



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:17 AM UTC

PDB ID : 3AR4 / pdb_00003ar4
Title : Calcium pump crystal structure with bound ATP and TG in the absence of Ca²⁺
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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

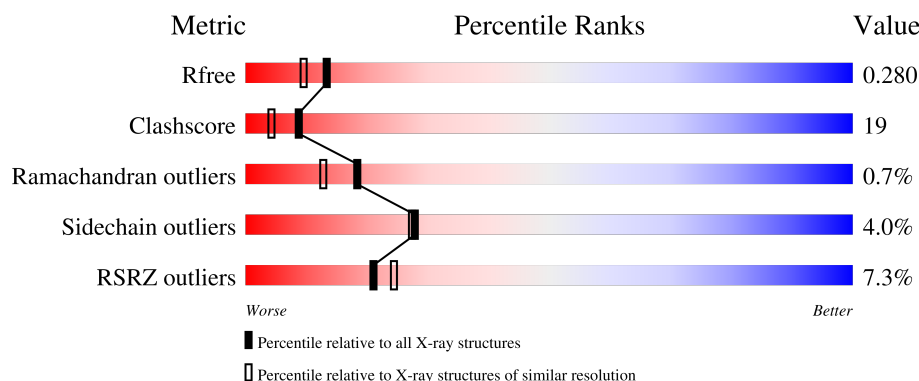
1 Overall quality at a glance

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	7% 64% 33% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8188 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.

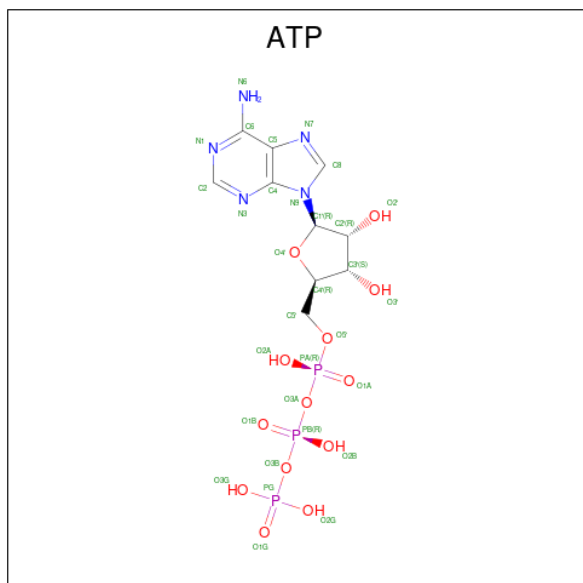
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

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	1A	ACE	-	acetylation	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

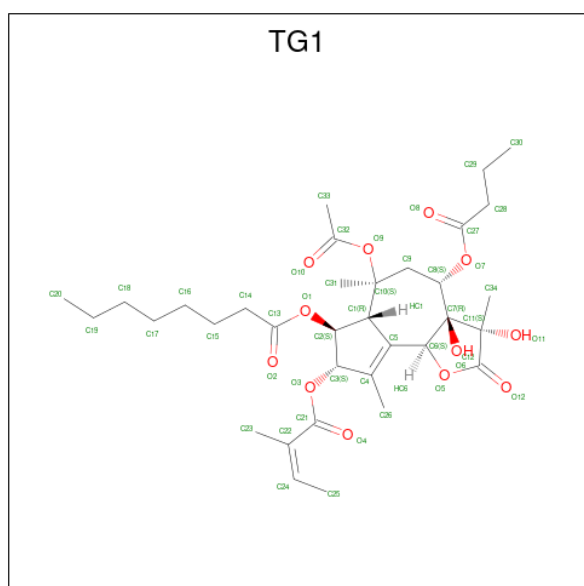


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

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

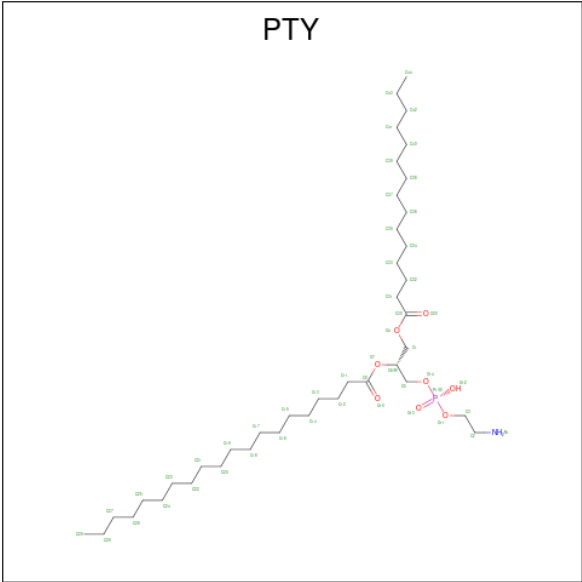
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



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

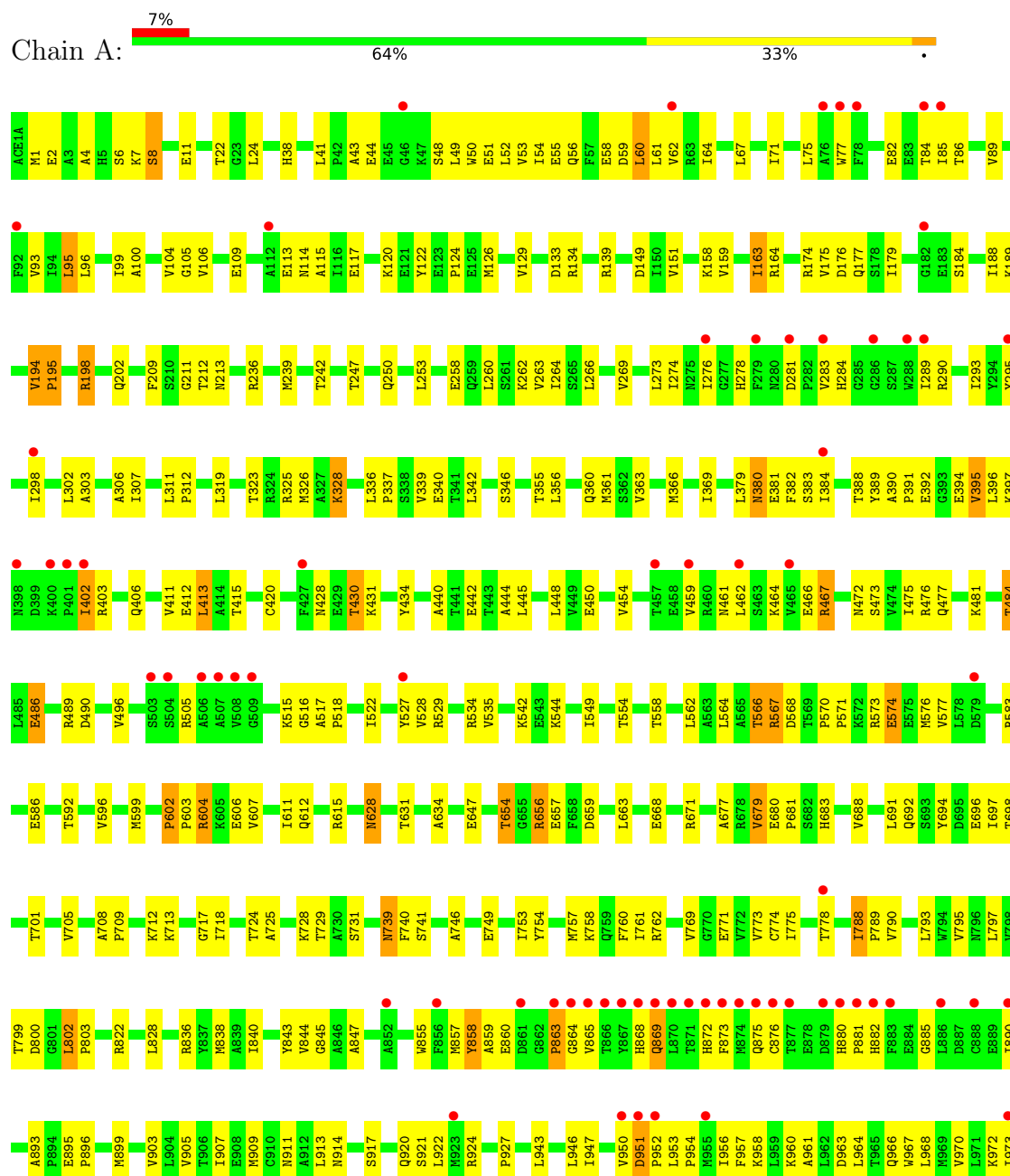
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	377	Total	O	0	0
			377	377		

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 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.38Å 71.38Å 590.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.15 14.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (14.97-2.15) 99.0 (14.97-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.281 0.237 , 0.280	Depositor DCC
R_{free} test set	4264 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8188	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: TG1, ATP, ACE, NA, PTY, MG

