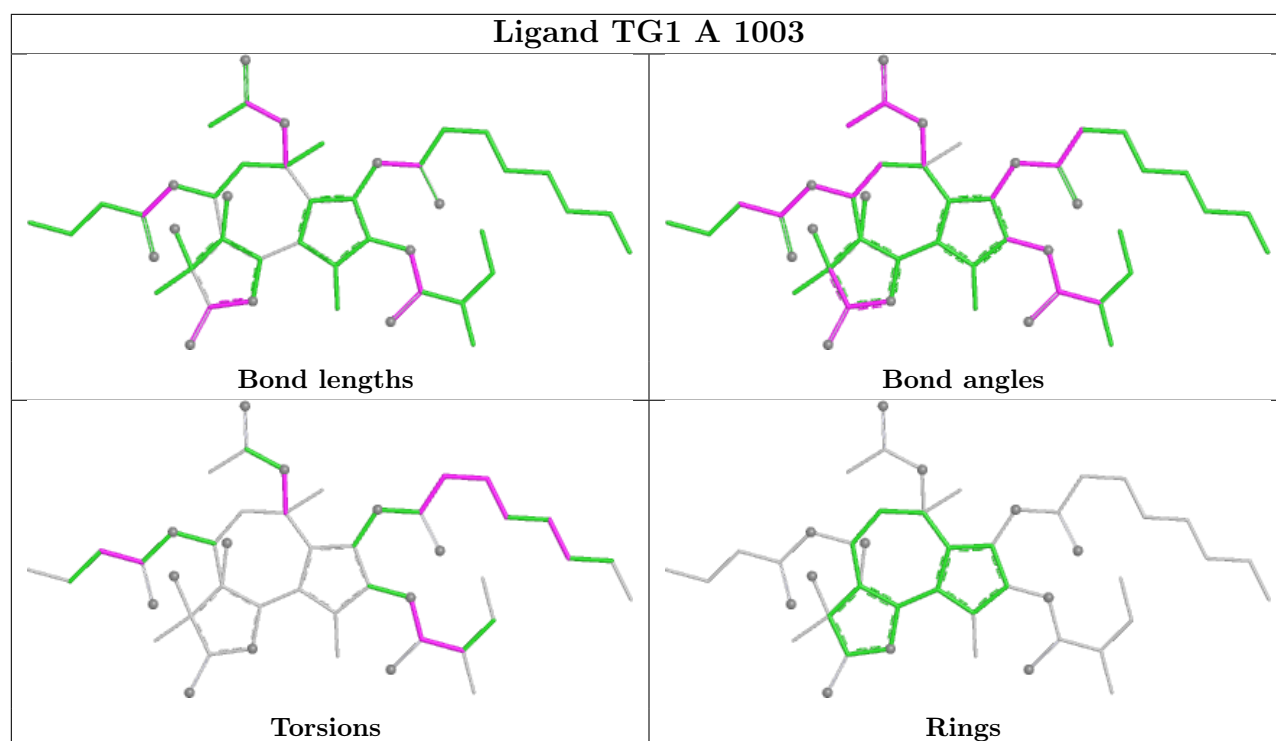
Bond angles



Torsions



Rings



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	994/995 (99%)	0.29	54 (5%) 31 35	36, 63, 120, 160	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	873	PHE	7.2
1	A	508	VAL	7.1
1	A	886	LEU	5.9
1	A	507	ALA	5.8
1	A	85	ILE	5.5
1	A	883	PHE	5.4
1	A	865	VAL	5.1
1	A	866	THR	4.8
1	A	868	HIS	4.6
1	A	885	GLY	4.3
1	A	506	ALA	4.2
1	A	881	PRO	4.2
1	A	84	THR	4.0
1	A	503	SER	3.3
1	A	864	GLY	3.3
1	A	884	GLU	3.2
1	A	78	PHE	3.0
1	A	862	GLY	3.0
1	A	465	VAL	2.9
1	A	874	MET	2.9
1	A	288	TRP	2.9
1	A	462	LEU	2.9
1	A	656	ARG	2.8
1	A	867	TYR	2.8
1	A	88	PHE	2.7
1	A	870	LEU	2.7
1	A	46	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	993	GLU	2.6
1	A	285	GLY	2.6
1	A	77	TRP	2.6
1	A	875	GLN	2.6
1	A	876	CYS	2.5
1	A	882	HIS	2.5
1	A	951	ASP	2.5
1	A	427	PHE	2.5
1	A	872	HIS	2.4
1	A	289	ILE	2.4
1	A	863	PRO	2.4
1	A	994	GLY	2.4
1	A	111	ASN	2.3
1	A	45	GLU	2.3
1	A	579	ASP	2.3
1	A	852	ALA	2.3
1	A	295	TYR	2.3
1	A	992	LEU	2.1
1	A	952	PRO	2.1
1	A	107	TRP	2.1
1	A	504	SER	2.1
1	A	103	ILE	2.1
1	A	110	ARG	2.1
1	A	476	ARG	2.1
1	A	855	TRP	2.1
1	A	505	ARG	2.0
1	A	92	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 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,

