W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:06 pm GMT

PDB ID : 4UU1

Title : CRYSTAL STRUCTURE OF (SR) CALCIUM-ATPASE E2(TG) IN THE PRESENCE OF DOPC

Authors : Drachmann, N.D.; Olesen, C.; Moeller, J.V.; Guo, Z.; Nissen, P.; Bublitz, M.

Deposited on : 2014-07-24

Resolution : 2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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.
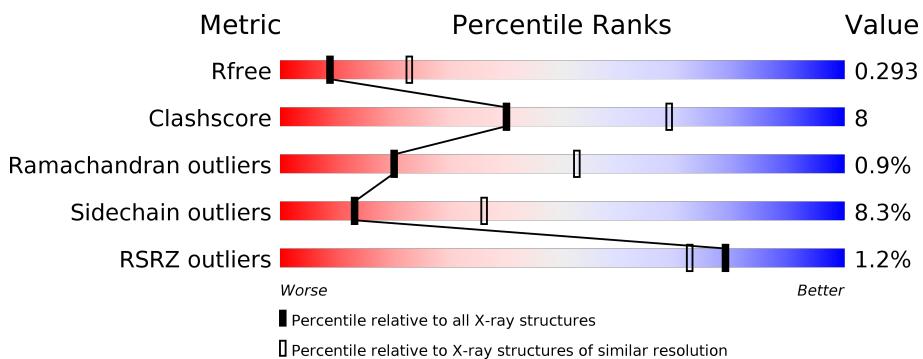
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	995	

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
2	TG1	A	1003	-	-	-	X
3	PCW	A	1101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	1302	-	-	-	X
5	ACP	A	1996	-	-	-	X

2 Entry composition ⓘ

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 7674	C 4878	N 1287	O 1452	S 57	0	0	0

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 (three-letter code: TG1) (formula: $C_{34}H_{50}O_{12}$).
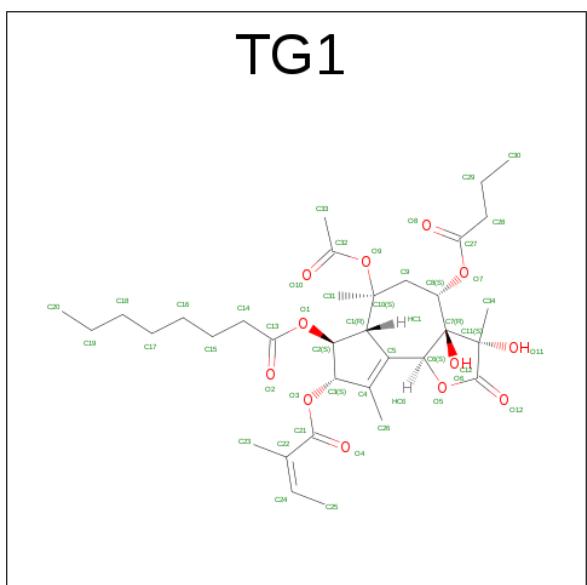
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 46	C 34	O 12	0	0

