



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:40 PM UTC

PDB ID : 4UU1 / pdb_00004uu1
Title : CRYSTAL STRUCTURE OF (SR) CALCIUM-ATPASE E2(TG) IN THE PRESENCE OF DOPC
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Deposited on : 2014-07-24
Resolution : 2.80 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

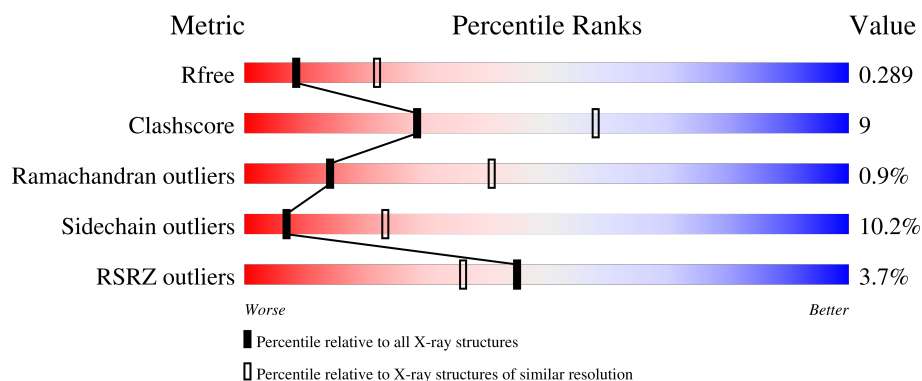
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	4% 73% 24% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7834 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.

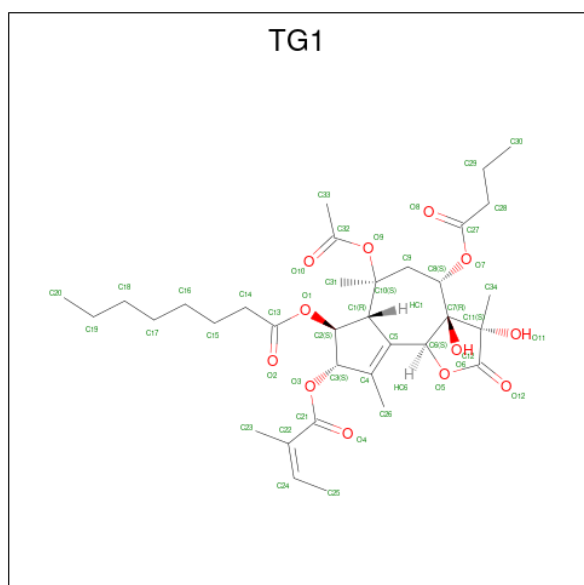
- Molecule 1 is a protein called SARCOPLASMIC ENDOPLASMIC RETICULUM CALCIUM ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7674	4878	1287	1452	57			

There is a discrepancy between the modelled and reference sequences:

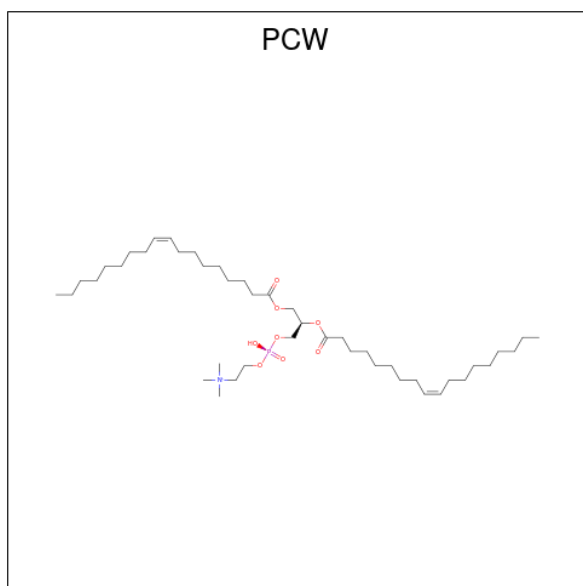
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP B6CAM1

- Molecule 2 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).



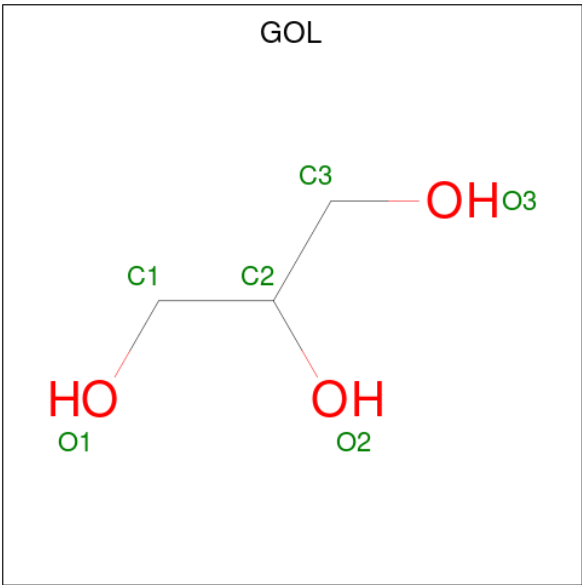
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			46	34	12		

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



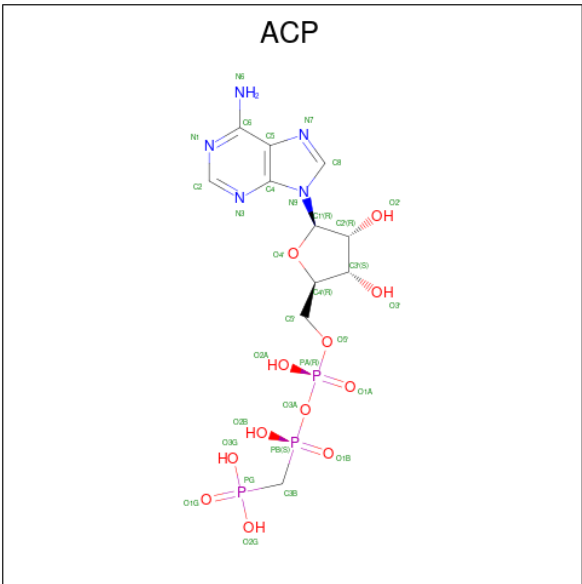
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	12	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			23	13	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		