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	0.42	0/7813	0.89	22/10594 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	838	MET	N-CA-C	-6.74	103.40	111.69
1	A	602	PRO	N-CA-C	6.50	118.62	110.70
1	A	159	VAL	CA-C-N	6.25	125.95	119.64
1	A	159	VAL	C-N-CA	6.25	125.95	119.64
1	A	698	THR	N-CA-C	6.22	119.38	109.24
1	A	654	THR	N-CA-C	-5.95	101.66	110.46
1	A	517	ALA	CA-C-N	5.79	125.26	119.24
1	A	517	ALA	C-N-CA	5.79	125.26	119.24
1	A	788	ILE	CA-C-N	5.71	126.97	119.84
1	A	788	ILE	C-N-CA	5.71	126.97	119.84
1	A	163	ILE	N-CA-C	5.65	116.61	108.48
1	A	739	ASN	N-CA-C	5.57	117.78	109.25
1	A	628	ASN	N-CA-C	-5.41	103.75	110.41
1	A	356	LEU	N-CA-C	-5.40	105.82	112.90
1	A	195	PRO	N-CA-C	5.33	121.70	113.75
1	A	8	SER	N-CA-C	-5.18	103.84	110.53
1	A	164	ARG	N-CA-C	-5.12	100.96	109.46
1	A	194	VAL	CA-C-N	5.12	125.15	119.32
1	A	194	VAL	C-N-CA	5.12	125.15	119.32
1	A	761	ILE	N-CA-C	-5.06	105.91	110.82
1	A	4	ALA	N-CA-C	5.03	117.42	111.33
1	A	395	VAL	N-CA-C	-5.00	104.60	110.05

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	7674	0	7765	293	0
2	A	31	0	12	3	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	46	0	50	2	0
6	A	57	0	33	1	0
7	A	377	0	0	16	0
All	All	8188	0	7860	293	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 19.

