



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:53 AM BST

PDB ID : 7BT2
Title : Crystal structure of the SERCA2a in the E2.ATP state
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Deposited on : 2020-03-31
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

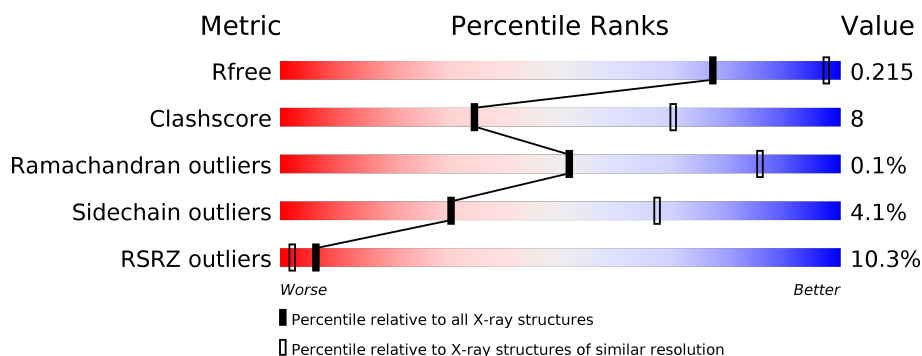
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	997	<div> <div>10%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCW	A	1003	-	-	-	X
4	PCW	A	1004	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PCW	A	1005	-	-	-	X
4	PCW	A	1006	-	-	-	X

2 Entry composition [i](#)

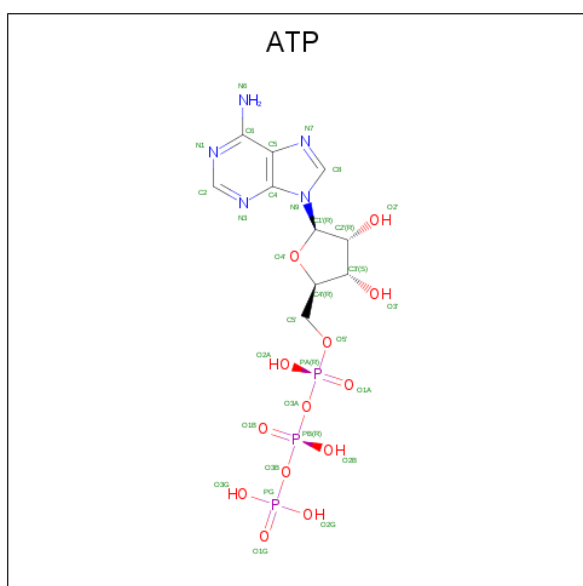
There are 6 unique types of molecules in this entry. The entry contains 7869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

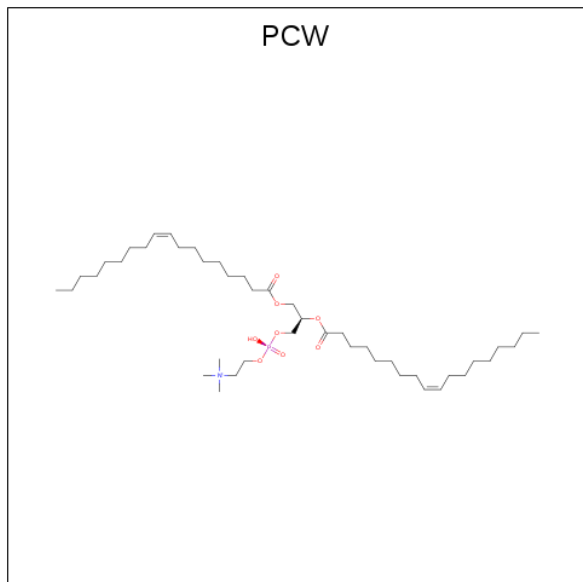
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	991	Total	C	N	O	S	0	0	0
			7639	4858	1284	1441	56			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by author).

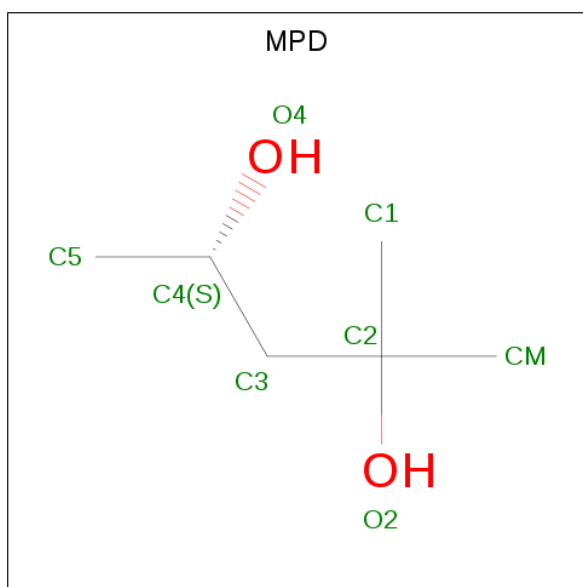


- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.60 Å 270.38 Å 97.34 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.00 14.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (14.99-3.00) 97.3 (14.99-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.61 Å)	Xtriage
Refinement program	PHENIX 1.9_1692, CNS	Depositor
R, R_{free}	0.192 , 0.222 0.193 , 0.215	Depositor DCC
R_{free} test set	2406 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7869	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: MPD, K, PCW, ATP

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	0.69	1/7778 (0.0%)	0.61	0/10552

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	CYS	CB-SG	-5.49	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	ILE	Peptide

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	7639	0	7752	129	0
2	A	31	0	12	0	0
3	A	1	0	0	0	0
4	A	88	0	72	3	0
5	A	8	0	14	0	0
6	A	102	0	0	2	0
All	All	7869	0	7850	130	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 8.