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).
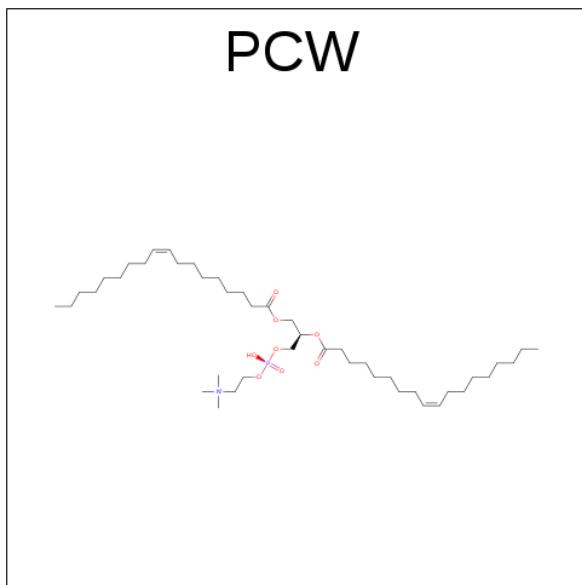
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 22	C 12	N 1	O 8	P 1	0	0
3	A	1	Total 23	C 13	N 1	O 8	P 1	0	0
3	A	1	Total 24	C 14	N 1	O 8	P 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
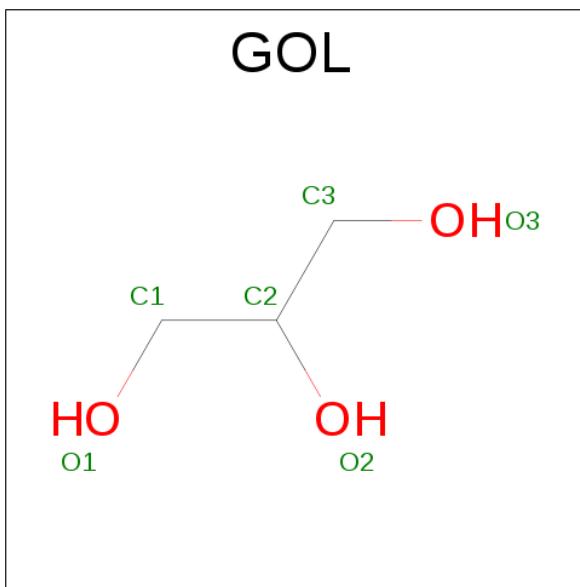
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
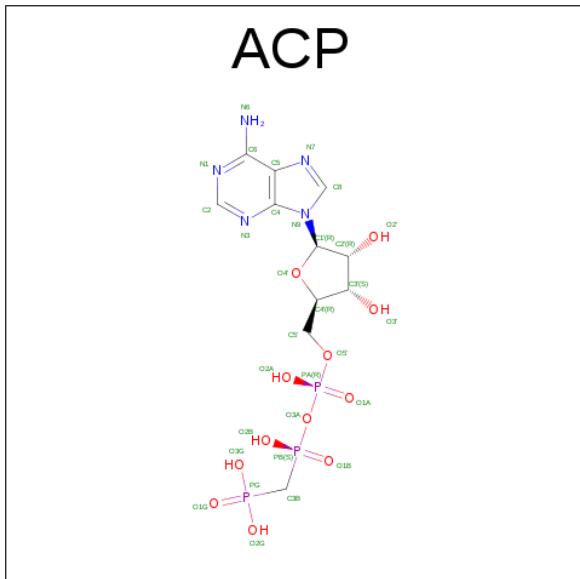
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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
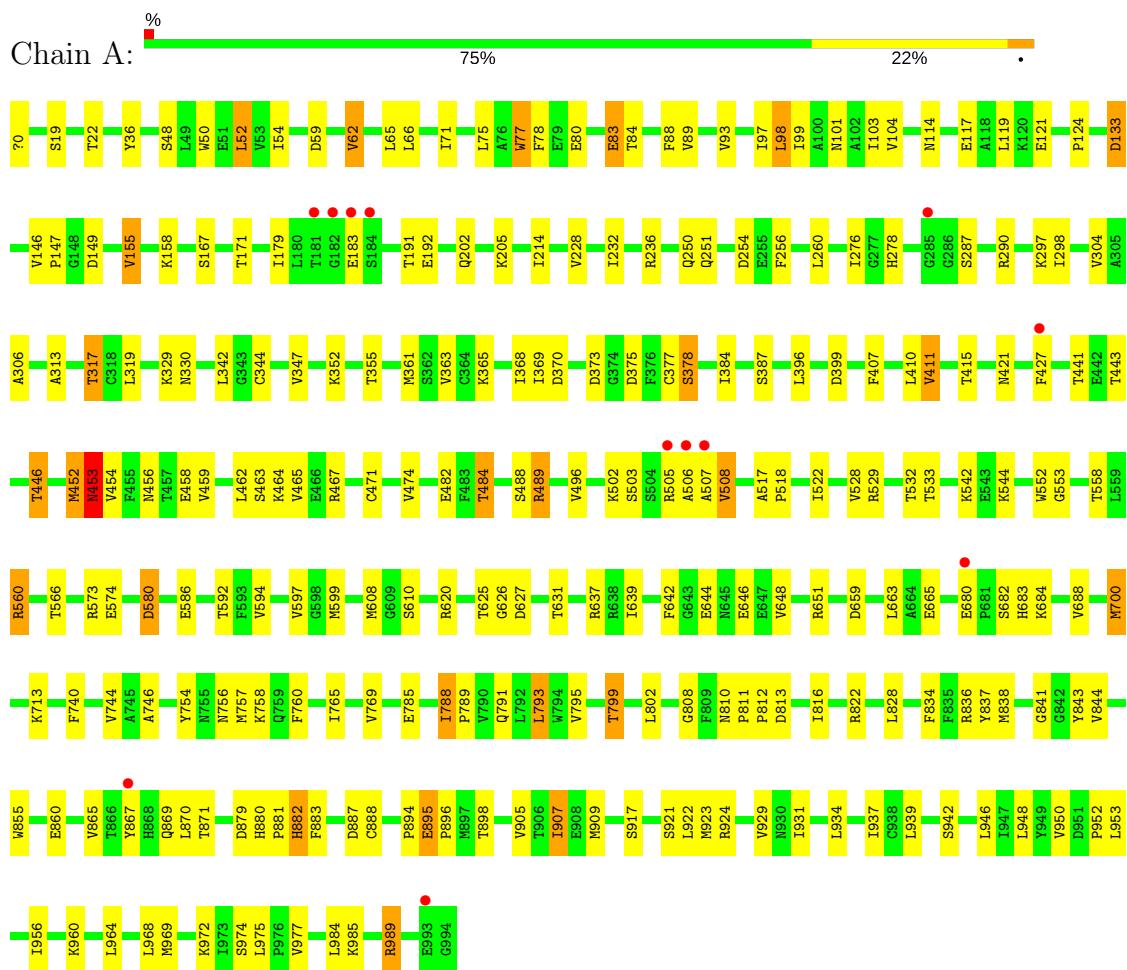
4 Data and refinement statistics ⓘ