All (293) 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:366:MET:HE2	1:A:384:ILE:HD11	1.43	0.97
1:A:328:LYS:HZ3	1:A:328:LYS:HA	1.37	0.88
1:A:290:ARG:HH12	1:A:875:GLN:HG2	1.39	0.87
1:A:328:LYS:HA	1:A:328:LYS:NZ	1.88	0.87
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.59	0.84
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.60	0.84
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.61	0.83
1:A:85:ILE:HG23	1:A:86:THR:HG22	1.61	0.82
1:A:462:LEU:HB3	1:A:466:GLU:HB2	1.63	0.81
1:A:963:ASP:H	1:A:966:GLN:NE2	1.80	0.79
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.62	0.79
1:A:963:ASP:H	1:A:966:GLN:HE21	1.29	0.78
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.66	0.78
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.66	0.77
1:A:739:ASN:HD22	1:A:740:PHE:N	1.85	0.75
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.68	0.74
1:A:924:ARG:HA	1:A:924:ARG:HE	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.88	0.73
1:A:583:ARG:HD2	7:A:2218:HOH:O	1.88	0.72
1:A:179:ILE:O	1:A:705:VAL:HG22	1.90	0.72
1:A:89:VAL:O	1:A:93:VAL:HG23	1.89	0.71
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.21	0.71
1:A:56:GLN:OE1	1:A:105:GLY:HA3	1.90	0.71
1:A:55:GLU:HA	1:A:58:GLU:HG3	1.73	0.70
1:A:680:GLU:HB2	1:A:683:HIS:CD2	2.26	0.70
1:A:397:LYS:HB2	1:A:402:ILE:HG21	1.74	0.69
1:A:264:ILE:HG23	1:A:302:LEU:HD12	1.75	0.69
1:A:836:ARG:O	1:A:840:ILE:HG12	1.93	0.68
1:A:312:PRO:HG2	7:A:2357:HOH:O	1.93	0.68
1:A:680:GLU:H	1:A:683:HIS:CD2	2.10	0.68
1:A:554:THR:HG21	7:A:2365:HOH:O	1.92	0.68
1:A:680:GLU:H	1:A:683:HIS:HD2	1.41	0.67
1:A:583:ARG:O	1:A:586:GLU:HG2	1.95	0.67
1:A:149:ASP:HB2	7:A:2356:HOH:O	1.94	0.67
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.77	0.67
1:A:663:LEU:HD12	1:A:663:LEU:H	1.59	0.66
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.77	0.66
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.77	0.66
1:A:758:LYS:O	1:A:762:ARG:HG3	1.96	0.66
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.78	0.66
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.78	0.65
1:A:174:ARG:NH2	1:A:188:ILE:HD11	2.12	0.65
1:A:968:LEU:O	1:A:972:LYS:HG3	1.97	0.65
1:A:606:GLU:OE1	1:A:606:GLU:N	2.28	0.64
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.79	0.64
1:A:174:ARG:CZ	1:A:188:ILE:HD11	2.28	0.64
1:A:397:LYS:HB2	1:A:402:ILE:CG2	2.26	0.64
1:A:290:ARG:HH22	1:A:875:GLN:HB3	1.63	0.63
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.98	0.63
1:A:857:MET:O	1:A:864:GLY:HA2	1.98	0.63
1:A:49:LEU:O	1:A:53:VAL:HG23	1.98	0.62
1:A:515:LYS:HE3	2:A:1002:ATP:N1	2.15	0.62
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.82	0.62
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.81	0.62
1:A:262:LYS:O	1:A:266:LEU:HD23	1.99	0.62
1:A:126:MET:HE2	1:A:139:ARG:HD3	1.82	0.61
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.81	0.61
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASP:O	1:A:212:THR:HG23	1.99	0.61
1:A:395:VAL:O	1:A:396:LEU:HD23	2.00	0.61
1:A:403:ARG:HG2	7:A:2133:HOH:O	2.01	0.60
1:A:402:ILE:HD13	1:A:402:ILE:H	1.65	0.60
1:A:459:VAL:HB	1:A:467:ARG:NE	2.16	0.59
1:A:472:ASN:HB3	1:A:476:ARG:HH12	1.68	0.59
1:A:567:ARG:CD	1:A:570:PRO:HA	2.32	0.59
1:A:873:PHE:CE1	1:A:881:PRO:HG3	2.37	0.59
1:A:529:ARG:CZ	1:A:592:THR:HG21	2.32	0.59
1:A:604:ARG:HG3	1:A:604:ARG:HH11	1.66	0.59
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.85	0.59
1:A:390:ALA:C	1:A:392:GLU:H	2.11	0.58
1:A:739:ASN:HD22	1:A:739:ASN:C	2.12	0.58
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.86	0.58
1:A:924:ARG:HA	1:A:924:ARG:NE	2.17	0.58
1:A:247:THR:H	1:A:250:GLN:NE2	2.02	0.58
1:A:554:THR:HG23	7:A:2155:HOH:O	2.03	0.57
1:A:325:ARG:HH12	1:A:753:ILE:HD11	1.68	0.57
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.04	0.57
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.38	0.57
1:A:654:THR:OG1	1:A:657:GLU:HG3	2.04	0.57
1:A:880:HIS:N	1:A:881:PRO:HD2	2.19	0.57
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.03	0.57
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.33	0.57
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.20	0.56
1:A:383:SER:O	1:A:384:ILE:HD13	2.05	0.56
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.20	0.56
1:A:974:SER:C	1:A:976:PRO:HD2	2.31	0.56
1:A:262:LYS:NZ	1:A:266:LEU:HD21	2.20	0.56
1:A:52:LEU:CD1	1:A:109:GLU:HG3	2.34	0.55
1:A:82:GLU:C	1:A:84:THR:H	2.14	0.55
1:A:881:PRO:HG2	1:A:882:HIS:H	1.71	0.55
1:A:48:SER:OG	1:A:51:GLU:HG3	2.05	0.55
1:A:346:SER:OG	1:A:696:GLU:OE2	2.23	0.55
1:A:769:VAL:HA	5:A:1003:TG1:H231	1.88	0.55
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.88	0.55
1:A:481:LYS:HD3	1:A:484:THR:HG22	1.89	0.55
1:A:236:ARG:HD3	1:A:236:ARG:C	2.31	0.55
1:A:663:LEU:HD12	1:A:663:LEU:N	2.22	0.55
1:A:52:LEU:HD23	1:A:106:VAL:HG13	1.89	0.55
1:A:339:VAL:HG23	1:A:340:GLU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.42	0.55
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.36	0.54
1:A:836:ARG:HG2	1:A:984:LEU:HB3	1.90	0.54
1:A:484:THR:HB	1:A:496:VAL:HG12	1.90	0.54
1:A:865:VAL:HB	1:A:868:HIS:CB	2.37	0.54
1:A:384:ILE:HD12	1:A:395:VAL:HG22	1.90	0.54
1:A:921:SER:HB3	1:A:982:GLU:OE1	2.08	0.54
1:A:668:GLU:O	1:A:671:ARG:HG2	2.08	0.54
1:A:951:ASP:HB2	1:A:952:PRO:HD3	1.90	0.53
1:A:411:VAL:HG22	1:A:454:VAL:HB	1.90	0.53
1:A:604:ARG:HG3	7:A:2033:HOH:O	2.07	0.53
1:A:60:LEU:HD12	1:A:258:GLU:OE1	2.08	0.53
1:A:289:ILE:O	1:A:293:ILE:HG13	2.08	0.53
1:A:459:VAL:HB	1:A:467:ARG:CD	2.39	0.53
1:A:899:MET:O	1:A:903:VAL:HG23	2.08	0.53
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.38	0.53
1:A:184:SER:HB2	7:A:2194:HOH:O	2.08	0.53
1:A:663:LEU:H	1:A:663:LEU:CD1	2.21	0.52
1:A:325:ARG:HH12	1:A:753:ILE:CD1	2.23	0.52
1:A:762:ARG:HD3	1:A:828:LEU:O	2.09	0.52
1:A:8:SER:OG	1:A:11:GLU:HG3	2.09	0.52
1:A:38:HIS:HE1	7:A:2386:HOH:O	1.93	0.52
1:A:311:LEU:N	1:A:312:PRO:HD2	2.24	0.52
1:A:326:MET:HE1	1:A:339:VAL:CG1	2.40	0.52
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.91	0.52
1:A:472:ASN:HB3	1:A:476:ARG:NH1	2.24	0.52
1:A:654:THR:HA	1:A:677:ALA:O	2.08	0.52
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.91	0.52
1:A:195:PRO:HA	7:A:2369:HOH:O	2.07	0.52
1:A:366:MET:CE	1:A:384:ILE:HD11	2.30	0.52
1:A:534:ARG:HG2	1:A:535:VAL:N	2.25	0.52
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.09	0.52
1:A:298:ILE:O	1:A:302:LEU:HB2	2.10	0.51
1:A:863:PRO:C	1:A:865:VAL:H	2.18	0.51
1:A:749:GLU:O	1:A:753:ILE:HG12	2.11	0.51
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.93	0.51
1:A:975:LEU:N	1:A:976:PRO:HD2	2.26	0.51
1:A:212:THR:HG22	1:A:213:ASN:N	2.25	0.51
1:A:379:LEU:HD11	1:A:544:LYS:HD2	1.93	0.51
1:A:757:MET:HA	1:A:760:PHE:CE2	2.45	0.51
1:A:122:TYR:O	1:A:211:GLY:HA2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LEU:O	1:A:968:LEU:HD13	2.11	0.50
1:A:771:GLU:O	1:A:775:ILE:HG12	2.12	0.50
1:A:890:ILE:C	1:A:890:ILE:HD12	2.37	0.50
1:A:263:VAL:HG11	5:A:1003:TG1:O4	2.12	0.50
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.23	0.50
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.50
1:A:303:ALA:O	1:A:307:ILE:HG12	2.11	0.50
1:A:656:ARG:HH11	1:A:656:ARG:HG2	1.76	0.50
1:A:361:MET:HG2	1:A:599:MET:SD	2.52	0.50
1:A:381:GLU:HG2	7:A:2371:HOH:O	2.12	0.50
1:A:574:GLU:H	1:A:574:GLU:CD	2.19	0.50
1:A:895:GLU:CD	1:A:895:GLU:H	2.19	0.50
1:A:273:LEU:HA	1:A:276:ILE:HG13	1.94	0.49
1:A:943:LEU:O	1:A:946:LEU:HB3	2.12	0.49
1:A:428:ASN:OD1	1:A:430:THR:HB	2.12	0.49
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.93	0.49
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.90	0.49
1:A:212:THR:CG2	1:A:213:ASN:N	2.76	0.49
1:A:242:THR:O	1:A:712:LYS:NZ	2.45	0.49
1:A:847:ALA:CA	1:A:973:ILE:HD11	2.37	0.49
1:A:323:THR:HA	1:A:326:MET:HE3	1.93	0.49
1:A:450:GLU:OE2	1:A:450:GLU:HA	2.11	0.49
1:A:571:PRO:HG2	1:A:576:MET:SD	2.53	0.49
1:A:198:ARG:O	1:A:198:ARG:HD3	2.13	0.49
1:A:680:GLU:N	1:A:683:HIS:CD2	2.80	0.49
1:A:701:THR:HA	1:A:718:ILE:O	2.13	0.49
1:A:947:ILE:HG22	1:A:953:LEU:HD13	1.94	0.49
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.77	0.48
1:A:659:ASP:OD1	1:A:683:HIS:HE1	1.96	0.48
1:A:739:ASN:ND2	1:A:741:SER:H	2.10	0.48
1:A:793:LEU:O	1:A:797:LEU:HD13	2.13	0.48
1:A:869:GLN:HB2	1:A:872:HIS:HD2	1.77	0.48
1:A:202:GLN:OE1	1:A:489:ARG:HD3	2.14	0.48
1:A:473:SER:O	1:A:477:GLN:HG2	2.14	0.48
1:A:688:VAL:O	1:A:692:GLN:HG3	2.12	0.48
1:A:905:VAL:O	1:A:909:MET:HG2	2.13	0.48
1:A:262:LYS:HZ3	1:A:266:LEU:HD21	1.79	0.48
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.95	0.48
1:A:50:TRP:O	1:A:54:ILE:HG12	2.14	0.48
1:A:577:VAL:HG23	1:A:583:ARG:NH1	2.29	0.48
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:HA	1:A:328:LYS:CE	2.43	0.48
1:A:60:LEU:O	1:A:64:ILE:HG12	2.14	0.47
1:A:573:ARG:HG3	7:A:2137:HOH:O	2.14	0.47
1:A:96:LEU:C	1:A:96:LEU:HD23	2.39	0.47
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.95	0.47
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.96	0.47
1:A:403:ARG:HB3	1:A:406:GLN:HG3	1.96	0.47
1:A:952:PRO:O	1:A:956:ILE:HG13	2.14	0.47
1:A:573:ARG:HG2	1:A:573:ARG:HH11	1.80	0.47
1:A:656:ARG:HG2	1:A:656:ARG:NH1	2.29	0.47
1:A:278:HIS:HA	1:A:281:ASP:OD2	2.14	0.47
1:A:680:GLU:N	1:A:683:HIS:HD2	2.11	0.47
1:A:880:HIS:H	1:A:881:PRO:HD2	1.78	0.47
1:A:882:HIS:NE2	1:A:885:GLY:HA3	2.30	0.47
1:A:260:LEU:CD2	1:A:307:ILE:HD13	2.44	0.47
1:A:75:LEU:C	1:A:77:TRP:H	2.22	0.47
1:A:534:ARG:NH2	1:A:568:ASP:HB2	2.30	0.47
1:A:1:MET:HE1	1:A:7:LYS:HG3	1.98	0.46
1:A:515:LYS:HE3	2:A:1002:ATP:C2	2.50	0.46
1:A:725:ALA:O	1:A:729:THR:HG23	2.15	0.46
1:A:1:MET:CE	1:A:7:LYS:HG3	2.44	0.46
1:A:71:ILE:O	1:A:75:LEU:HD13	2.16	0.46
1:A:366:MET:HA	1:A:596:VAL:O	2.16	0.46
1:A:402:ILE:HD13	1:A:402:ILE:N	2.30	0.46
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.98	0.46
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.44	0.46
1:A:800:ASP:C	1:A:803:PRO:HD2	2.41	0.46
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.98	0.46
1:A:534:ARG:HH21	1:A:568:ASP:CB	2.28	0.46
1:A:858:TYR:CD1	1:A:858:TYR:N	2.84	0.46
1:A:442:GLU:OE2	1:A:515:LYS:NZ	2.49	0.46
1:A:95:LEU:HD22	1:A:99:ILE:HD11	1.98	0.46
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.50	0.46
1:A:346:SER:HB3	1:A:697:ILE:H	1.80	0.45
1:A:295:TYR:O	1:A:298:ILE:HG12	2.17	0.45
1:A:274:ILE:O	1:A:274:ILE:HG22	2.14	0.45
1:A:604:ARG:HB2	1:A:607:VAL:CG2	2.46	0.45
1:A:149:ASP:CB	7:A:2356:HOH:O	2.60	0.45
1:A:459:VAL:C	1:A:461:ASN:H	2.23	0.45
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.80	0.45
1:A:534:ARG:HH21	1:A:568:ASP:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.32	0.44
1:A:124:PRO:HB3	1:A:158:LYS:HB3	1.99	0.44
1:A:516:GLY:HA2	2:A:1002:ATP:N3	2.33	0.44
1:A:420:CYS:SG	1:A:515:LYS:HE2	2.58	0.44
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.99	0.44
1:A:114:ASN:OD1	1:A:117:GLU:HG2	2.17	0.44
1:A:209:PHE:O	1:A:212:THR:HB	2.18	0.44
1:A:361:MET:HE2	1:A:440:ALA:HB3	2.00	0.44
1:A:611:ILE:O	1:A:615:ARG:HG3	2.18	0.44
1:A:967:TRP:O	1:A:970:VAL:HB	2.17	0.44
1:A:604:ARG:CG	1:A:604:ARG:NH1	2.79	0.43
1:A:668:GLU:CD	1:A:671:ARG:HD3	2.43	0.43
1:A:52:LEU:CD2	1:A:106:VAL:HG13	2.49	0.43
1:A:2:GLU:HG3	7:A:2291:HOH:O	2.19	0.43
1:A:380:ASN:HD22	1:A:382:PHE:HZ	1.66	0.43
1:A:688:VAL:HG11	1:A:713:LYS:HG2	2.01	0.43
1:A:960:LYS:O	1:A:961:ALA:C	2.61	0.43
1:A:126:MET:CE	1:A:139:ARG:HD3	2.49	0.43
1:A:325:ARG:HD2	1:A:749:GLU:OE2	2.19	0.43
1:A:628:ASN:ND2	1:A:631:THR:H	2.17	0.43
1:A:788:ILE:HD13	1:A:958:LYS:HD2	2.01	0.43
1:A:855:TRP:HA	1:A:859:ALA:CB	2.49	0.43
1:A:67:LEU:HD12	1:A:67:LEU:O	2.19	0.43
1:A:115:ALA:HB1	1:A:239:MET:HE1	2.00	0.43
1:A:795:VAL:HA	1:A:799:THR:HB	2.01	0.43
1:A:369:ILE:HG13	1:A:528:VAL:HG11	1.99	0.43
1:A:133:ASP:O	1:A:134:ARG:HG3	2.19	0.42
1:A:388:THR:OG1	1:A:389:TYR:N	2.52	0.42
1:A:6:SER:HA	1:A:194:VAL:O	2.20	0.42
1:A:273:LEU:HA	1:A:276:ILE:CG1	2.48	0.42
1:A:922:LEU:HD22	1:A:927:PRO:HG3	2.02	0.42
1:A:990:ASN:HD21	6:A:1012:PTY:C2	2.32	0.42
1:A:724:THR:O	1:A:728:LYS:HG3	2.20	0.42
1:A:100:ALA:O	1:A:104:VAL:HG23	2.20	0.42
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.01	0.42
1:A:692:GLN:C	1:A:694:TYR:H	2.27	0.42
1:A:273:LEU:HA	1:A:276:ILE:CD1	2.50	0.42
1:A:326:MET:HG2	1:A:749:GLU:HG2	2.01	0.42
1:A:360:GLN:HB2	7:A:2237:HOH:O	2.20	0.42
1:A:988:ALA:O	1:A:992:LEU:HB2	2.19	0.42
1:A:607:VAL:O	1:A:611:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ALA:HB3	1:A:709:PRO:HD3	2.02	0.41
1:A:754:TYR:HD1	1:A:757:MET:HE3	1.85	0.41
1:A:917:SER:OG	1:A:920:GLN:HB2	2.20	0.41
1:A:775:ILE:C	1:A:778:THR:HG22	2.44	0.41
1:A:950:VAL:O	1:A:954:PRO:HD2	2.20	0.41
1:A:415:THR:HA	1:A:475:ILE:HG21	2.01	0.41
1:A:434:TYR:HE1	1:A:464:LYS:HE3	1.86	0.41
1:A:115:ALA:CB	1:A:239:MET:HE1	2.51	0.41
1:A:790:VAL:HG12	1:A:957:PHE:CD1	2.56	0.41
1:A:428:ASN:CG	1:A:431:LYS:HD3	2.46	0.41
1:A:950:VAL:O	1:A:952:PRO:HD2	2.20	0.41
1:A:554:THR:O	1:A:554:THR:HG22	2.20	0.41
1:A:573:ARG:HG2	1:A:573:ARG:NH1	2.36	0.41
1:A:43:ALA:HA	1:A:120:LYS:HZ3	1.85	0.41
1:A:175:VAL:HG12	1:A:177:GLN:HG3	2.02	0.41
1:A:269:VAL:O	1:A:273:LEU:HG	2.20	0.41
1:A:336:LEU:O	1:A:339:VAL:HG22	2.21	0.41
1:A:951:ASP:O	1:A:952:PRO:C	2.64	0.41
1:A:290:ARG:NH2	1:A:875:GLN:HB3	2.33	0.41
1:A:534:ARG:HH21	1:A:568:ASP:CG	2.29	0.41
1:A:361:MET:CG	1:A:599:MET:SD	3.08	0.40
1:A:382:PHE:CD1	1:A:382:PHE:N	2.89	0.40
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.51	0.40
1:A:41:LEU:HD13	1:A:236:ARG:HG3	2.04	0.40
1:A:406:GLN:HG2	7:A:2224:HOH:O	2.22	0.40
1:A:518:PRO:HB3	1:A:549:ILE:HD13	2.02	0.40
1:A:529:ARG:HH21	1:A:534:ARG:HB2	1.86	0.40
1:A:774:CYS:O	1:A:778:THR:HG22	2.21	0.40
1:A:486:GLU:CD	1:A:486:GLU:H	2.28	0.40
1:A:717:GLY:O	1:A:731:SER:HB2	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%)	932 (94%)	54 (5%)	7 (1%)	18	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	951	ASP
1	A	858	TYR
1	A	869	GLN
1	A	505	ARG
1	A	430	THR
1	A	863	PRO
1	A	391	PRO