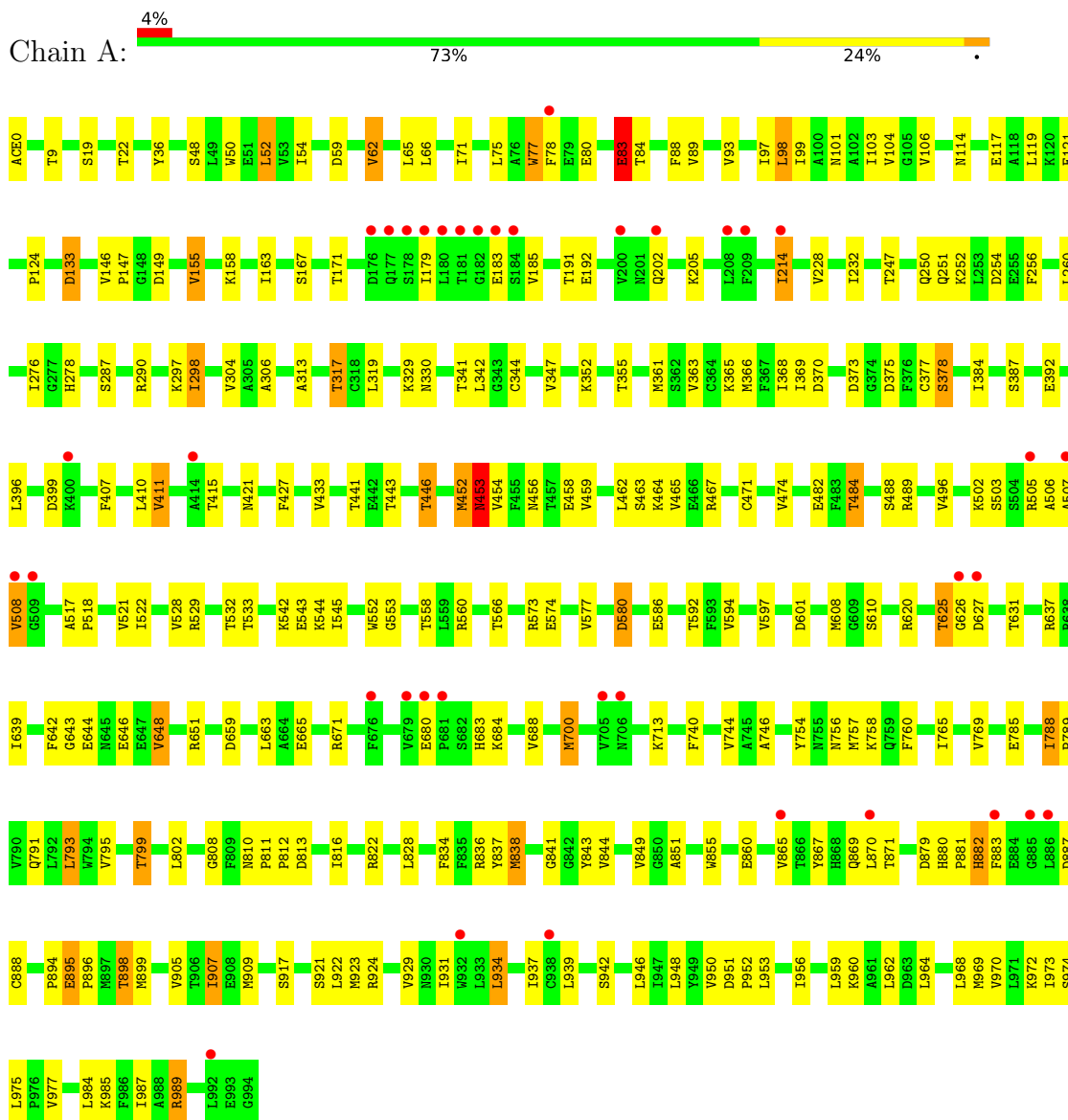
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.70Å 71.70Å 591.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.80 73.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.80) 100.0 (73.92-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.293 0.231 , 0.289	Depositor DCC
R_{free} test set	1995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7834	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: TG1, K, GOL, PCW, ACE, ACP, 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	0.56	0/7813	0.89	7/10594 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	THR	N-CA-C	5.68	117.43	108.96
1	A	951	ASP	CA-C-N	-5.65	112.70	118.85
1	A	951	ASP	C-N-CA	-5.65	112.70	118.85
1	A	83	GLU	N-CA-C	-5.50	106.62	113.55
1	A	163	ILE	N-CA-C	5.11	115.26	108.11
1	A	934	LEU	N-CA-C	-5.09	105.63	111.07
1	A	643	GLY	N-CA-C	-5.01	105.90	112.82

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	137	0
2	A	46	0	50	3	0
3	A	69	0	60	6	0
4	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	0	14	3	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
All	All	7834	0	7905	139	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 9.