All (130) 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:862:PRO:HG2	1:A:889:ILE:HG21	1.41	1.02
1:A:679:GLU:H	1:A:682:HIS:HD2	1.14	0.93
1:A:61:LEU:HD13	1:A:303:ALA:HB1	1.55	0.86
1:A:987:ALA:HA	1:A:991:LEU:HB2	1.69	0.74
1:A:986:VAL:O	1:A:990:TYR:HB2	1.87	0.74
1:A:856:ILE:O	1:A:863:ARG:HD3	1.90	0.72
1:A:828:ILE:HA	1:A:832:LEU:HD23	1.72	0.71
1:A:989:ASN:ND2	1:A:989:ASN:O	2.22	0.71
1:A:61:LEU:HD12	1:A:307:ILE:HD11	1.74	0.69
1:A:484:THR:HB	1:A:496:VAL:HG12	1.75	0.68
1:A:679:GLU:H	1:A:682:HIS:CD2	2.04	0.66
1:A:61:LEU:CD1	1:A:307:ILE:HD11	2.25	0.66
1:A:48:THR:O	1:A:52:LEU:HB2	1.96	0.66
1:A:357:THR:O	1:A:603:ARG:NH1	2.29	0.66
1:A:938:LEU:O	1:A:942:LEU:HG	1.97	0.64
1:A:64:ILE:HG23	1:A:67:LEU:HD21	1.80	0.63
1:A:579:ASP:HB3	1:A:582:ASN:ND2	2.13	0.62
1:A:75:LEU:HD21	1:A:290:ARG:NH2	2.14	0.61
1:A:60:LEU:HD23	1:A:63:ARG:HH21	1.63	0.61
1:A:527:ILE:HD13	1:A:540:VAL:HG11	1.83	0.61
1:A:75:LEU:O	1:A:79:GLU:N	2.34	0.60
1:A:571:ARG:HE	1:A:571:ARG:N	2.01	0.59
1:A:52:LEU:HD23	1:A:106:VAL:HG22	1.85	0.59
1:A:61:LEU:HD12	1:A:307:ILE:CD1	2.33	0.59
1:A:342:LEU:HD12	1:A:715:ILE:HD13	1.85	0.59
1:A:543:LYS:NZ	6:A:1103:HOH:O	2.36	0.58
1:A:772:VAL:HG23	1:A:844:GLY:HA3	1.85	0.58
1:A:604:ILE:HG13	1:A:605:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LYS:NZ	6:A:1106:HOH:O	2.37	0.57
1:A:47:LYS:HA	1:A:110:ARG:HH22	1.69	0.57
1:A:831:TRP:HB2	4:A:1004:PCW:O1P	2.04	0.57
1:A:961:LEU:HD11	1:A:966:TRP:HE3	1.70	0.55
1:A:918:ASN:O	1:A:988:ARG:HD2	2.07	0.55
1:A:776:LEU:HB3	1:A:848:VAL:HG21	1.88	0.55
1:A:351:ASP:HA	1:A:623:ILE:O	2.07	0.54
1:A:189:LYS:HG3	1:A:205:LYS:O	2.08	0.53
1:A:572:ARG:HD2	1:A:577:LEU:HD11	1.91	0.53
1:A:107:TRP:O	1:A:111:ASN:ND2	2.42	0.53
1:A:274:ILE:O	1:A:276:ILE:HG22	2.09	0.53
1:A:412:GLU:OE1	1:A:528:ARG:HD2	2.10	0.52
1:A:342:LEU:HD21	1:A:745:ALA:HB1	1.92	0.52
1:A:863:ARG:HB2	1:A:863:ARG:NH1	2.25	0.52
1:A:696:ILE:HD11	1:A:823:PRO:HG3	1.92	0.51
1:A:189:LYS:NZ	1:A:207:MET:O	2.31	0.51
1:A:59:ASP:OD2	1:A:101:ASN:ND2	2.44	0.51
1:A:483:PHE:CE1	1:A:572:ARG:HD3	2.45	0.51
1:A:61:LEU:HD13	1:A:303:ALA:CB	2.32	0.51
1:A:1:MET:HE1	1:A:7:LYS:HG3	1.93	0.51
1:A:48:THR:OG1	1:A:51:GLU:HB3	2.11	0.50
1:A:230:THR:HG22	1:A:232:ILE:H	1.76	0.50
1:A:65:LEU:HG	1:A:94:ILE:HG23	1.94	0.50
1:A:863:ARG:HG3	1:A:863:ARG:O	2.12	0.50
1:A:412:GLU:OE2	1:A:565:THR:HG21	2.11	0.50
1:A:989:ASN:C	1:A:989:ASN:HD22	2.13	0.49
1:A:326:MET:HG3	1:A:748:GLU:HG2	1.94	0.49
1:A:752:ILE:O	1:A:756:MET:HG3	2.12	0.49
1:A:276:ILE:O	1:A:276:ILE:HG23	2.13	0.49
1:A:201:ASN:HA	1:A:204:LYS:HD3	1.94	0.49
1:A:301:ALA:HA	1:A:788:PRO:HG3	1.94	0.49
1:A:759:PHE:HA	1:A:762:TYR:HB3	1.95	0.49
1:A:377:CYS:HB3	1:A:540:VAL:HG22	1.95	0.48
1:A:349:CYS:HB3	1:A:623:ILE:HD12	1.95	0.48
1:A:45:GLU:C	1:A:47:LYS:H	2.17	0.48
1:A:653:THR:HA	1:A:676:ALA:O	2.14	0.48
1:A:812:ASP:N	1:A:812:ASP:OD1	2.44	0.48
1:A:163:ILE:HB	1:A:208:LEU:HB2	1.95	0.48
1:A:986:VAL:HG13	1:A:987:ALA:N	2.29	0.47
1:A:436:LYS:HE2	1:A:438:GLY:O	2.15	0.47
1:A:571:ARG:HE	1:A:571:ARG:H	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:ALA:H	1:A:863:ARG:NH1	2.12	0.47
1:A:483:PHE:CD1	1:A:572:ARG:HD3	2.49	0.47
1:A:319:LEU:HD22	1:A:339:VAL:HG21	1.95	0.47
1:A:756:MET:HA	1:A:759:PHE:CE1	2.49	0.47
1:A:769:GLY:HA3	1:A:843:VAL:HG22	1.97	0.47
1:A:755:ASN:HB3	1:A:807:GLY:HA2	1.97	0.47
1:A:670:LEU:HD13	1:A:693:PHE:CE2	2.50	0.46
1:A:65:LEU:HD13	1:A:300:VAL:HG11	1.98	0.46
1:A:528:ARG:HH22	1:A:567:ASP:CG	2.19	0.46
1:A:943:HIS:O	1:A:946:ILE:HG22	2.15	0.46
1:A:794:VAL:HA	1:A:798:THR:HB	1.97	0.46
1:A:283:VAL:HG13	1:A:284:HIS:CD2	2.51	0.46
1:A:736:ASP:O	1:A:737:ASP:HB2	2.16	0.46
1:A:162:ASP:OD2	1:A:231:GLU:HG2	2.17	0.45
1:A:658:ASP:OD2	1:A:682:HIS:HE1	1.99	0.45
1:A:95:LEU:HD12	1:A:98:LEU:HD12	1.97	0.45
1:A:783:PRO:HD3	1:A:869:LEU:HG	1.98	0.45
1:A:135:LYS:H	1:A:135:LYS:HD3	1.81	0.45
1:A:119:LEU:HD22	1:A:323:THR:HG21	1.98	0.45
1:A:923:ARG:HD2	1:A:923:ARG:HA	1.71	0.45
1:A:483:PHE:CE1	1:A:572:ARG:HB2	2.52	0.44
1:A:734:LEU:HD22	1:A:741:THR:HB	1.99	0.44
1:A:267:ILE:O	1:A:271:VAL:HG23	2.18	0.44
1:A:75:LEU:HD21	1:A:290:ARG:HH21	1.82	0.44
1:A:307:ILE:HG21	1:A:307:ILE:HD13	1.65	0.44
1:A:50:LEU:O	1:A:54:ILE:HG13	2.17	0.44
1:A:20:GLU:OE2	1:A:166:THR:CB	2.66	0.44
1:A:23:GLY:HA3	1:A:130:TYR:O	2.18	0.43
1:A:527:ILE:HG22	1:A:592:PHE:HB3	2.00	0.43
1:A:783:PRO:HG2	1:A:855:PHE:HE2	1.83	0.43
1:A:180:LEU:HD11	1:A:201:ASN:HD22	1.83	0.43
1:A:67:LEU:HD12	1:A:68:ALA:N	2.33	0.43
1:A:855:PHE:HD1	1:A:855:PHE:HA	1.72	0.43
1:A:570:LEU:HA	1:A:571:ARG:HH21	1.83	0.43
1:A:505:ARG:O	1:A:505:ARG:HD3	2.19	0.43
1:A:8:THR:HA	1:A:193:PRO:HG3	2.01	0.42
1:A:20:GLU:OE2	1:A:166:THR:HB	2.18	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.87	0.42
1:A:259:GLN:O	1:A:263:VAL:HG23	2.19	0.42
1:A:525:THR:HG23	1:A:589:ASN:HA	2.02	0.42
1:A:772:VAL:O	1:A:776:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:O	1:A:277:GLY:C	2.58	0.42
1:A:271:VAL:O	1:A:274:ILE:HG22	2.19	0.42
1:A:416:ILE:HD11	1:A:565:THR:HG22	2.01	0.42
1:A:324:ARG:NH1	4:A:1006:PCW:H72	2.35	0.42
4:A:1006:PCW:H11	4:A:1006:PCW:C5	2.50	0.42
1:A:932:LEU:O	1:A:936:ILE:HG12	2.19	0.42
1:A:361:MET:HA	1:A:599:LEU:O	2.20	0.41
1:A:548:ILE:HA	1:A:548:ILE:HD13	1.79	0.41
1:A:556:ASP:HB3	1:A:558:LEU:HD21	2.01	0.41
1:A:60:LEU:O	1:A:64:ILE:HG13	2.20	0.41
1:A:983:LEU:HA	1:A:986:VAL:HG12	2.03	0.41
1:A:61:LEU:HD11	1:A:307:ILE:HD11	2.02	0.41
1:A:628:LYS:HD2	1:A:653:THR:HG23	2.03	0.41
1:A:890:PHE:HD1	1:A:890:PHE:HA	1.76	0.41
1:A:308:PRO:HA	1:A:767:ASN:HD21	1.86	0.41
1:A:153:ILE:N	1:A:153:ILE:HD13	2.36	0.41
1:A:986:VAL:HG13	1:A:987:ALA:H	1.86	0.41
1:A:711:LYS:HG3	1:A:729:ALA:HB1	2.04	0.40
1:A:875:CYS:HB2	1:A:890:PHE:HE2	1.86	0.40
1:A:65:LEU:HD13	1:A:300:VAL:HG21	2.02	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	989/997 (99%)	955 (97%)	33 (3%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	988	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	845/850 (99%)	810 (96%)	35 (4%)	30 67