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 73.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.80) 100.0 (73.91-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.293 0.221 , 0.293	Depositor DCC
R_{free} test set	1995 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, TG1, ACE, K, PCW, ACP

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	0.58	0/10594

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	128	0
2	A	46	0	50	2	0
3	A	69	0	60	6	0
4	A	12	0	16	0	0
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	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: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: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:580:ASP:N	1:A:580:ASP:OD1	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: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:560:ARG:HE	5:A:1996:ACP:H2'	1.69	0.57
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.87	0.57
1:A:909:MET:HE3	1:A:937:ILE:HA	1.85	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
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: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:865:VAL:HG12	1:A:867:TYR:HB2	1.91	0.53
1:A:66:LEU:HD12	1:A:98:LEU:HD23	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:837:TYR:HB2	2:A:1003:TG1:H331	1.92	0.52
1:A:421:ASN:ND2	1:A:446:THR:HG22	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:52:LEU:N	2.42	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:855:TRP:CE3	1:A:896:PRO:HB3	2.46	0.51
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.92	0.51
1:A:894:PRO:O	1:A:898:THR:HG23	2.11	0.51
1:A:89:VAL:O	1:A:93:VAL:HG23	2.11	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:923:MET:HB2	3:A:1102:PCW:H31	1.93	0.50
1:A:969:MET:HE3	1:A:972:LYS:HB3	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:361:MET:HE1	1:A:599:MET:HG3	1.95	0.48
1:A:155:VAL:HA	1:A:214:ILE:HG22	1.95	0.48
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
3:A:1102:PCW:H62	3:A:1102:PCW:H32	1.94	0.48
1:A:65:LEU:HA	1:A:65:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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
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:75:LEU:C	1:A:77:TRP:H	2.24	0.42
1:A:909:MET:HE3	1:A:937:ILE:HG23	2.01	0.42
1:A:250:GLN:HE21	3:A:1101:PCW:H71	1.85	0.41
1:A:80:GLU:CB	1:A:83:GLU:HB3	2.49	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:HA	1:A:793:LEU:HD13	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:319:LEU:HD21	1:A:757:MET:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:LYS:HD3	1:A:700:MET:HE1	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%)	20	52

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%)	770 (92%)	70 (8%)	13	36

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	121	GLU
1	A	133	ASP
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	191	THR
1	A	192	GLU
1	A	228	VAL
1	A	236	ARG
1	A	251	GLN
1	A	254	ASP
1	A	278	HIS
1	A	297	LYS
1	A	304	VAL
1	A	317	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	396	LEU

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Mol	Chain	Res	Type
1	A	399	ASP
1	A	411	VAL
1	A	441	THR
1	A	446	THR
1	A	452	MET
1	A	453	ASN
1	A	484	THR
1	A	489	ARG
1	A	503	SER
1	A	532	THR
1	A	533	THR
1	A	560	ARG
1	A	574	GLU
1	A	580	ASP
1	A	586	GLU
1	A	597	VAL
1	A	665	GLU
1	A	680	GLU
1	A	682	SER
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	860	GLU
1	A	870	LEU
1	A	879	ASP
1	A	882	HIS
1	A	895	GLU
1	A	907	ILE
1	A	917	SER
1	A	922	LEU
1	A	931	ILE
1	A	975	LEU
1	A	989	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
2	TG1	A	1003	-	43,48,48	1.91	8 (18%)	47,72,72	3.35	13 (27%)
3	PCW	A	1101	-	21,21,53	1.67	5 (23%)	26,29,61	1.33	1 (3%)
3	PCW	A	1102	-	22,22,53	1.54	5 (22%)	27,30,61	0.95	1 (3%)
3	PCW	A	1103	-	23,23,53	1.62	5 (21%)	28,31,61	1.14	2 (7%)
4	GOL	A	1301	-	5,5,5	0.36	0	5,5,5	0.26	0
4	GOL	A	1302	-	5,5,5	0.25	0	5,5,5	0.39	0
5	ACP	A	1996	7	27,33,33	1.66	5 (18%)	30,52,52	2.23	8 (26%)