All (139) 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:453:ASN:ND2	1:A:471:CYS:SG	2.45	0.90
1:A:560:ARG:NH2	5:A:1996:ACP:H8	1.91	0.86
1:A:484:THR:HB	1:A:496:VAL:HG12	1.60	0.84
1:A:838:MET:HE1	2:A:1003:TG1:H141	1.67	0.76
1:A:361:MET:HE3	1:A:601:ASP:HB2	1.70	0.74
1:A:377:CYS:HB3	1:A:544:LYS:HD2	1.68	0.73
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.73	0.69
1:A:812:PRO:HB3	1:A:816:ILE:HD11	1.74	0.69
1:A:347:VAL:HG22	1:A:620:ARG:HB3	1.73	0.69
1:A:443:THR:HA	1:A:446:THR:HG23	1.76	0.68
1:A:452:MET:O	1:A:454:VAL:N	2.28	0.66
1:A:287:SER:HB3	1:A:290:ARG:HB2	1.78	0.66
1:A:80:GLU:OE2	1:A:290:ARG:NH2	2.30	0.64
1:A:80:GLU:HB2	1:A:83:GLU:HB3	1.79	0.64
1:A:421:ASN:HD21	1:A:446:THR:HG22	1.63	0.63
1:A:580:ASP:N	1:A:580:ASP:OD1	2.30	0.63
1:A:133:ASP:N	1:A:133:ASP:OD1	2.32	0.62
1:A:411:VAL:O	1:A:415:THR:HG23	1.99	0.61
1:A:813:ASP:O	1:A:816:ILE:HG13	2.02	0.60
1:A:522:ILE:HG22	1:A:542:LYS:HE3	1.85	0.58
1:A:836:ARG:HG3	1:A:984:LEU:HD13	1.86	0.58
1:A:482:GLU:OE1	1:A:573:ARG:NH1	2.38	0.57
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.87	0.57
1:A:560:ARG:HE	5:A:1996:ACP:H2'	1.69	0.57
1:A:953:LEU:HA	1:A:956:ILE:HD12	1.87	0.56
1:A:769:VAL:HG12	1:A:841:GLY:HA3	1.87	0.56
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.40	0.56
1:A:898:THR:HG21	1:A:960:LYS:H	1.70	0.56
1:A:19:SER:OG	1:A:22:THR:HB	2.06	0.55
1:A:202:GLN:OE1	1:A:489:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ASP:OD1	1:A:888:CYS:N	2.29	0.54
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.88	0.54
1:A:969:MET:HE2	1:A:973:ILE:HG13	1.89	0.53
1:A:366:MET:HE1	1:A:452:MET:HE2	1.90	0.53
1:A:459:VAL:HA	1:A:462:LEU:HD13	1.90	0.53
1:A:560:ARG:HH21	5:A:1996:ACP:H8	1.72	0.53
1:A:370:ASP:HB3	1:A:378:SER:OG	2.09	0.53
1:A:625:THR:OG1	1:A:626:GLY:N	2.40	0.53
1:A:66:LEU:HD12	1:A:98:LEU:HD23	1.91	0.53
1:A:865:VAL:HG12	1:A:867:TYR:HB2	1.91	0.53
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.91	0.53
1:A:791:GLN:O	1:A:795:VAL:HG23	2.09	0.52
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.44	0.52
1:A:421:ASN:ND2	1:A:446:THR:HG22	2.25	0.52
1:A:837:TYR:HB2	2:A:1003:TG1:H331	1.92	0.52
1:A:48:SER:O	1:A:52:LEU:N	2.42	0.52
1:A:319:LEU:HD21	1:A:757:MET:HE1	1.91	0.52
1:A:688:VAL:HG11	1:A:713:LYS:HG2	1.90	0.52
1:A:974:SER:O	1:A:977:VAL:HG23	2.10	0.52
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.92	0.51
1:A:855:TRP:CE3	1:A:896:PRO:HB3	2.46	0.51
1:A:89:VAL:O	1:A:93:VAL:HG23	2.11	0.51
1:A:894:PRO:O	1:A:898:THR:HG23	2.11	0.51
1:A:205:LYS:HZ1	1:A:488:SER:HB3	1.76	0.51
1:A:313:ALA:O	1:A:317:THR:OG1	2.29	0.51
1:A:453:ASN:HB3	1:A:456:ASN:HA	1.92	0.51
1:A:907:ILE:HG12	1:A:977:VAL:HG21	1.92	0.50
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.92	0.50
1:A:811:PRO:HG3	1:A:929:VAL:HG12	1.93	0.50
1:A:659:ASP:OD1	1:A:683:HIS:NE2	2.44	0.50
1:A:99:ILE:O	1:A:103:ILE:HG12	2.11	0.50
1:A:553:GLY:O	1:A:631:THR:HG22	2.12	0.50
1:A:909:MET:HE3	1:A:937:ILE:HA	1.92	0.50
1:A:923:MET:HB2	3:A:1102:PCW:H31	1.93	0.50
1:A:881:PRO:O	1:A:883:PHE:N	2.45	0.49
1:A:757:MET:HA	1:A:760:PHE:CE2	2.47	0.49
1:A:205:LYS:NZ	1:A:488:SER:HB3	2.27	0.49
1:A:502:LYS:HB2	1:A:505:ARG:HB3	1.95	0.49
1:A:663:LEU:HD22	1:A:663:LEU:H	1.77	0.49
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.95	0.48
1:A:851:ALA:HB1	1:A:899:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:O	1:A:507:ALA:N	2.46	0.48
1:A:627:ASP:HB3	1:A:631:THR:OG1	2.13	0.48
1:A:909:MET:HE3	1:A:937:ILE:HG23	1.94	0.48
3:A:1102:PCW:H32	3:A:1102:PCW:H62	1.94	0.48
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.63	0.48
1:A:646:GLU:OE2	1:A:651:ARG:NH2	2.46	0.48
1:A:104:VAL:HG11	3:A:1101:PCW:H32	1.97	0.47
1:A:98:LEU:O	1:A:101:ASN:HB3	2.15	0.47
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.95	0.47
1:A:648:VAL:HG13	1:A:651:ARG:HB2	1.97	0.47
1:A:119:LEU:HD22	1:A:232:ILE:HD11	1.96	0.47
1:A:363:VAL:HG12	1:A:384:ILE:HD13	1.96	0.47
1:A:756:ASN:OD1	1:A:810:ASN:HB2	2.14	0.47
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.97	0.47
1:A:36:TYR:CG	1:A:147:PRO:HG2	2.49	0.47
1:A:754:TYR:O	1:A:758:LYS:HB2	2.15	0.46
1:A:642:PHE:CZ	1:A:648:VAL:HG11	2.50	0.46
1:A:464:LYS:HA	1:A:467:ARG:HB3	1.98	0.46
1:A:608:MET:SD	1:A:639:ILE:HA	2.55	0.46
1:A:898:THR:HG21	1:A:960:LYS:N	2.31	0.46
1:A:75:LEU:C	1:A:77:TRP:H	2.24	0.46
1:A:700:MET:HB3	1:A:700:MET:HE3	1.60	0.46
1:A:124:PRO:HB3	1:A:158:LYS:HB3	1.98	0.46
1:A:802:LEU:HD13	1:A:939:LEU:HD23	1.97	0.46
1:A:471:CYS:O	1:A:474:VAL:HG22	2.17	0.45
1:A:256:PHE:CZ	1:A:765:ILE:HD12	2.52	0.45
1:A:329:LYS:O	1:A:330:ASN:HB2	2.16	0.45
1:A:407:PHE:HB2	1:A:410:LEU:HB2	1.97	0.45
1:A:684:LYS:HD3	1:A:700:MET:HE1	1.98	0.45
1:A:834:PHE:CD1	2:A:1003:TG1:H332	2.52	0.45
1:A:529:ARG:NH1	1:A:592:THR:HG21	2.32	0.45
1:A:71:ILE:O	1:A:75:LEU:HG	2.17	0.44
1:A:463:SER:O	1:A:467:ARG:N	2.51	0.44
1:A:924:ARG:HG2	3:A:1102:PCW:H82	1.99	0.44
1:A:543:GLU:C	1:A:545:ILE:H	2.25	0.44
1:A:788:ILE:HD13	1:A:789:PRO:HD2	1.99	0.44
1:A:843:TYR:HE1	1:A:907:ILE:HD11	1.83	0.43
1:A:276:ILE:HD12	1:A:276:ILE:HA	1.88	0.43
1:A:319:LEU:CD2	1:A:757:MET:HE1	2.47	0.43
1:A:948:LEU:HD23	1:A:948:LEU:HA	1.87	0.43
1:A:811:PRO:HG3	1:A:929:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:HB3	1:A:62:VAL:HG13	2.00	0.43
1:A:344:CYS:SG	1:A:822:ARG:NH2	2.92	0.43
1:A:985:LYS:O	1:A:989:ARG:HD2	2.19	0.43
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.99	0.43
1:A:844:VAL:HG22	1:A:907:ILE:HG21	2.01	0.43
1:A:969:MET:HE3	1:A:972:LYS:HD3	2.01	0.42
3:A:1101:PCW:H72	3:A:1101:PCW:H41	1.83	0.42
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.84	0.42
1:A:637:ARG:NH1	1:A:644:GLU:O	2.53	0.42
1:A:880:HIS:N	1:A:881:PRO:HD2	2.35	0.42
1:A:899:MET:HE3	1:A:899:MET:HB3	1.76	0.42
1:A:80:GLU:CB	1:A:83:GLU:HB3	2.49	0.41
1:A:250:GLN:HE21	3:A:1101:PCW:H71	1.85	0.41
1:A:942:SER:O	1:A:946:LEU:N	2.50	0.41
1:A:298:ILE:HD13	1:A:298:ILE:HA	1.90	0.41
1:A:921:SER:H	1:A:989:ARG:NH2	2.19	0.41
1:A:648:VAL:CG1	1:A:651:ARG:HB2	2.50	0.41
1:A:793:LEU:HD13	1:A:793:LEU:HA	1.64	0.41
1:A:114:ASN:HB3	1:A:117:GLU:HB2	2.03	0.41
1:A:427:PHE:HB3	1:A:465:VAL:HA	2.03	0.41
1:A:452:MET:O	1:A:454:VAL:HG13	2.21	0.40
1:A:566:THR:HG23	1:A:594:VAL:HG21	2.03	0.40
1:A:934:LEU:HD23	1:A:934:LEU:HA	1.97	0.40
1:A:964:LEU:O	1:A:968:LEU:HG	2.20	0.40
1:A:507:ALA:O	1:A:508:VAL:HG22	2.21	0.40
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.56	0.40
1:A:895:GLU:H	1:A:895:GLU:HG2	1.31	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%)	921 (93%)	63 (6%)	9 (1%)	14	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	453	ASN
1	A	882	HIS
1	A	506	ALA
1	A	508	VAL
1	A	78	PHE
1	A	871	THR
1	A	458	GLU
1	A	558	THR
1	A	785	GLU