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	20	GLU
1	A	45	GLU
1	A	48	THR
1	A	84	THR
1	A	135	LYS
1	A	149	ASP
1	A	153	ILE
1	A	172	THR
1	A	253	LEU
1	A	311	LEU
1	A	413	LEU
1	A	445	LEU
1	A	484	THR
1	A	486	GLU
1	A	505	ARG
1	A	508	MET
1	A	548	ILE
1	A	561	LEU
1	A	565	THR
1	A	571	ARG
1	A	599	LEU
1	A	605	GLU
1	A	612	LEU
1	A	670	LEU
1	A	690	LEU
1	A	812	ASP
1	A	836	TYR
1	A	843	VAL
1	A	855	PHE

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Mol	Chain	Res	Type
1	A	863	ARG
1	A	944	PHE
1	A	961	LEU
1	A	989	ASN
1	A	991	LEU

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

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	ASN
1	A	132	GLN
1	A	177	GLN
1	A	284	HIS
1	A	403	ASN
1	A	566	HIS
1	A	582	ASN
1	A	682	HIS
1	A	767	ASN
1	A	874	GLN
1	A	957	GLN
1	A	989	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	PCW	A	1003	-	21,21,53	1.40	2 (9%)	27,29,61	0.85	1 (3%)
4	PCW	A	1006	-	21,21,53	1.01	0	27,29,61	0.55	0
2	ATP	A	1001	-	26,33,33	1.10	2 (7%)	31,52,52	0.95	2 (6%)
5	MPD	A	1007	-	7,7,7	0.73	0	9,10,10	0.58	0
4	PCW	A	1005	-	21,21,53	1.07	1 (4%)	27,29,61	0.62	1 (3%)
4	PCW	A	1004	-	21,21,53	1.03	1 (4%)	27,29,61	0.69	0