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%)	28	27

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

Mol	Chain	Res	Type
1	A	22	THR
1	A	44	GLU
1	A	60	LEU
1	A	95	LEU
1	A	113	GLU
1	A	189	LYS
1	A	198	ARG
1	A	253	LEU
1	A	319	LEU
1	A	328	LYS
1	A	380	ASN
1	A	394	GLU

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Mol	Chain	Res	Type
1	A	402	ILE
1	A	413	LEU
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	490	ASP
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	604	ARG
1	A	612	GLN
1	A	647	GLU
1	A	656	ARG
1	A	679	VAL
1	A	691	LEU
1	A	789	PRO
1	A	802	LEU
1	A	822	ARG
1	A	860	GLU
1	A	876	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	360	GLN
1	A	461	ASN
1	A	472	ASN
1	A	510	ASN
1	A	628	ASN
1	A	683	HIS
1	A	739	ASN
1	A	914	ASN
1	A	919	ASN
1	A	920	GLN
1	A	966	GLN
1	A	990	ASN

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 8 ligands modelled in this entry, 3 are 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$
6	PTY	A	1011	-	18,18,49	1.28	3 (16%)	21,23,54	1.17	2 (9%)
5	TG1	A	1003	-	44,48,48	1.70	13 (29%)	47,72,72	1.66	9 (19%)
6	PTY	A	1013	-	18,18,49	1.26	3 (16%)	21,23,54	1.35	3 (14%)
6	PTY	A	1012	-	18,18,49	1.32	3 (16%)	21,23,54	1.53	4 (19%)
2	ATP	A	1002	3	32,33,33	1.59	5 (15%)	48,52,52	0.99	2 (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
6	PTY	A	1011	-	-	5/20/20/53	-
5	TG1	A	1003	-	-	10/33/99/99	0/3/3/3
6	PTY	A	1013	-	-	10/20/20/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PTY	A	1012	-	-	6/20/20/53	-
2	ATP	A	1002	3	-	2/22/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	ATP	PB-O3A	4.86	1.64	1.59
5	A	1003	TG1	O4-C21	3.99	1.29	1.21
5	A	1003	TG1	C3-C4	3.67	1.55	1.50
2	A	1002	ATP	C2-N1	3.63	1.40	1.33
5	A	1003	TG1	C34-C11	3.63	1.58	1.53
2	A	1002	ATP	C4-N3	3.62	1.41	1.34
5	A	1003	TG1	C1-C2	3.42	1.60	1.54
5	A	1003	TG1	C1-C5	2.96	1.56	1.51
5	A	1003	TG1	C9-C10	2.88	1.59	1.54
6	A	1012	PTY	C1-C6	2.83	1.59	1.50
5	A	1003	TG1	C11-C7	2.76	1.59	1.55
6	A	1011	PTY	C1-C6	2.75	1.59	1.50
2	A	1002	ATP	PA-O3A	2.55	1.62	1.59
6	A	1013	PTY	C1-C6	2.45	1.58	1.50
6	A	1013	PTY	P1-O13	2.42	1.59	1.50
2	A	1002	ATP	PB-O3B	2.40	1.62	1.59
6	A	1011	PTY	P1-O13	2.38	1.59	1.50
5	A	1003	TG1	C31-C10	2.36	1.57	1.52
5	A	1003	TG1	O7-C27	2.36	1.40	1.34
6	A	1012	PTY	P1-O13	2.28	1.58	1.50
5	A	1003	TG1	O1-C13	2.28	1.40	1.34
6	A	1013	PTY	C5-C6	2.25	1.57	1.50
5	A	1003	TG1	C2-C3	2.25	1.57	1.53
6	A	1012	PTY	C5-C6	2.18	1.57	1.50
5	A	1003	TG1	C9-C8	2.17	1.55	1.52
5	A	1003	TG1	O6-C7	2.13	1.46	1.43
6	A	1011	PTY	C5-C6	2.07	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	TG1	C10-O9-C32	5.76	134.87	121.36
6	A	1013	PTY	O7-C8-C11	3.78	117.83	111.09
5	A	1003	TG1	O12-C12-C11	-3.71	124.52	128.28
6	A	1012	PTY	O12-P1-O13	-3.68	95.33	112.44
6	A	1011	PTY	O7-C8-C11	3.40	117.14	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	TG1	O7-C8-C9	3.18	112.32	106.63
6	A	1012	PTY	O7-C8-C11	3.09	116.60	111.09
5	A	1003	TG1	O5-C12-O12	2.87	125.31	121.60
5	A	1003	TG1	O3-C21-O4	2.77	128.56	123.40
5	A	1003	TG1	C7-C6-C5	2.69	122.47	115.41
5	A	1003	TG1	C24-C22-C21	2.68	130.85	120.79
2	A	1002	ATP	N3-C2-N1	-2.46	124.86	128.58
6	A	1011	PTY	O4-C1-C6	2.41	115.34	108.40
2	A	1002	ATP	C2'-C1'-N9	2.40	119.28	113.30
6	A	1012	PTY	O4-C1-C6	2.37	115.23	108.40
6	A	1013	PTY	P1-O14-C5	2.29	134.46	121.35
5	A	1003	TG1	C23-C22-C21	-2.25	110.33	116.12
5	A	1003	TG1	O4-C21-C22	-2.22	118.23	125.28
6	A	1012	PTY	O14-P1-O13	2.15	117.46	108.94
6	A	1013	PTY	O4-C1-C6	2.12	114.52	108.40