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%)	754 (90%)	86 (10%)	7	23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	52	LEU
1	A	62	VAL
1	A	77	TRP
1	A	83	GLU
1	A	84	THR
1	A	88	PHE
1	A	97	ILE
1	A	98	LEU
1	A	106	VAL
1	A	121	GLU
1	A	133	ASP

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Mol	Chain	Res	Type
1	A	146	VAL
1	A	149	ASP
1	A	155	VAL
1	A	167	SER
1	A	171	THR
1	A	179	ILE
1	A	183	GLU
1	A	185	VAL
1	A	191	THR
1	A	192	GLU
1	A	214	ILE
1	A	228	VAL
1	A	247	THR
1	A	251	GLN
1	A	252	LYS
1	A	254	ASP
1	A	278	HIS
1	A	297	LYS
1	A	298	ILE
1	A	304	VAL
1	A	317	THR
1	A	341	THR
1	A	352	LYS
1	A	368	ILE
1	A	373	ASP
1	A	375	ASP
1	A	378	SER
1	A	387	SER
1	A	392	GLU
1	A	396	LEU
1	A	399	ASP
1	A	411	VAL
1	A	433	VAL
1	A	441	THR
1	A	446	THR
1	A	452	MET
1	A	453	ASN
1	A	484	THR
1	A	503	SER
1	A	521	VAL
1	A	532	THR
1	A	533	THR

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Mol	Chain	Res	Type
1	A	574	GLU
1	A	577	VAL
1	A	580	ASP
1	A	586	GLU
1	A	597	VAL
1	A	648	VAL
1	A	665	GLU
1	A	671	ARG
1	A	680	GLU
1	A	700	MET
1	A	788	ILE
1	A	793	LEU
1	A	799	THR
1	A	828	LEU
1	A	838	MET
1	A	849	VAL
1	A	860	GLU
1	A	870	LEU
1	A	879	ASP
1	A	882	HIS
1	A	895	GLU
1	A	898	THR
1	A	907	ILE
1	A	917	SER
1	A	922	LEU
1	A	931	ILE
1	A	959	LEU
1	A	962	LEU
1	A	970	VAL
1	A	975	LEU
1	A	987	ILE
1	A	989	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	213	ASN
1	A	238	GLN
1	A	453	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PCW	A	1102	-	22,22,53	1.58	5 (22%)	28,30,61	0.90	1 (3%)
3	PCW	A	1101	-	21,21,53	1.72	6 (28%)	27,29,61	1.37	1 (3%)
4	GOL	A	1302	-	5,5,5	0.24	0	5,5,5	0.48	0
4	GOL	A	1301	-	5,5,5	0.32	0	5,5,5	0.29	0
5	ACP	A	1996	7	31,33,33	1.80	8 (25%)	47,52,52	1.93	9 (19%)
2	TG1	A	1003	-	44,48,48	2.18	11 (25%)	47,72,72	3.46	14 (29%)
3	PCW	A	1103	-	23,23,53	1.65	6 (26%)	29,31,61	1.04	2 (6%)

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
3	PCW	A	1102	-	-	10/25/25/57	-
3	PCW	A	1101	-	-	13/23/23/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1302	-	-	0/4/4/4	-
4	GOL	A	1301	-	-	2/4/4/4	-
5	ACP	A	1996	7	-	5/19/38/38	0/3/3/3
2	TG1	A	1003	-	-	15/33/99/99	0/3/3/3
3	PCW	A	1103	-	-	9/27/27/57	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	TG1	O12-C12	8.47	1.39	1.20
3	A	1101	PCW	O2-C31	4.96	1.46	1.35
2	A	1003	TG1	C4-C5	4.87	1.54	1.33
2	A	1003	TG1	O5-C12	4.28	1.41	1.35
3	A	1102	PCW	O2-C31	4.22	1.46	1.34
3	A	1103	PCW	O2-C31	4.07	1.45	1.34
5	A	1996	ACP	PG-O1G	4.03	1.58	1.50
3	A	1103	PCW	O3-C11	3.81	1.44	1.33
2	A	1003	TG1	C3-C4	3.79	1.55	1.50
2	A	1003	TG1	C24-C22	3.73	1.53	1.31
2	A	1003	TG1	O7-C8	-3.35	1.40	1.46
5	A	1996	ACP	PB-O2B	-3.31	1.48	1.56
5	A	1996	ACP	C8-N9	3.29	1.43	1.37
2	A	1003	TG1	O9-C10	-3.01	1.43	1.48
5	A	1996	ACP	PG-O3G	-2.76	1.48	1.55
5	A	1996	ACP	PB-O1B	2.58	1.57	1.51
3	A	1103	PCW	C6-N	-2.46	1.42	1.50
3	A	1101	PCW	C6-N	-2.44	1.42	1.50
2	A	1003	TG1	C11-C7	2.43	1.58	1.55
3	A	1102	PCW	C6-N	-2.43	1.42	1.50
3	A	1102	PCW	O3-C11	2.33	1.44	1.33
5	A	1996	ACP	C5-C4	2.28	1.43	1.39
3	A	1103	PCW	C7-N	-2.26	1.43	1.50
5	A	1996	ACP	PA-O3A	-2.20	1.57	1.59
3	A	1102	PCW	C7-N	-2.17	1.43	1.50
3	A	1101	PCW	O3-C11	2.16	1.43	1.33
2	A	1003	TG1	C1-C5	2.16	1.54	1.51
3	A	1101	PCW	C7-N	-2.13	1.43	1.50
3	A	1101	PCW	C32-C31	2.09	1.56	1.49
3	A	1103	PCW	C8-N	-2.05	1.44	1.50
3	A	1101	PCW	C8-N	-2.04	1.44	1.50
2	A	1003	TG1	O3-C21	2.03	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	TG1	C9-C8	2.03	1.55	1.52
3	A	1102	PCW	C8-N	-2.02	1.44	1.50
3	A	1103	PCW	C5-N	-2.01	1.45	1.51
5	A	1996	ACP	PG-O2G	2.00	1.59	1.55

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	TG1	O12-C12-C11	-14.95	113.16	128.28
2	A	1003	TG1	O5-C12-O12	-11.60	106.59	121.60
5	A	1996	ACP	PB-O3A-PA	7.19	155.85	132.37
5	A	1996	ACP	O2G-PG-O1G	-6.49	95.60	112.39
2	A	1003	TG1	C26-C4-C3	-5.62	111.87	121.24
3	A	1101	PCW	O2-C31-C32	5.44	120.79	111.09
2	A	1003	TG1	C10-O9-C32	5.02	133.13	121.36
2	A	1003	TG1	C10-C1-C5	4.25	120.85	115.07
2	A	1003	TG1	C23-C22-C24	-4.02	107.70	123.12
2	A	1003	TG1	C26-C4-C5	-3.78	120.63	130.03
2	A	1003	TG1	O3-C21-O4	-3.76	116.39	123.40
2	A	1003	TG1	O5-C6-C5	-3.52	105.94	111.17
5	A	1996	ACP	O5'-PA-O1A	-3.28	95.94	108.94
2	A	1003	TG1	O7-C8-C9	3.24	112.42	106.63
3	A	1103	PCW	O3-C11-C12	3.19	120.82	111.15
5	A	1996	ACP	O3A-PA-O1A	-3.04	101.56	110.70
2	A	1003	TG1	C23-C22-C21	-2.94	108.57	116.12
5	A	1996	ACP	O2A-PA-O5'	2.83	120.40	107.57
2	A	1003	TG1	O9-C32-C33	-2.80	105.94	110.67
5	A	1996	ACP	C1'-N9-C8	2.64	132.94	127.09
5	A	1996	ACP	O2A-PA-O3A	2.59	114.28	107.27
3	A	1103	PCW	O2-C31-C32	2.57	120.36	110.93
3	A	1102	PCW	O2-C31-C32	2.53	120.23	110.93
5	A	1996	ACP	O3G-PG-C3B	2.47	112.39	106.40
2	A	1003	TG1	C11-C7-C8	2.44	117.69	114.44
5	A	1996	ACP	O2G-PG-C3B	2.35	112.09	106.40
2	A	1003	TG1	C6-C5-C4	-2.23	116.44	126.58