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	PCW	A	1003	-	-	6/23/23/57	-
4	PCW	A	1006	-	-	9/23/23/57	-
2	ATP	A	1001	-	-	7/18/38/38	0/3/3/3
5	MPD	A	1007	-	-	2/5/5/5	-
4	PCW	A	1005	-	-	3/23/23/57	-
4	PCW	A	1004	-	-	9/23/23/57	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ATP	C8-N7	-3.39	1.28	1.34
4	A	1003	PCW	O2-C2	2.91	1.53	1.46
4	A	1003	PCW	O2-C31	2.63	1.41	1.35
2	A	1001	ATP	O5'-C5'	-2.38	1.35	1.44
4	A	1004	PCW	C1-C2	2.03	1.56	1.50
4	A	1005	PCW	P-O3P	-2.01	1.51	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ATP	O4'-C1'-C2'	-3.48	101.84	106.93
4	A	1003	PCW	O3-C3-C2	3.19	117.72	108.43
4	A	1005	PCW	O3-C3-C2	2.42	115.49	108.43
2	A	1001	ATP	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	PCW	C1-O3P-P-O1P
4	A	1003	PCW	C1-O3P-P-O2P
4	A	1003	PCW	C1-O3P-P-O4P
4	A	1006	PCW	C5-C4-O4P-P
4	A	1006	PCW	C32-C31-O2-C2
4	A	1006	PCW	O31-C31-O2-C2
2	A	1001	ATP	C5'-O5'-PA-O1A
4	A	1004	PCW	C1-O3P-P-O1P
4	A	1004	PCW	C1-O3P-P-O2P
4	A	1004	PCW	C1-O3P-P-O4P
4	A	1004	PCW	C4-O4P-P-O1P
4	A	1004	PCW	C4-O4P-P-O2P
4	A	1005	PCW	O11-C11-O3-C3
4	A	1004	PCW	O11-C11-O3-C3
4	A	1004	PCW	C12-C11-O3-C3
4	A	1005	PCW	C12-C11-O3-C3
2	A	1001	ATP	O4'-C4'-C5'-O5'
2	A	1001	ATP	C3'-C4'-C5'-O5'
4	A	1004	PCW	C4-O4P-P-O3P
2	A	1001	ATP	C5'-O5'-PA-O3A
4	A	1006	PCW	C4-O4P-P-O2P
2	A	1001	ATP	C5'-O5'-PA-O2A
4	A	1003	PCW	O4P-C4-C5-N
4	A	1006	PCW	O4P-C4-C5-N
4	A	1005	PCW	O4P-C4-C5-N
4	A	1004	PCW	O4P-C4-C5-N
4	A	1006	PCW	C4-O4P-P-O3P
2	A	1001	ATP	PA-O3A-PB-O2B
4	A	1003	PCW	C3-C2-O2-C31
4	A	1006	PCW	C1-C2-O2-C31
2	A	1001	ATP	PA-O3A-PB-O1B
5	A	1007	MPD	C2-C3-C4-C5
4	A	1003	PCW	C4-O4P-P-O1P
4	A	1006	PCW	C1-O3P-P-O2P

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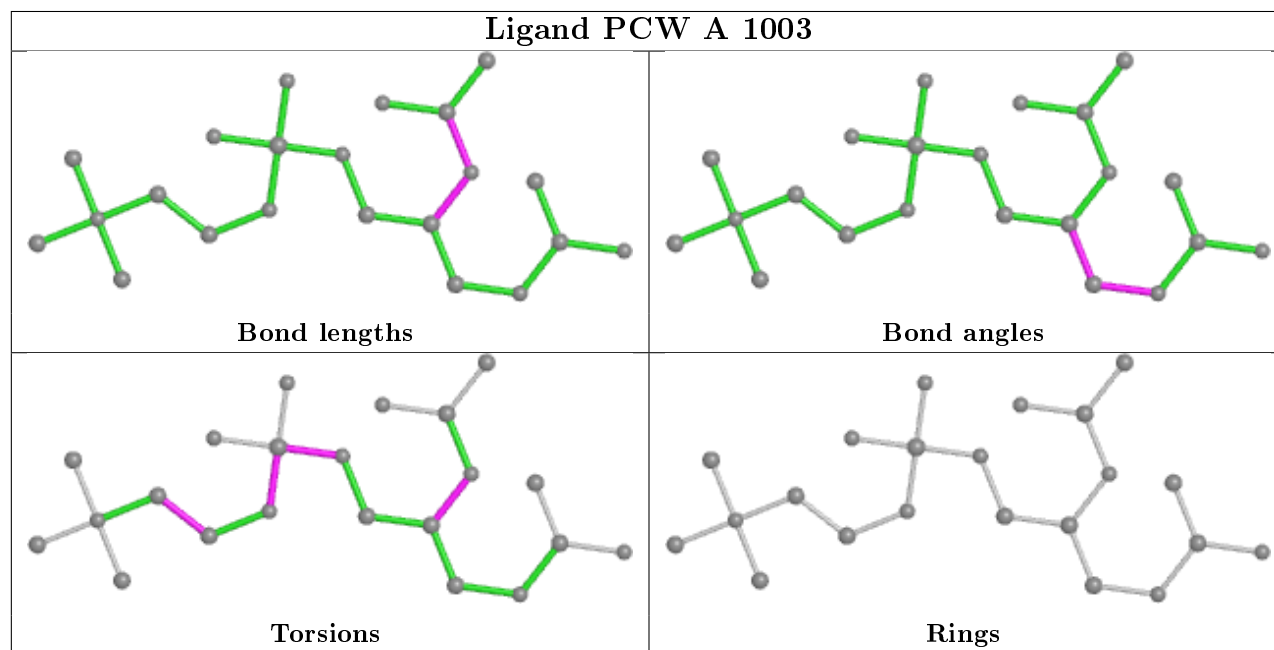
Mol	Chain	Res	Type	Atoms
4	A	1006	PCW	C3-C2-O2-C31
5	A	1007	MPD	C2-C3-C4-O4

There are no ring outliers.