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1011	PTY	N1-C2-C3-O11
6	A	1011	PTY	C11-C8-O7-C6
6	A	1013	PTY	N1-C2-C3-O11
6	A	1013	PTY	C11-C8-O7-C6
6	A	1013	PTY	C5-O14-P1-O11
6	A	1013	PTY	C5-O14-P1-O12
6	A	1013	PTY	C5-O14-P1-O13
6	A	1012	PTY	C11-C8-O7-C6
6	A	1011	PTY	O10-C8-O7-C6
6	A	1013	PTY	O10-C8-O7-C6
6	A	1011	PTY	C31-C30-O4-C1
6	A	1012	PTY	C31-C30-O4-C1
6	A	1013	PTY	C31-C30-O4-C1
6	A	1012	PTY	O10-C8-O7-C6
6	A	1011	PTY	O30-C30-O4-C1
6	A	1012	PTY	O30-C30-O4-C1
6	A	1013	PTY	O30-C30-O4-C1
5	A	1003	TG1	O3-C21-C22-C23
5	A	1003	TG1	O3-C21-C22-C24
5	A	1003	TG1	O4-C21-C22-C23
5	A	1003	TG1	C15-C16-C17-C18
5	A	1003	TG1	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
6	A	1013	PTY	O4-C1-C6-O7
2	A	1002	ATP	PA-O3A-PB-O1B
5	A	1003	TG1	O4-C21-C22-C24
6	A	1012	PTY	C5-O14-P1-O12
6	A	1013	PTY	O4-C1-C6-C5
5	A	1003	TG1	C22-C21-O3-C3
5	A	1003	TG1	C9-C10-O9-C32
6	A	1012	PTY	O14-C5-C6-O7
5	A	1003	TG1	O1-C13-C14-C15
5	A	1003	TG1	O2-C13-C14-C15
2	A	1002	ATP	PA-O3A-PB-O2B

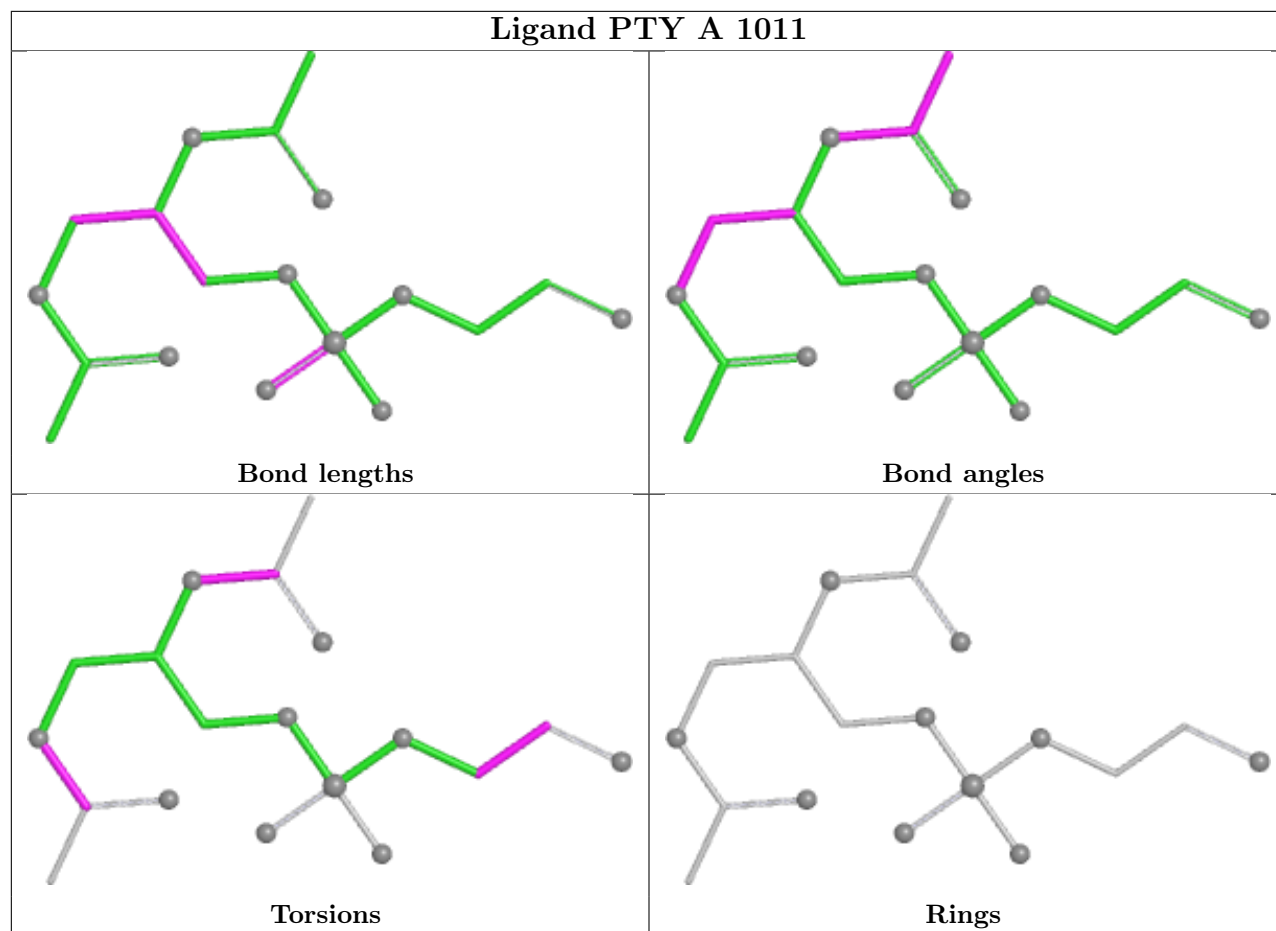
There are no ring outliers.