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	TG1	O4-C21-O3-C3
2	A	1003	TG1	O3-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	A	1003	TG1	C21-C22-C24-C25
3	A	1101	PCW	C4-O4P-P-O1P
3	A	1101	PCW	C4-O4P-P-O2P
3	A	1101	PCW	C4-O4P-P-O3P
3	A	1102	PCW	O4P-C4-C5-N
3	A	1102	PCW	C1-O3P-P-O1P
3	A	1102	PCW	C1-O3P-P-O2P
3	A	1103	PCW	C12-C11-O3-C3
3	A	1103	PCW	O11-C11-O3-C3
3	A	1103	PCW	C1-O3P-P-O1P
3	A	1103	PCW	C1-O3P-P-O2P
3	A	1103	PCW	C1-O3P-P-O4P
3	A	1103	PCW	C4-O4P-P-O3P
4	A	1301	GOL	O1-C1-C2-C3
5	A	1996	ACP	PB-C3B-PG-O1G
5	A	1996	ACP	PB-C3B-PG-O2G
5	A	1996	ACP	PB-C3B-PG-O3G
3	A	1101	PCW	C32-C31-O2-C2
3	A	1101	PCW	O31-C31-O2-C2
3	A	1101	PCW	C12-C11-O3-C3
3	A	1101	PCW	O11-C11-O3-C3
2	A	1003	TG1	O10-C32-O9-C10
3	A	1101	PCW	C3-C2-O2-C31
4	A	1301	GOL	O1-C1-C2-O2
2	A	1003	TG1	C27-C28-C29-C30
3	A	1102	PCW	C1-C2-C3-O3
2	A	1003	TG1	C22-C21-O3-C3
2	A	1003	TG1	C15-C16-C17-C18
2	A	1003	TG1	O4-C21-C22-C24
3	A	1101	PCW	C1-C2-C3-O3
2	A	1003	TG1	C16-C17-C18-C19
3	A	1102	PCW	C32-C31-O2-C2
3	A	1101	PCW	O3P-C1-C2-O2
3	A	1102	PCW	O31-C31-O2-C2
3	A	1101	PCW	O4P-C4-C5-N
3	A	1103	PCW	O4P-C4-C5-N
3	A	1102	PCW	O3P-C1-C2-C3
3	A	1103	PCW	O3P-C1-C2-C3
3	A	1102	PCW	O3P-C1-C2-O2
3	A	1103	PCW	O3P-C1-C2-O2
3	A	1101	PCW	O2-C2-C3-O3
3	A	1102	PCW	O2-C2-C3-O3

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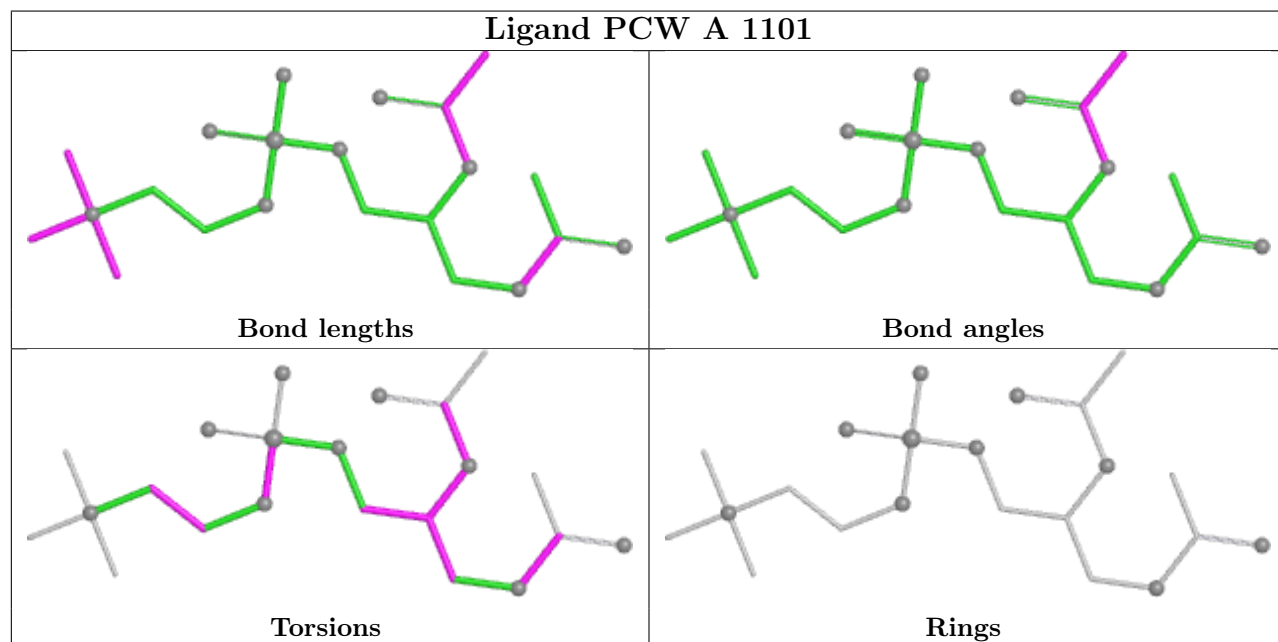
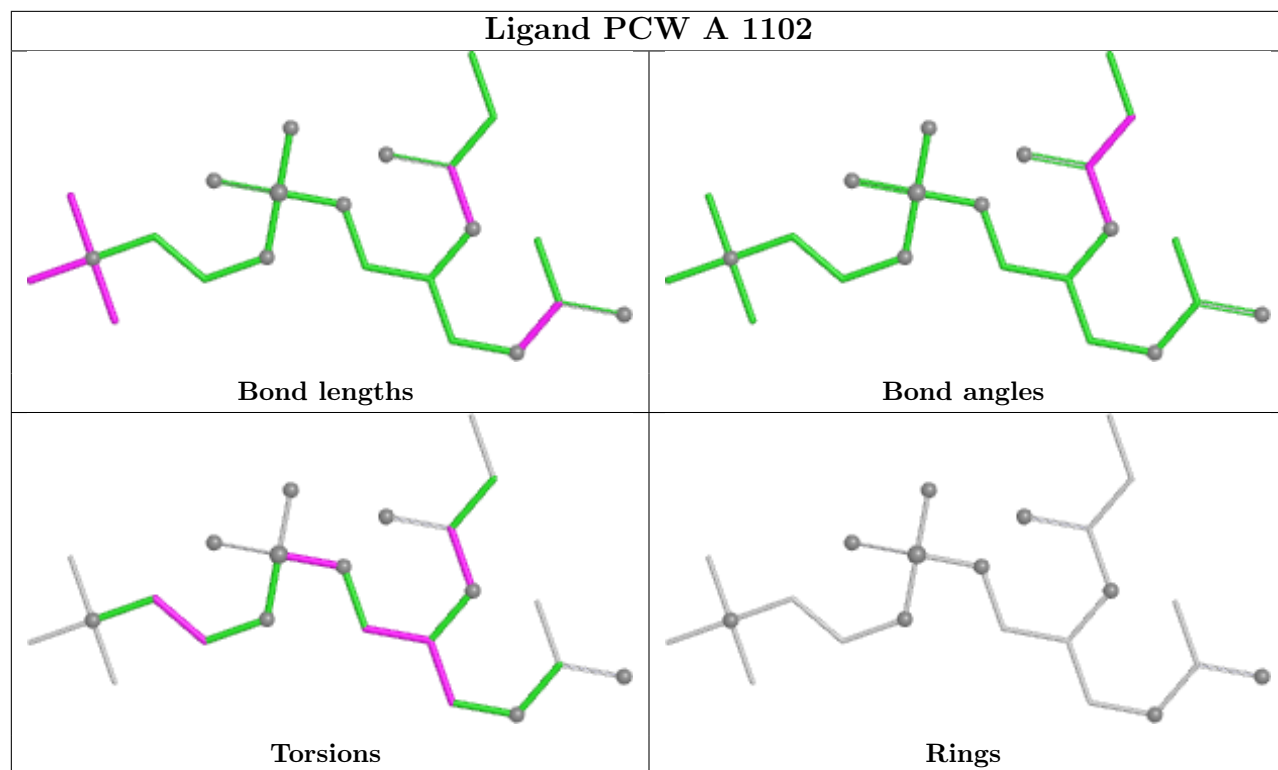
Mol	Chain	Res	Type	Atoms
3	A	1102	PCW	C1-O3P-P-O4P
5	A	1996	ACP	C5'-O5'-PA-O1A
2	A	1003	TG1	C33-C32-O9-C10
2	A	1003	TG1	C13-C14-C15-C16
2	A	1003	TG1	O2-C13-O1-C2
2	A	1003	TG1	C9-C10-O9-C32
5	A	1996	ACP	PG-C3B-PB-O1B
3	A	1101	PCW	O3P-C1-C2-C3
2	A	1003	TG1	O4-C21-C22-C23
2	A	1003	TG1	O1-C13-C14-C15