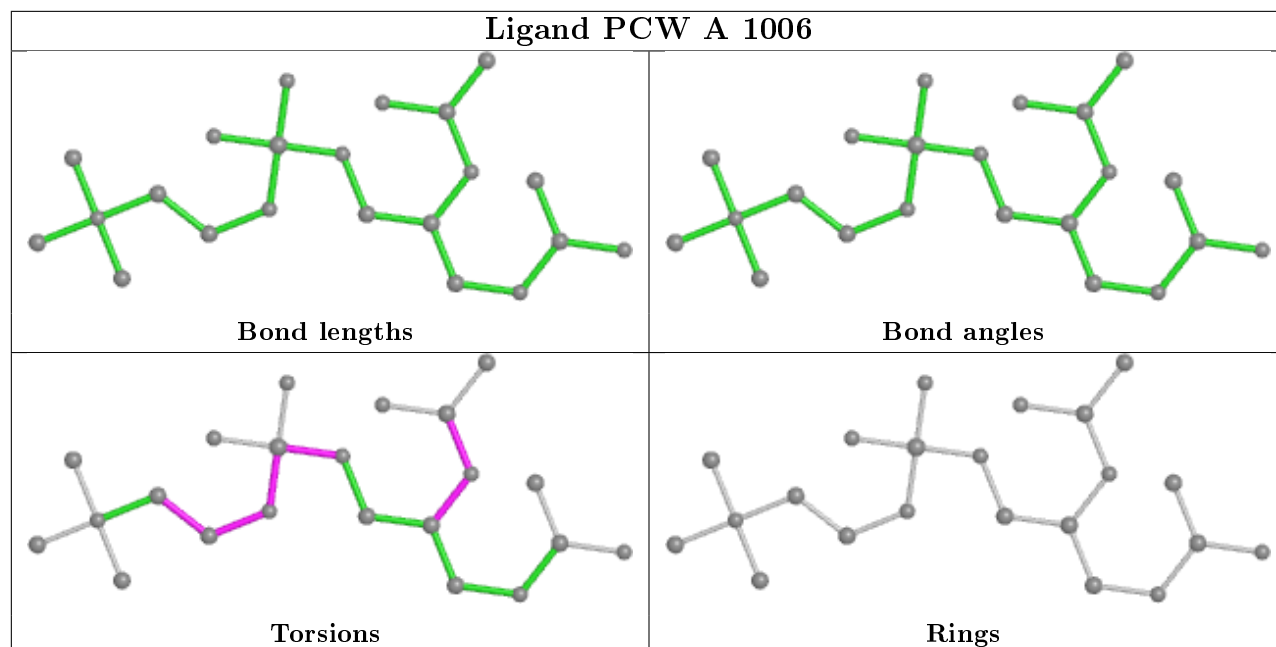
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1006	PCW	2	0
4	A	1004	PCW	1	0

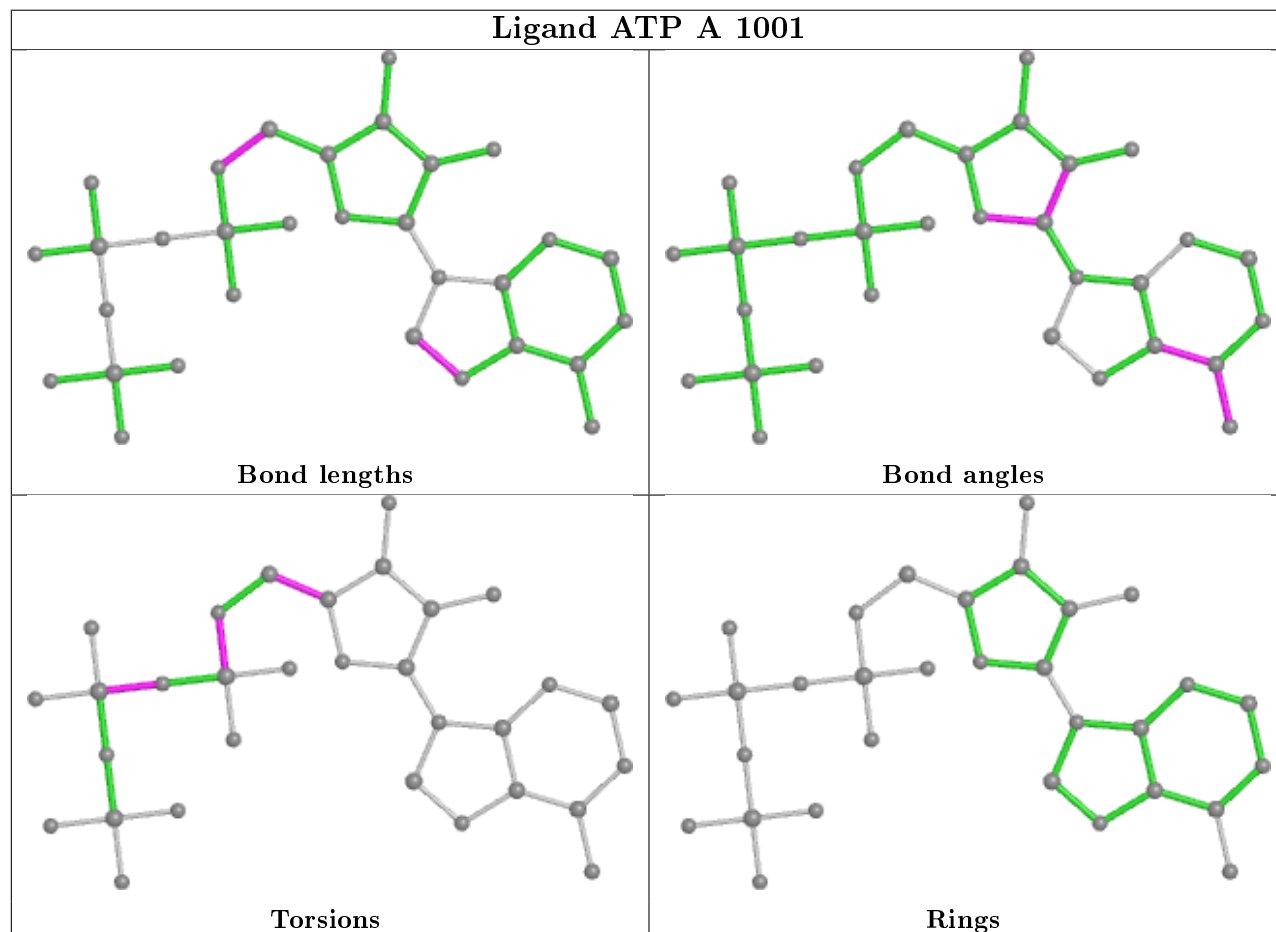
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