3 monomers are involved in 6 short contacts:

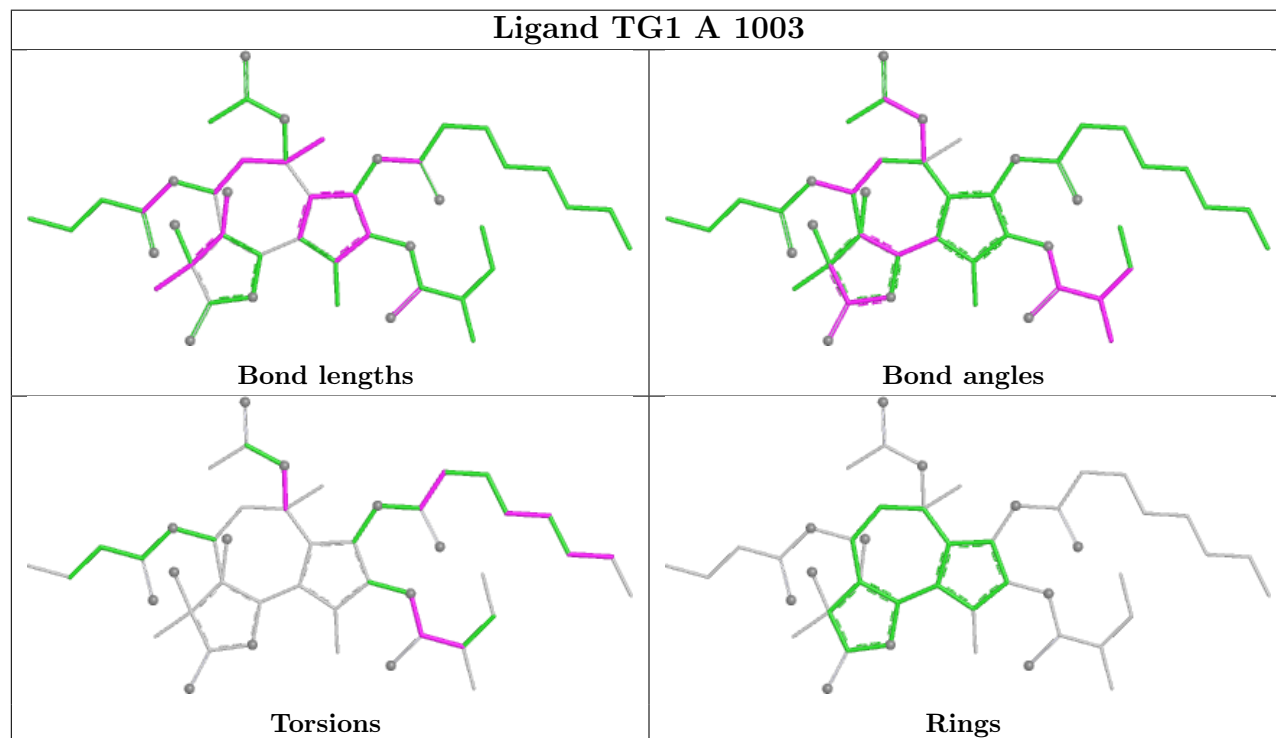
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	TG1	2	0
6	A	1012	PTY	1	0
2	A	1002	ATP	3	0

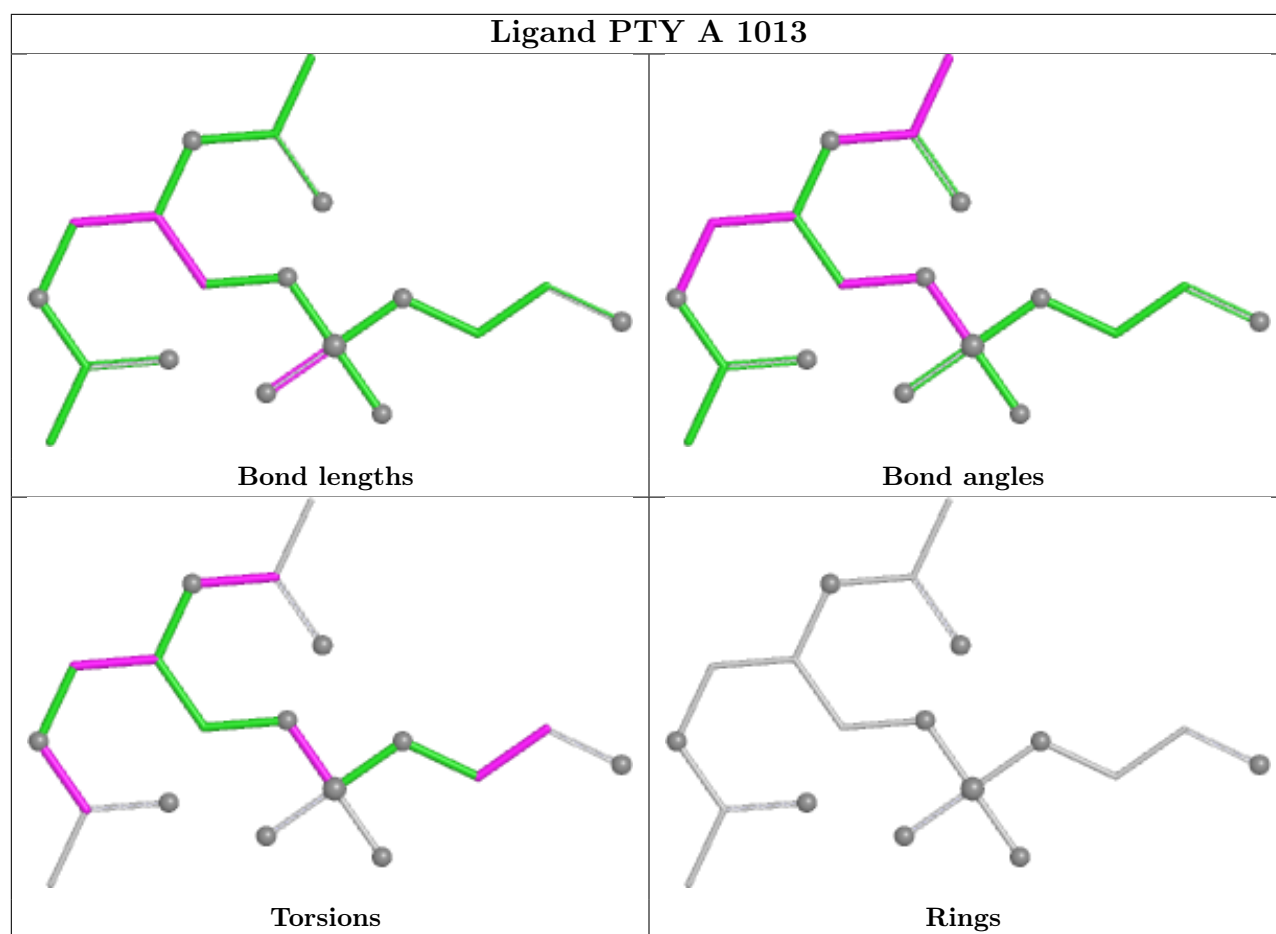
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