There are no ring outliers.

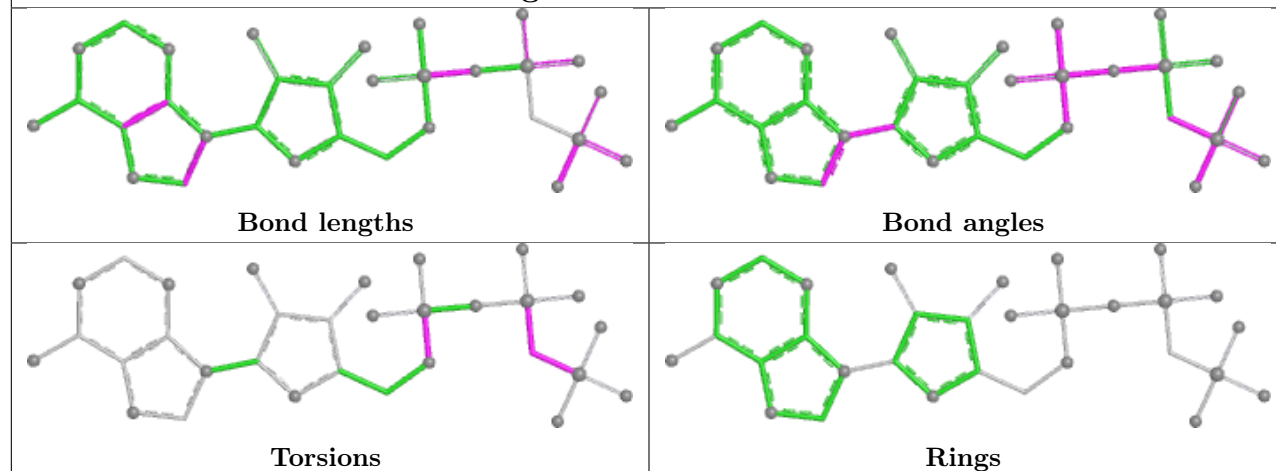
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	PCW	3	0
3	A	1101	PCW	3	0
5	A	1996	ACP	3	0
2	A	1003	TG1	3	0

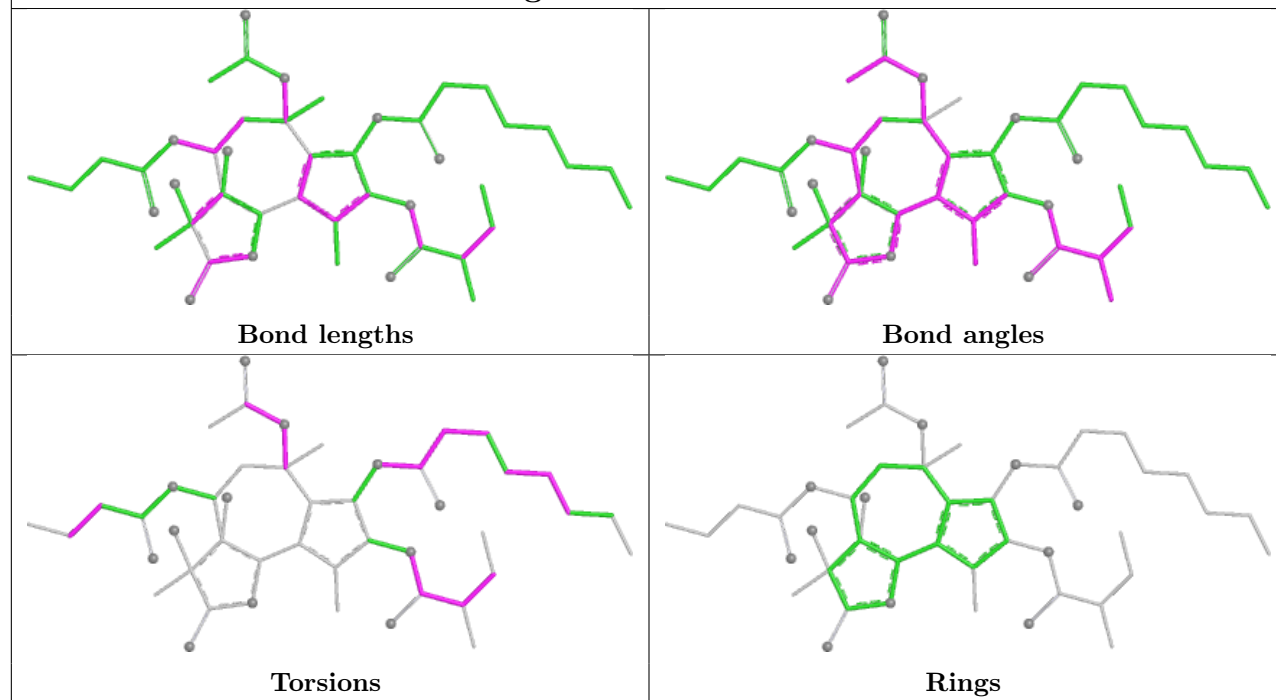
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