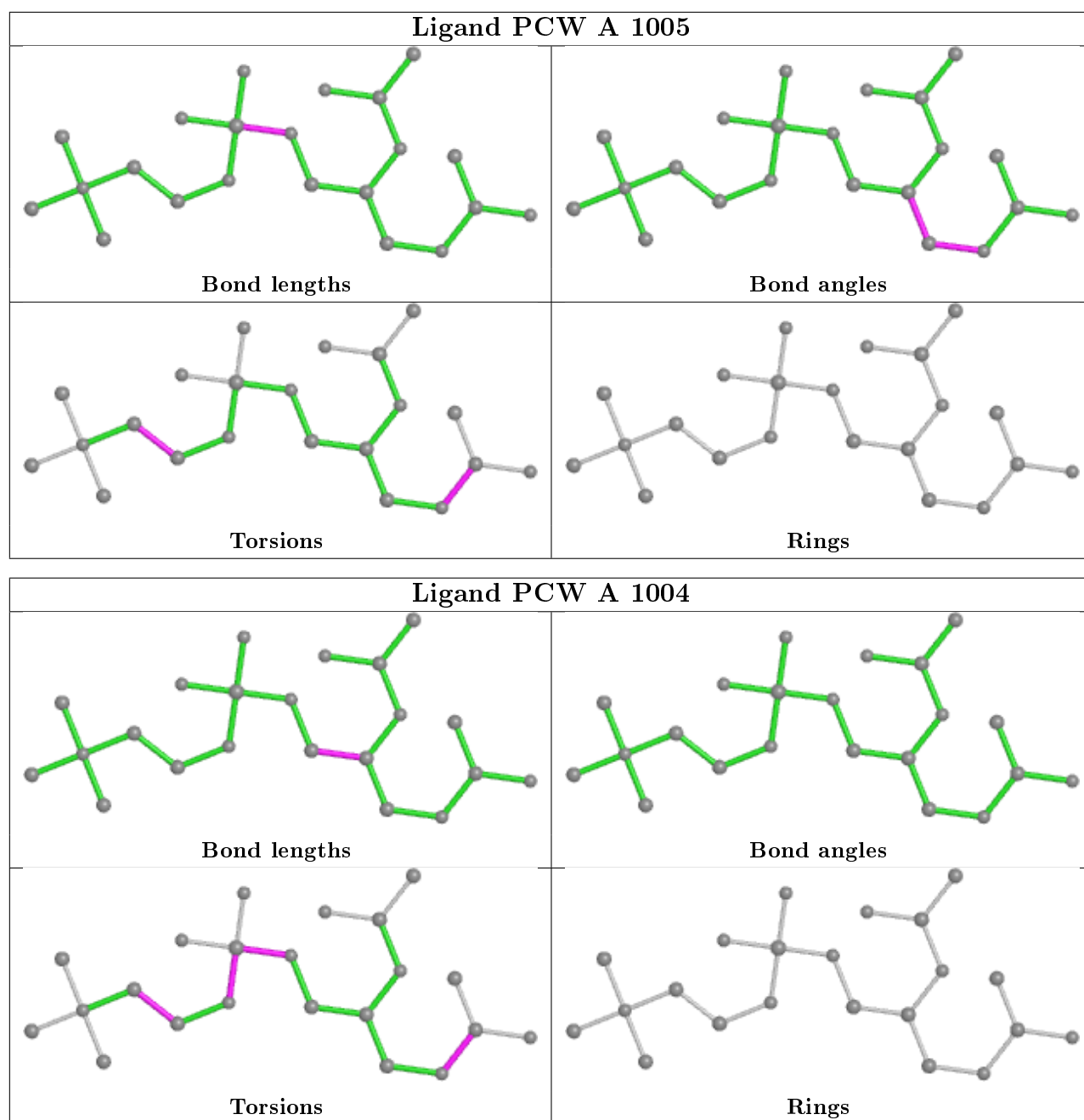


Ligand PCW A 1006



Ligand ATP A 1001





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	991/997 (99%)	0.08	102 (10%) 6 2	38, 96, 249, 336	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	SER	9.9
1	A	283	VAL	9.7
1	A	83	GLU	9.3
1	A	281	ASP	8.9
1	A	74	VAL	8.2
1	A	880	PRO	7.6
1	A	284	HIS	7.3
1	A	72	SER	7.2
1	A	877	GLU	7.1
1	A	73	PHE	7.1
1	A	883	GLU	6.9
1	A	57	PHE	6.7
1	A	66	LEU	6.6
1	A	240	VAL	6.5
1	A	265	SER	6.5
1	A	77	TRP	6.3
1	A	282	PRO	6.3
1	A	111	ASN	6.2
1	A	70	CYS	5.9
1	A	286	GLY	5.9
1	A	86	THR	5.9
1	A	278	HIS	5.8
1	A	82	GLU	5.8
1	A	69	ALA	5.8
1	A	876	LYS	5.4
1	A	85	ILE	5.4
1	A	84	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	241	ALA	5.3
1	A	292	ALA	5.1
1	A	275	ASN	5.0
1	A	280	ASN	5.0
1	A	81	GLY	4.9
1	A	46	GLY	4.8
1	A	89	VAL	4.7
1	A	110	ARG	4.6
1	A	64	ILE	4.6
1	A	42	PRO	4.5
1	A	53	VAL	4.5
1	A	888	ALA	4.4
1	A	285	GLY	4.4
1	A	950	GLU	4.3
1	A	50	LEU	4.3
1	A	242	THR	4.2
1	A	90	GLU	4.2
1	A	288	TRP	4.2
1	A	88	PHE	4.2
1	A	245	GLU	4.1
1	A	58	GLU	4.1
1	A	243	GLU	4.0
1	A	873	LEU	3.9
1	A	95	LEU	3.9
1	A	289	ILE	3.9
1	A	87	ALA	3.8
1	A	55	GLU	3.7
1	A	239	MET	3.7
1	A	258	GLU	3.6
1	A	274	ILE	3.5
1	A	108	GLN	3.5
1	A	56	GLN	3.5
1	A	71	ILE	3.5
1	A	99	VAL	3.5
1	A	80	GLU	3.4
1	A	238	GLU	3.4
1	A	107	TRP	3.3
1	A	276	ILE	3.3
1	A	92	PHE	3.3
1	A	269	ILE	3.3
1	A	262	LYS	3.2
1	A	874	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	54	ILE	3.0
1	A	91	PRO	3.0
1	A	109	GLU	2.9
1	A	859	ASP	2.9
1	A	244	GLN	2.9
1	A	117	GLU	2.9
1	A	878	ASP	2.9
1	A	61	LEU	2.8
1	A	279	PHE	2.8
1	A	49	LEU	2.7
1	A	134	ARG	2.7
1	A	68	ALA	2.6
1	A	273	ILE	2.6
1	A	41	LEU	2.5
1	A	236	ARG	2.5
1	A	268	CYS	2.5
1	A	51	GLU	2.5
1	A	234	LYS	2.5
1	A	271	VAL	2.5
1	A	879	ASN	2.4
1	A	948	TYR	2.4
1	A	267	ILE	2.4
1	A	270	ALA	2.4
1	A	884	GLY	2.4
1	A	101	ASN	2.3
1	A	93	VAL	2.2
1	A	375	ASP	2.2
1	A	272	TRP	2.2
1	A	45	GLU	2.1
1	A	44	GLU	2.1
1	A	277	GLY	2.1
1	A	293	ILE	2.0
1	A	67	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