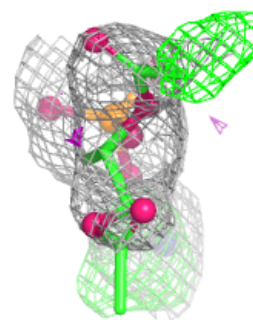
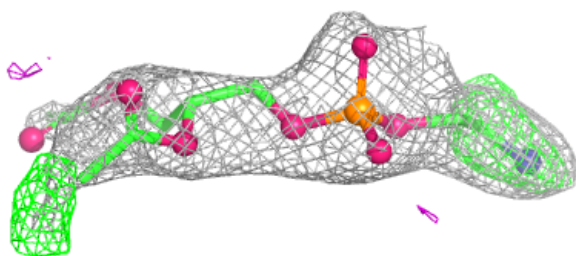
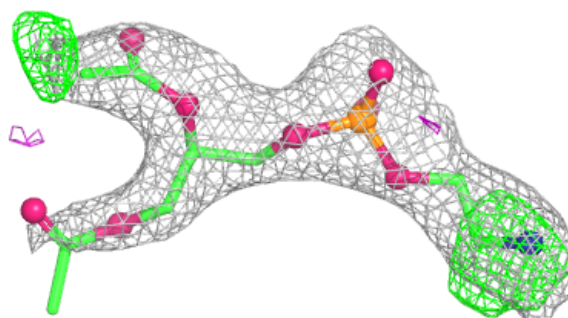
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PTY	A	1013	19/50	0.65	0.18	114,119,122,123	0
5	PTY	A	1012	19/50	0.72	0.18	104,105,105,105	0
5	PTY	A	1011	19/50	0.76	0.20	125,128,130,130	0
4	128	A	1002	46/46	0.84	0.13	56,89,105,108	0
3	TG1	A	1003	46/46	0.90	0.11	64,70,78,78	0
2	NA	A	1000	1/1	0.94	0.05	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.

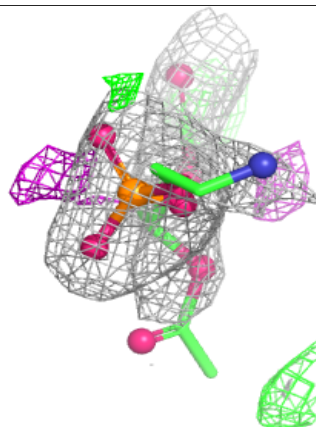
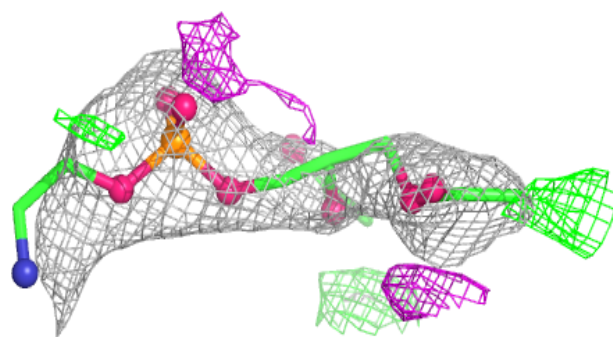
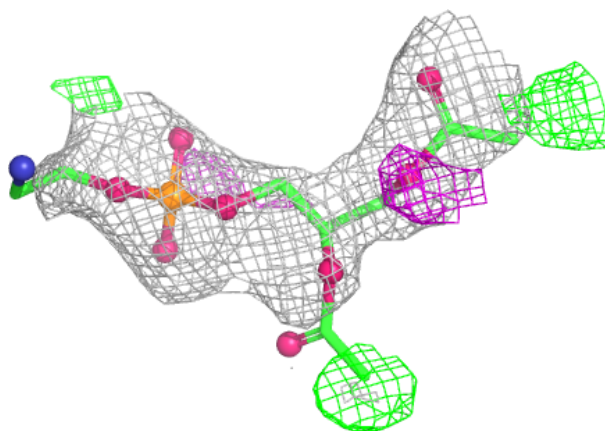
Electron density around PTY A 1013:

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



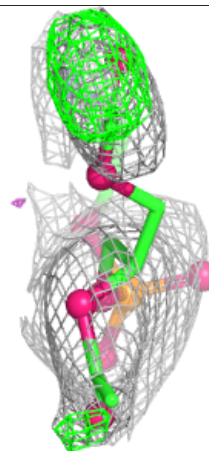
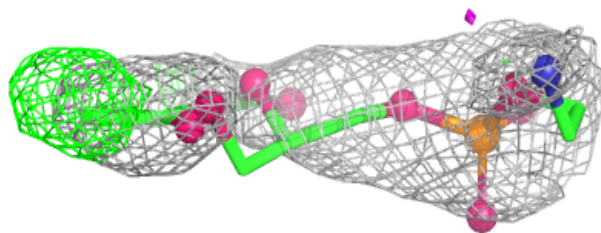
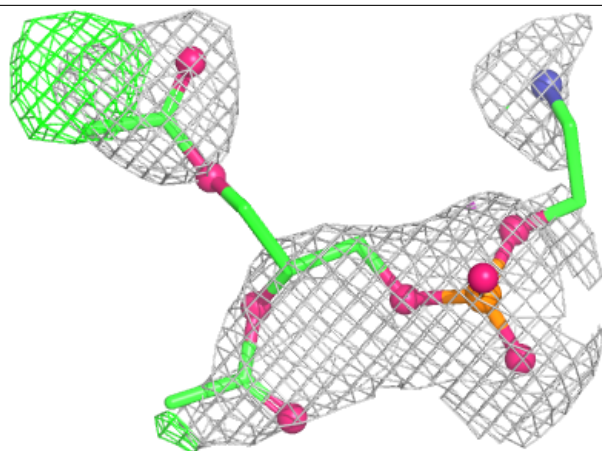
Electron density around PTY A 1012:

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



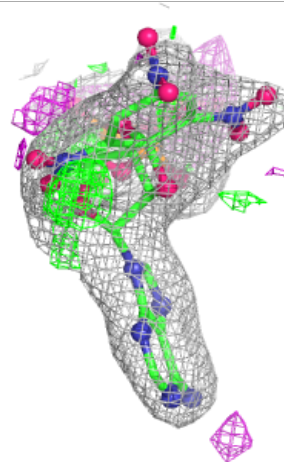
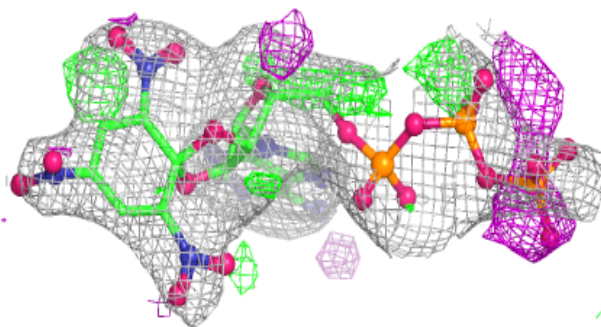
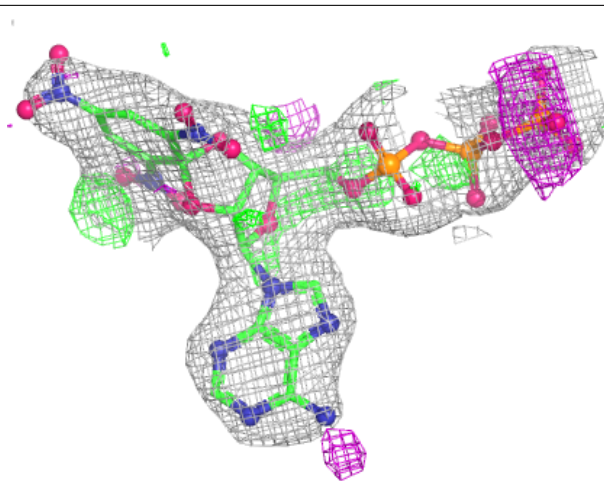
Electron density around PTY A 1011:

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



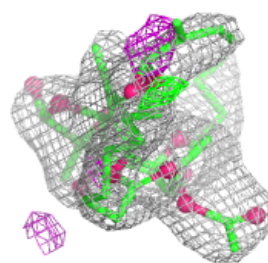
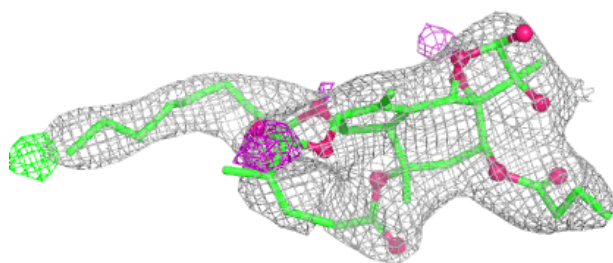
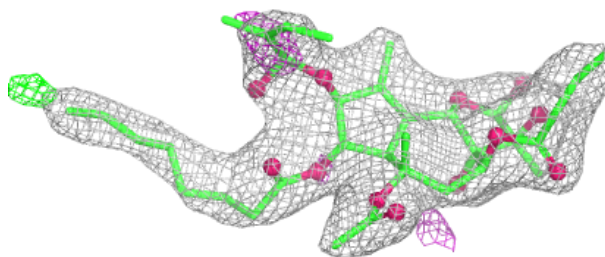
Electron density around 128 A 1002:

$2mF_o-DF_c$ (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.