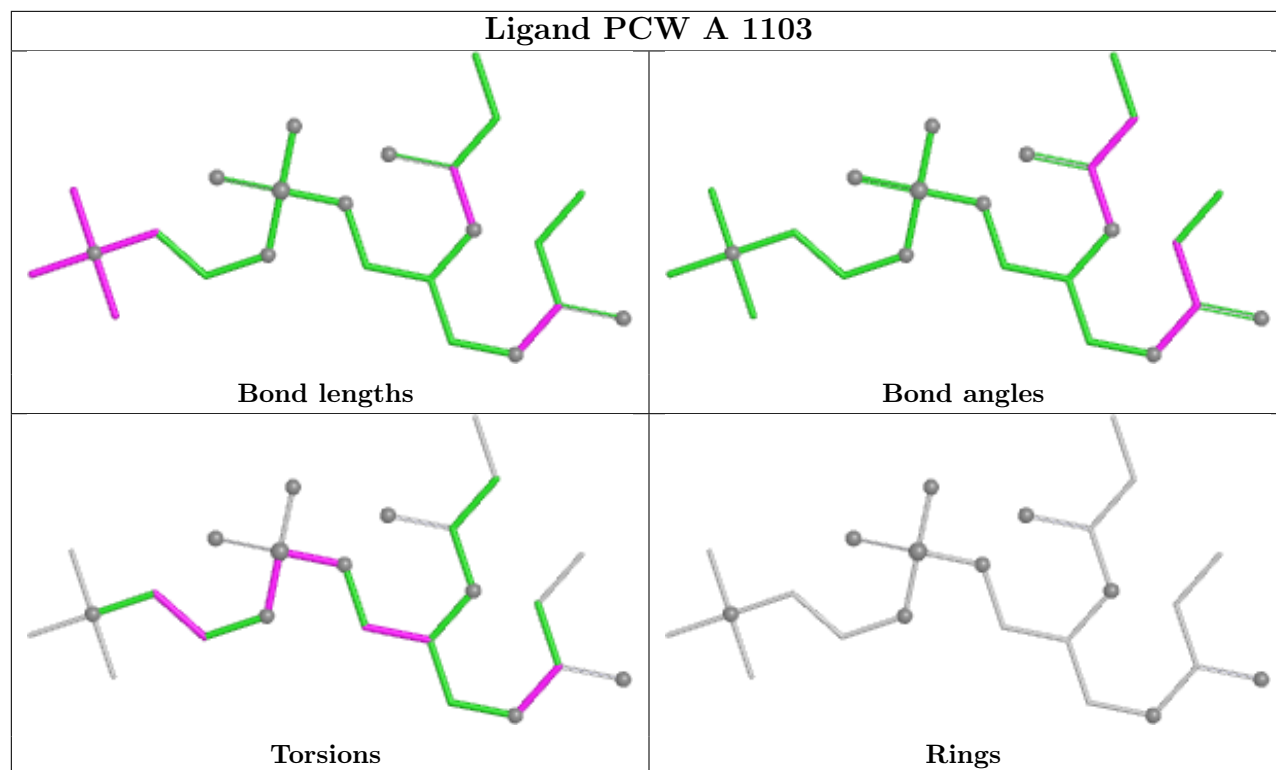


Ligand ACP A 1996



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%)	0.07	37 (3%) 45 36	47, 86, 146, 213	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	GLU	7.3
1	A	181	THR	5.8
1	A	183	GLU	5.7
1	A	182	GLY	4.7
1	A	626	GLY	4.0
1	A	681	PRO	3.6
1	A	627	ASP	3.6
1	A	938	CYS	3.4
1	A	184	SER	3.4
1	A	177	GLN	3.3
1	A	932	TRP	3.0
1	A	508	VAL	3.0
1	A	509	GLY	3.0
1	A	200	VAL	3.0
1	A	865	VAL	2.8
1	A	214	ILE	2.8
1	A	180	LEU	2.7
1	A	179	ILE	2.6
1	A	78	PHE	2.6
1	A	178	SER	2.5
1	A	870	LEU	2.5
1	A	886	LEU	2.5
1	A	209	PHE	2.5
1	A	505	ARG	2.5
1	A	414	ALA	2.4
1	A	507	ALA	2.4
1	A	992	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	885	GLY	2.3
1	A	176	ASP	2.3
1	A	202	GLN	2.2
1	A	883	PHE	2.2
1	A	706	ASN	2.1
1	A	679	VAL	2.1
1	A	400	LYS	2.1
1	A	676	PHE	2.1
1	A	208	LEU	2.0
1	A	705	VAL	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](#)

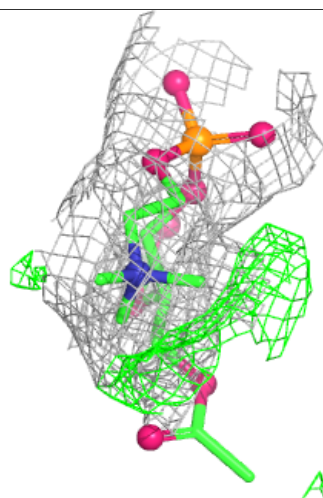
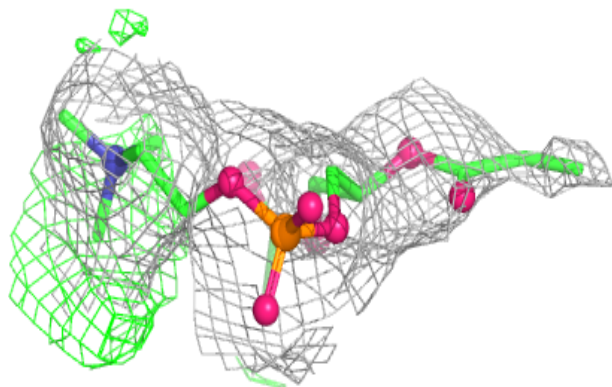
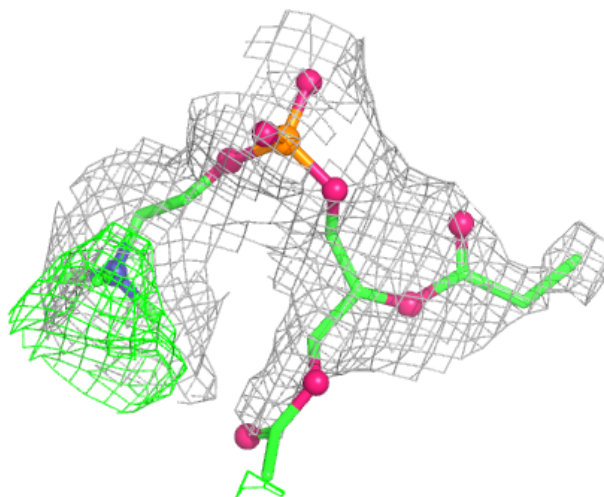
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	PCW	A	1102	23/54	0.60	0.19	70,134,142,165	0
3	PCW	A	1101	22/54	0.74	0.18	96,129,186,189	0
3	PCW	A	1103	24/54	0.74	0.13	59,123,150,150	0
4	GOL	A	1302	6/6	0.76	0.21	62,86,87,92	6
5	ACP	A	1996	31/31	0.78	0.15	50,94,129,172	31
7	MG	A	2002	1/1	0.86	0.16	159,159,159,159	0
4	GOL	A	1301	6/6	0.88	0.14	81,86,102,116	0
2	TG1	A	1003	46/46	0.94	0.10	60,90,111,114	0
6	K	A	2001	1/1	0.98	0.04	90,90,90,90	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.