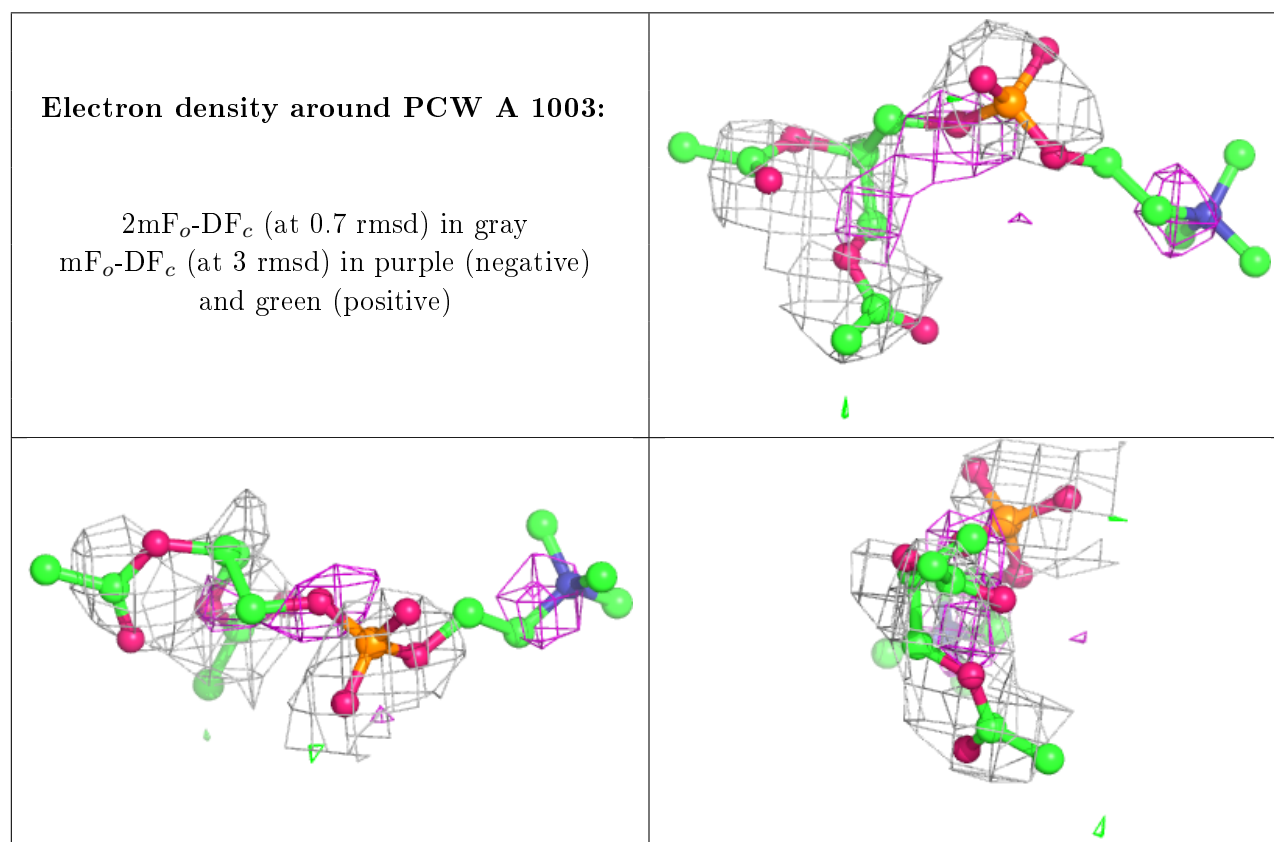
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

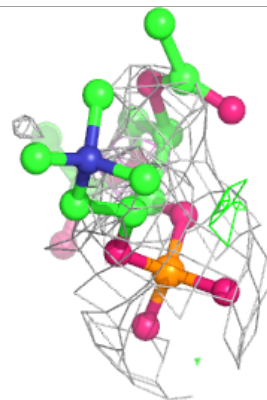
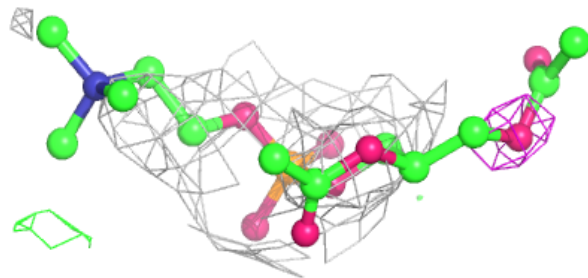
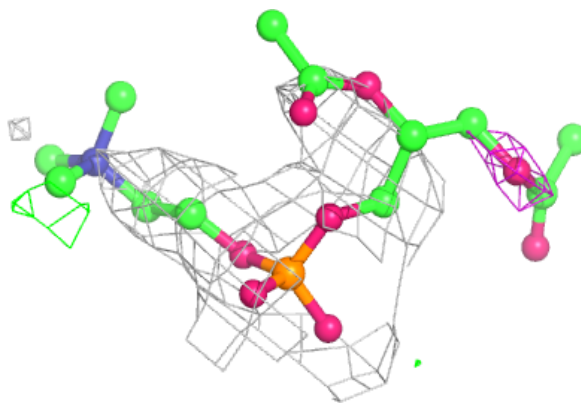
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PCW	A	1003	22/54	0.50	0.58	125,163,203,206	0
4	PCW	A	1005	22/54	0.55	0.54	126,157,172,175	0
4	PCW	A	1006	22/54	0.66	0.52	118,150,226,233	0
4	PCW	A	1004	22/54	0.70	0.46	105,152,219,230	0
5	MPD	A	1007	8/8	0.88	0.27	63,75,88,94	0
3	K	A	1002	1/1	0.97	0.06	66,66,66,66	0
2	ATP	A	1001	31/31	0.98	0.14	48,49,75,79	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.