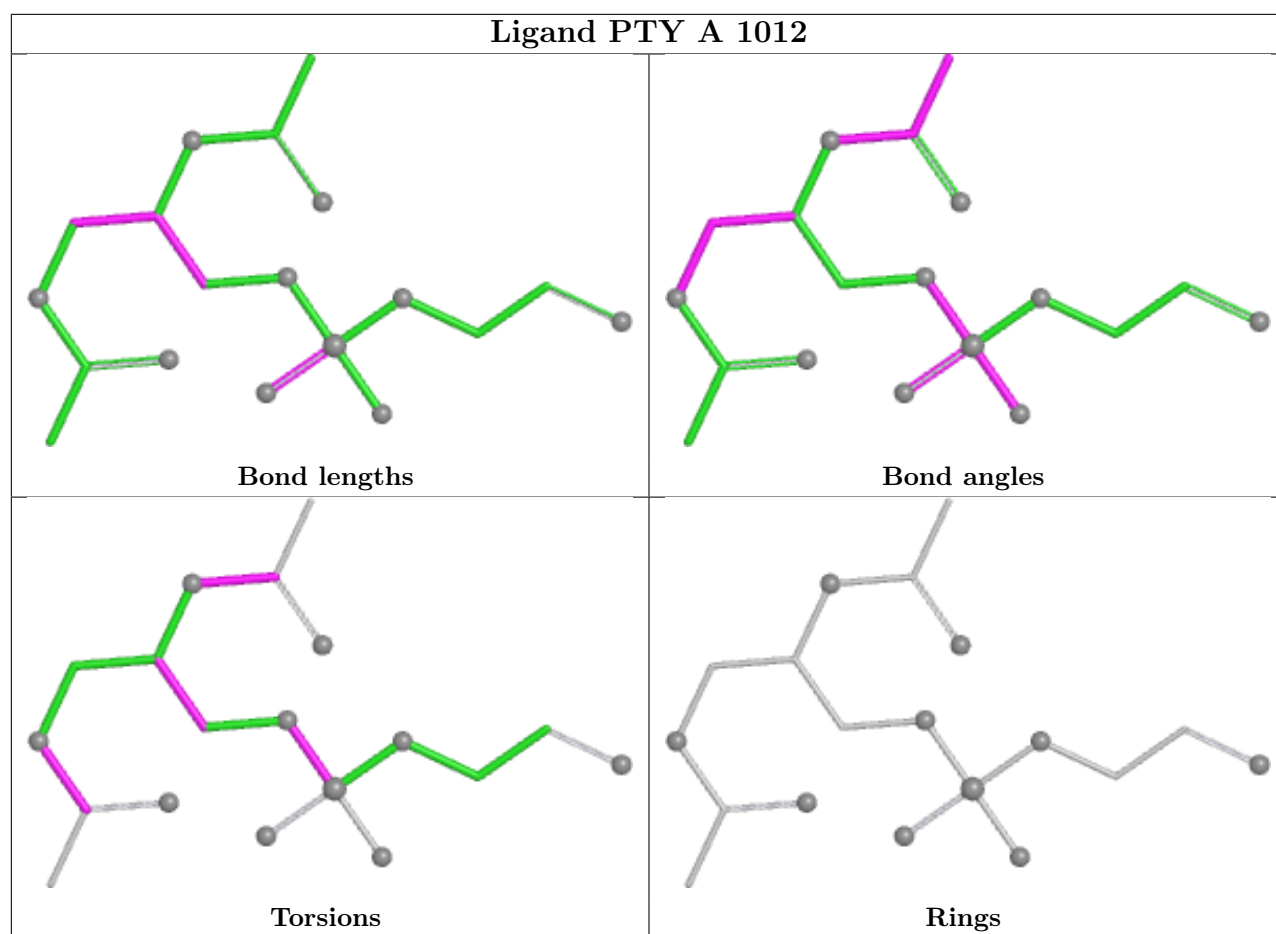
Ligand PTY A 1011

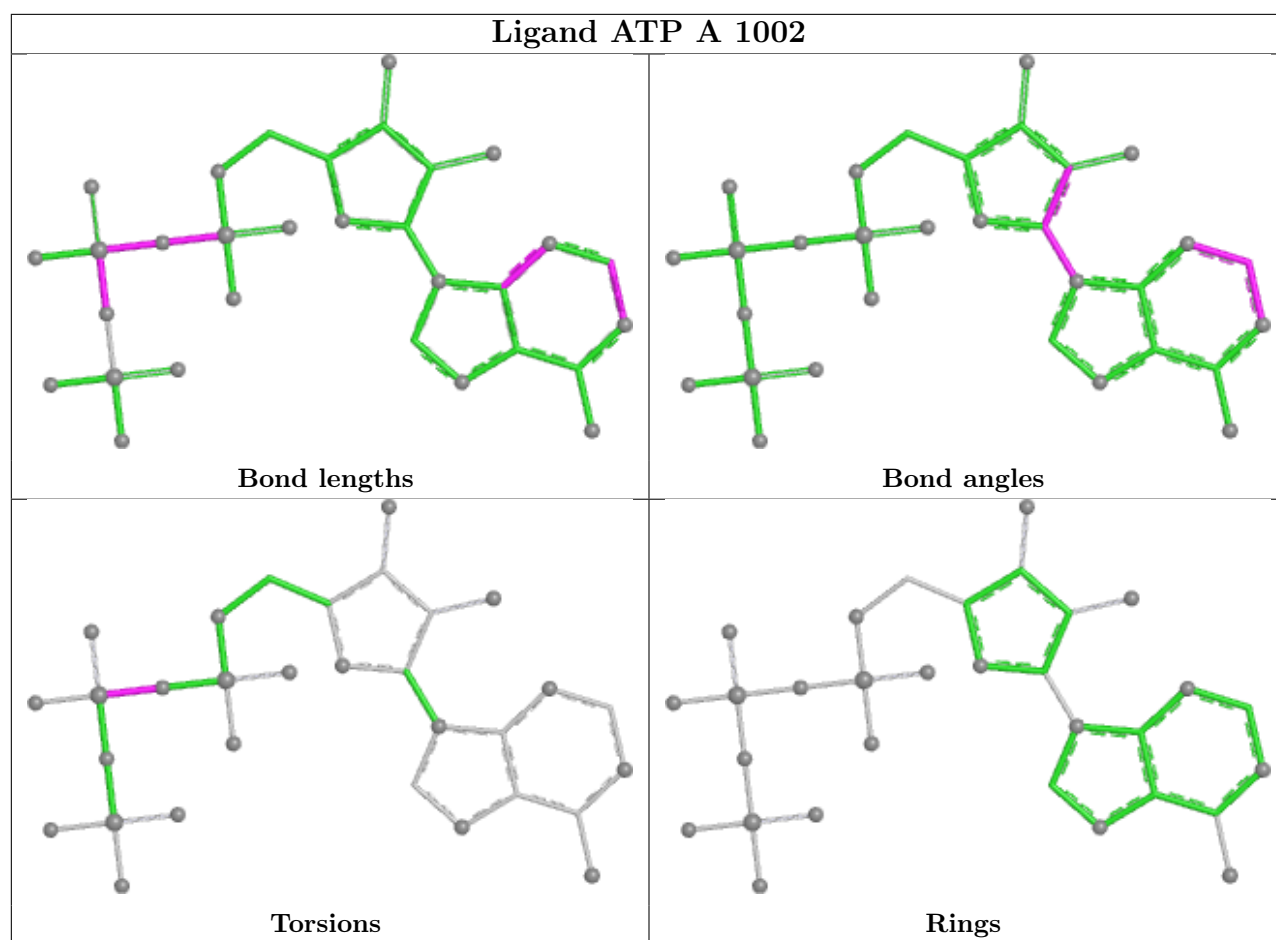


Ligand TG1 A 1003









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	994/995 (99%)	0.49	73 (7%) 21 24	28, 55, 107, 152	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	865	VAL	8.9
1	A	873	PHE	8.1
1	A	85	ILE	7.7
1	A	883	PHE	6.8
1	A	508	VAL	5.8
1	A	507	ALA	4.9
1	A	870	LEU	4.9
1	A	506	ALA	4.8
1	A	864	GLY	4.6
1	A	866	THR	4.5
1	A	867	TYR	4.3
1	A	288	TRP	4.1
1	A	888	CYS	4.1
1	A	503	SER	4.0
1	A	882	HIS	4.0
1	A	874	MET	3.9
1	A	402	ILE	3.8
1	A	279	PHE	3.8
1	A	952	PRO	3.6
1	A	877	THR	3.6
1	A	950	VAL	3.5
1	A	880	HIS	3.5
1	A	76	ALA	3.5
1	A	459	VAL	3.4
1	A	504	SER	3.4
1	A	868	HIS	3.4
1	A	276	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	872	HIS	3.2
1	A	869	GLN	3.2
1	A	886	LEU	3.1
1	A	890	ILE	3.1
1	A	991	TYR	3.0
1	A	951	ASP	3.0
1	A	77	TRP	2.9
1	A	295	TYR	2.9
1	A	283	VAL	2.8
1	A	84	THR	2.8
1	A	863	PRO	2.8
1	A	879	ASP	2.8
1	A	861	ASP	2.8
1	A	871	THR	2.8
1	A	401	PRO	2.8
1	A	427	PHE	2.7
1	A	457	THR	2.7
1	A	876	CYS	2.7
1	A	579	ASP	2.7
1	A	852	ALA	2.6
1	A	46	GLY	2.6
1	A	398	ASN	2.6
1	A	881	PRO	2.6
1	A	973	ILE	2.6
1	A	384	ILE	2.5
1	A	993	GLU	2.5
1	A	78	PHE	2.4
1	A	112	ALA	2.4
1	A	465	VAL	2.4
1	A	875	GLN	2.3
1	A	955	MET	2.3
1	A	286	GLY	2.3
1	A	856	PHE	2.2
1	A	289	ILE	2.2
1	A	778	THR	2.2
1	A	992	LEU	2.2
1	A	62	VAL	2.2
1	A	923	MET	2.2
1	A	92	PHE	2.1
1	A	182	GLY	2.1
1	A	298	ILE	2.1
1	A	462	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	TYR	2.1
1	A	509	GLY	2.1
1	A	281	ASP	2.0
1	A	400	LYS	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](#)

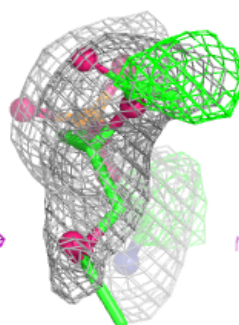
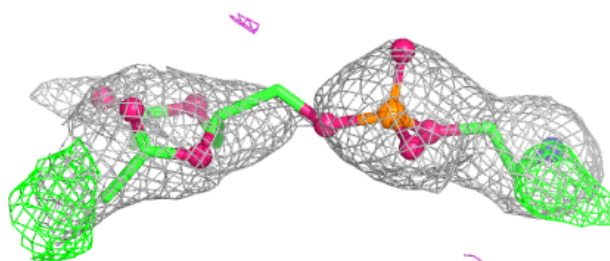
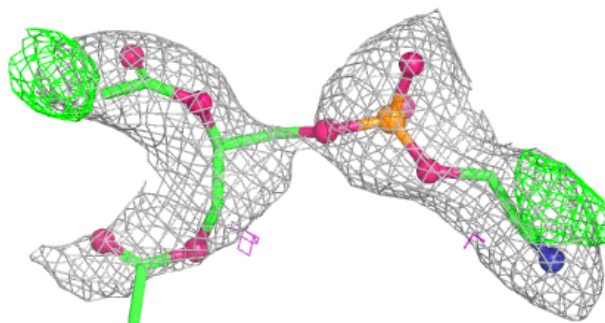
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	PTY	A	1013	19/50	0.63	0.17	99,108,108,108	0
6	PTY	A	1012	19/50	0.66	0.25	109,113,116,116	0
6	PTY	A	1011	19/50	0.78	0.18	114,115,117,117	0
5	TG1	A	1003	46/46	0.85	0.14	61,68,84,86	0
3	MG	A	1001	1/1	0.88	0.07	65,65,65,65	0
2	ATP	A	1002	31/31	0.95	0.07	42,52,62,64	0
4	NA	A	1000	1/1	0.98	0.06	43,43,43,43	0
3	MG	A	997	1/1	1.00	0.03	58,58,58,58	0