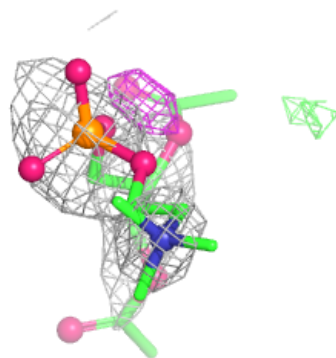
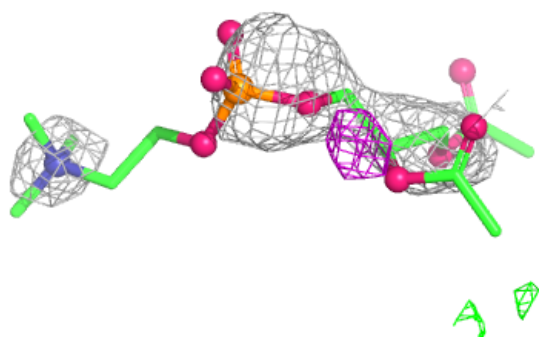
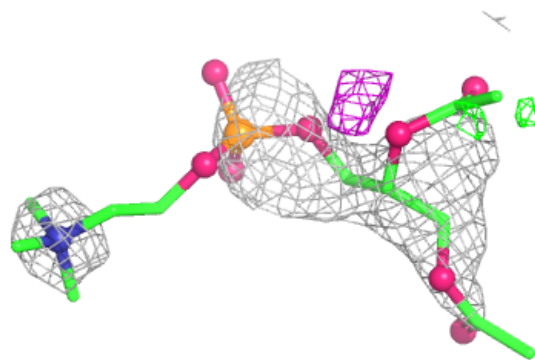
Electron density around PCW A 1102:

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

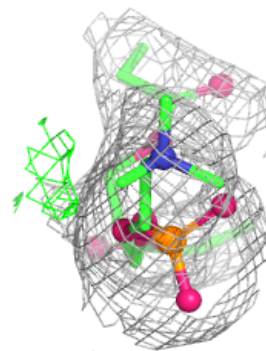
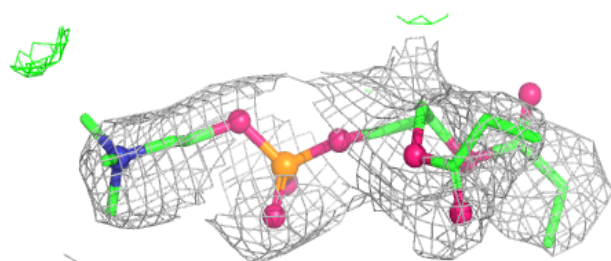
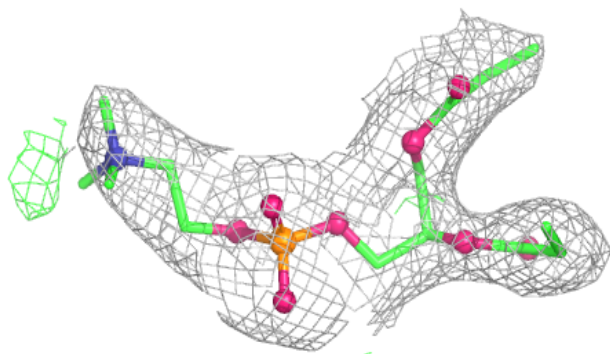


Electron density around PCW A 1101:

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

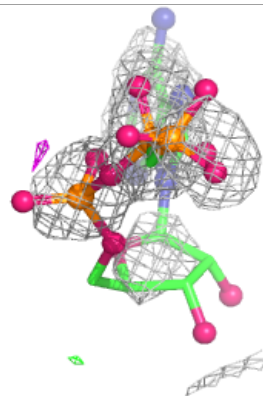
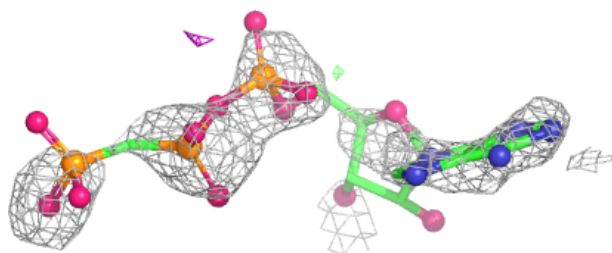
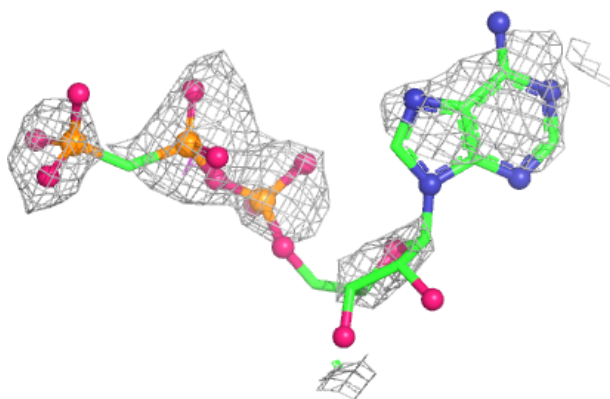
**Electron density around PCW A 1103:**

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

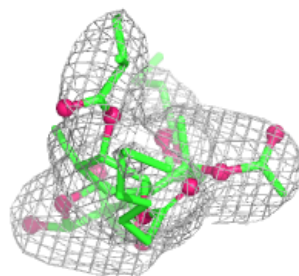
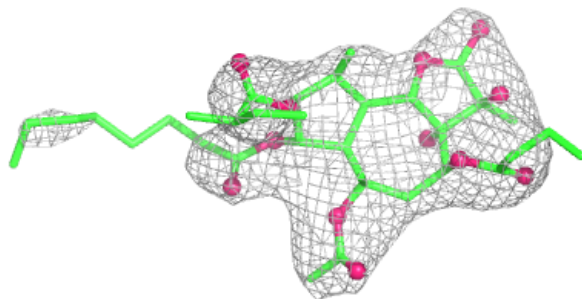
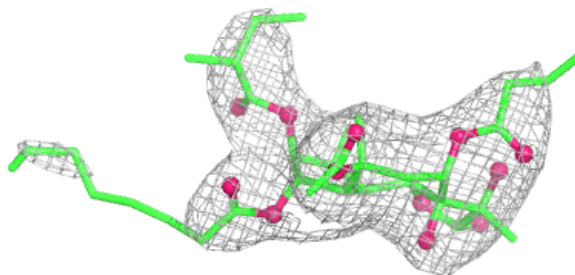


Electron density around ACP A 1996:

$2mF_o-DF_c$ (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.