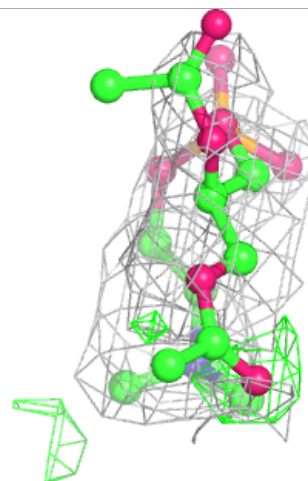
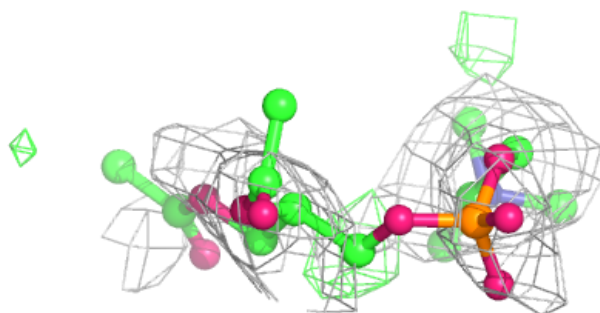
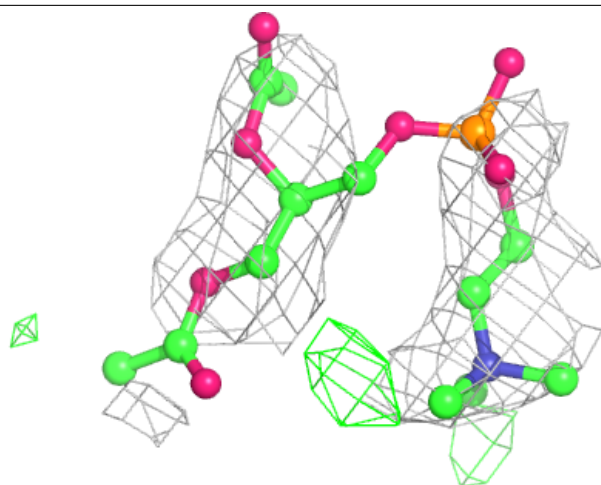
Electron density around PCW A 1005:

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



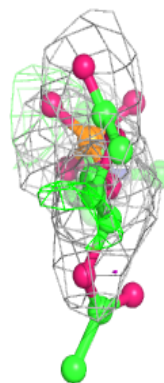
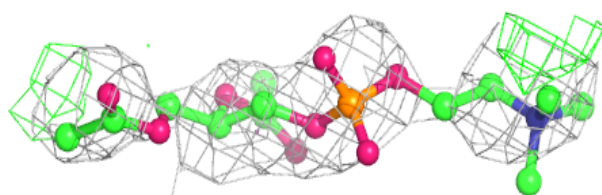
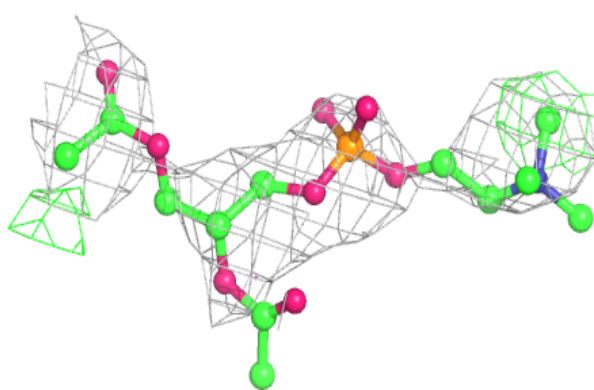
Electron density around PCW A 1006:

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

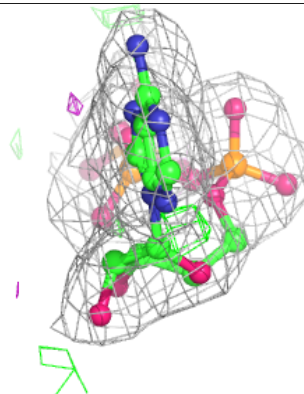
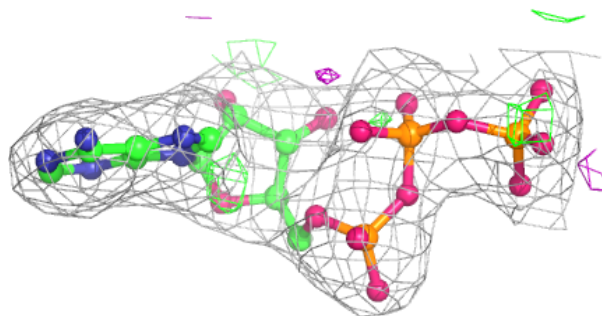
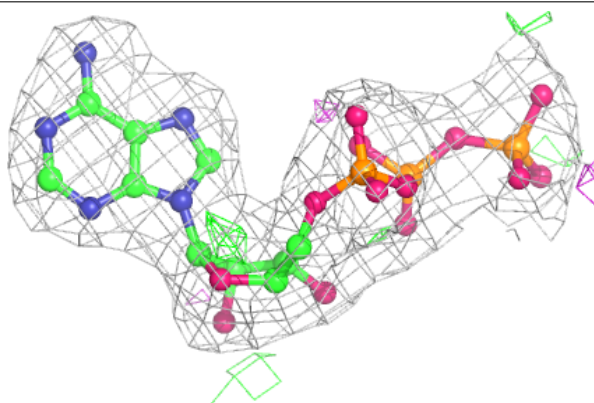


Electron density around PCW A 1004:

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

**Electron density around ATP A 1001:**

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



6.5 Other polymers

There are no such residues in this entry.