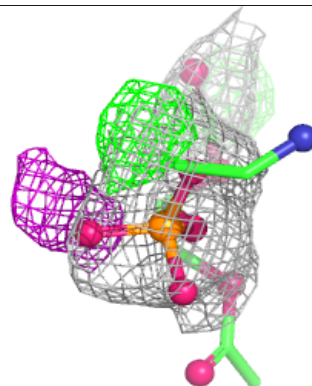
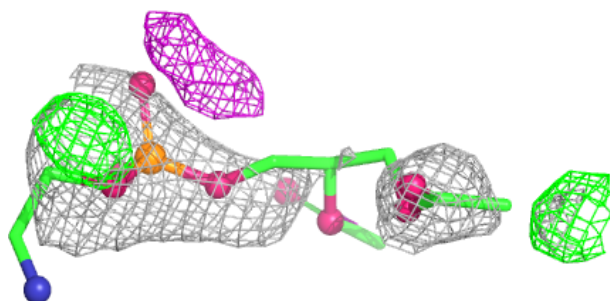
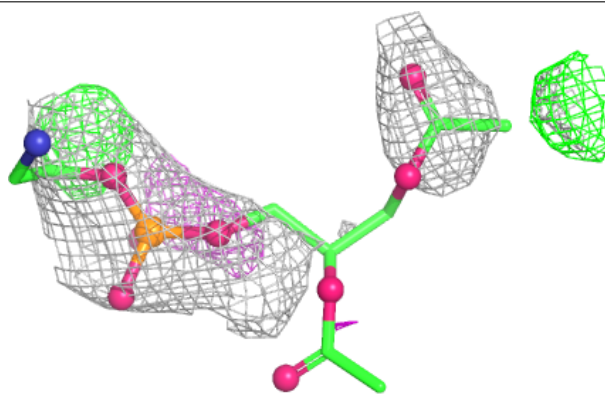
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

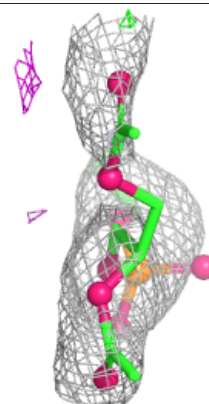
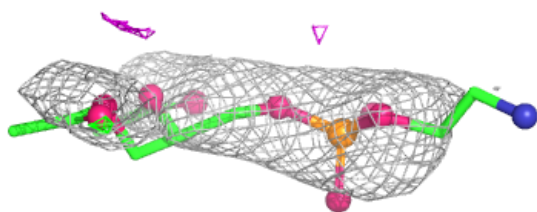
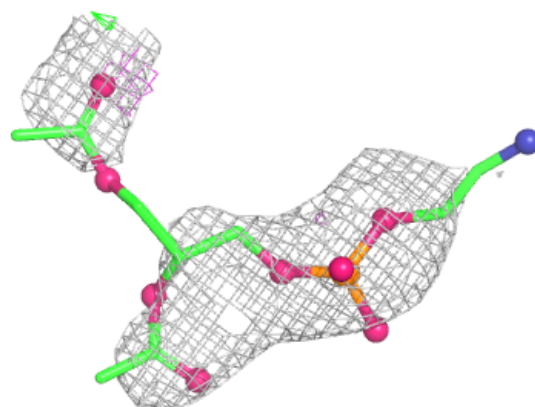
**Electron density around PTY A 1012:**

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

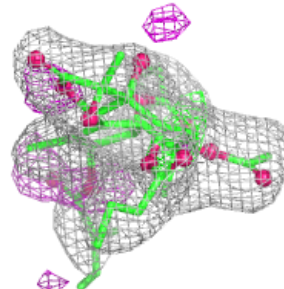
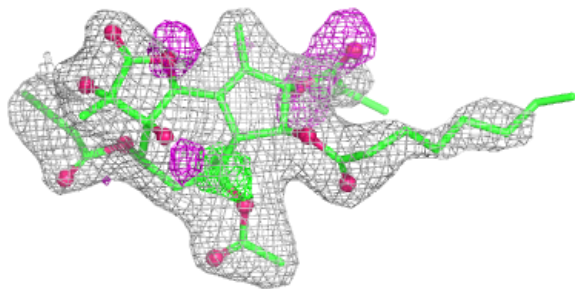
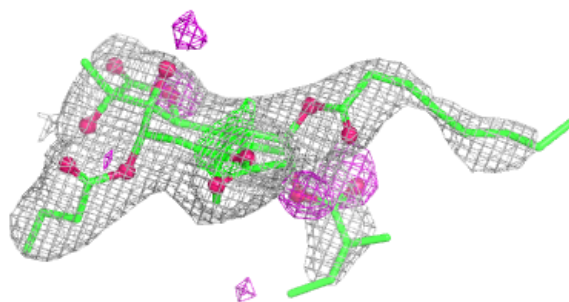


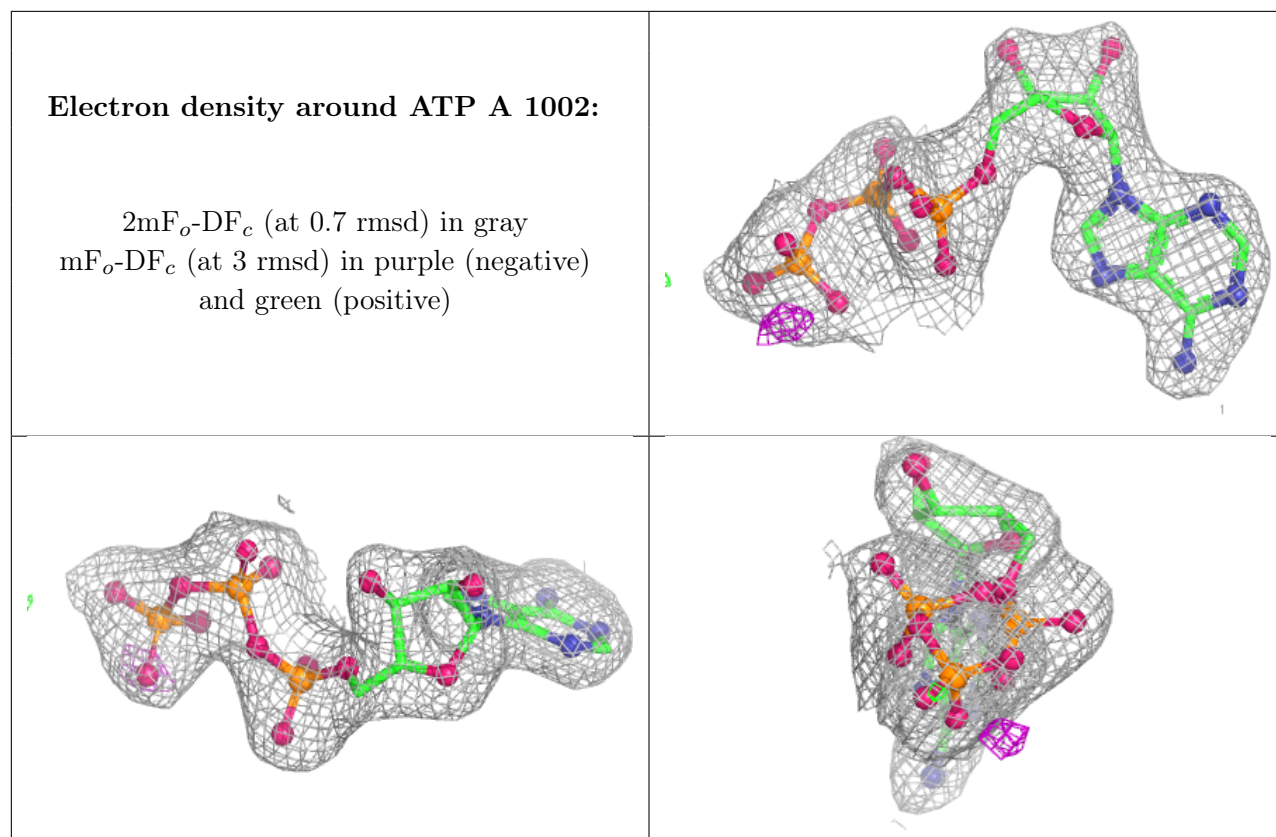
Electron density around PTY A 1011:

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

**Electron density around 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.