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
2	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
3	PCW	A	1101	-	-	0/23/23/57	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCW	A	1102	-	-	0/25/25/57	0/0/0/0
3	PCW	A	1103	-	-	0/27/27/57	0/0/0/0
4	GOL	A	1301	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1302	-	-	0/4/4/4	0/0/0/0
5	ACP	A	1996	7	-	0/15/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1996	ACP	PB-O2B	-3.31	1.48	1.56
2	A	1003	TG1	O7-C8	-3.11	1.40	1.46
2	A	1003	TG1	O9-C10	-2.94	1.43	1.48
5	A	1996	ACP	PG-O3G	-2.58	1.48	1.54
3	A	1103	PCW	C6-N	-2.45	1.42	1.50
3	A	1101	PCW	C6-N	-2.44	1.42	1.50
3	A	1102	PCW	C6-N	-2.42	1.42	1.50
3	A	1103	PCW	C7-N	-2.25	1.43	1.50
3	A	1102	PCW	C7-N	-2.17	1.43	1.50
3	A	1101	PCW	C7-N	-2.12	1.43	1.50
3	A	1103	PCW	C8-N	-2.05	1.44	1.50
3	A	1101	PCW	C8-N	-2.03	1.44	1.50
3	A	1102	PCW	C8-N	-2.02	1.44	1.50
3	A	1101	PCW	O3-C11	2.08	1.43	1.33
2	A	1003	TG1	C1-C5	2.09	1.54	1.51
3	A	1102	PCW	O3-C11	2.25	1.44	1.33
5	A	1996	ACP	C2-N3	2.35	1.36	1.32
5	A	1996	ACP	PB-O1B	2.36	1.57	1.51
2	A	1003	TG1	C11-C7	2.62	1.58	1.55
2	A	1003	TG1	C9-C8	2.62	1.55	1.52
2	A	1003	TG1	C24-C22	3.41	1.53	1.30
5	A	1996	ACP	PG-O1G	3.76	1.58	1.50
3	A	1103	PCW	O3-C11	3.78	1.44	1.33
3	A	1103	PCW	O2-C31	3.96	1.45	1.34
2	A	1003	TG1	O5-C12	4.02	1.41	1.35
3	A	1102	PCW	O2-C31	4.10	1.46	1.34
3	A	1101	PCW	O2-C31	4.78	1.46	1.35
2	A	1003	TG1	O12-C12	7.92	1.39	1.20

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	TG1	O12-C12-C11	-15.88	113.16	128.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1003	TG1	O5-C12-O12	-10.90	106.59	121.63
5	A	1996	ACP	O2G-PG-O1G	-6.24	95.60	112.32
2	A	1003	TG1	C26-C4-C3	-4.92	111.87	120.89
2	A	1003	TG1	C23-C22-C24	-3.57	107.70	123.38
2	A	1003	TG1	C26-C4-C5	-3.53	120.63	129.77
2	A	1003	TG1	O3-C21-O4	-3.46	116.39	123.31
2	A	1003	TG1	O5-C12-C11	-3.41	105.18	110.15
5	A	1996	ACP	O5'-PA-O1A	-3.30	95.94	109.25
2	A	1003	TG1	C23-C22-C21	-2.88	108.57	116.01
2	A	1003	TG1	C7-C11-C12	-2.53	95.39	100.64
2	A	1003	TG1	O9-C32-C33	-2.38	105.94	110.73
5	A	1996	ACP	C1'-N9-C4	-2.37	122.54	126.64
5	A	1996	ACP	O1B-PB-C3B	2.11	114.19	108.97
5	A	1996	ACP	O2G-PG-C3B	2.35	112.09	106.40
2	A	1003	TG1	O7-C8-C9	2.39	112.42	107.30
2	A	1003	TG1	O11-C11-C12	2.40	113.01	105.94
5	A	1996	ACP	O3G-PG-C3B	2.47	112.39	106.40
5	A	1996	ACP	O2A-PA-O5'	2.60	120.40	108.14
3	A	1102	PCW	O2-C31-C32	3.12	120.23	110.74
3	A	1103	PCW	O2-C31-C32	3.16	120.36	110.74
3	A	1103	PCW	O3-C11-C12	3.53	120.82	111.35
2	A	1003	TG1	C10-O9-C32	4.48	133.13	121.83
3	A	1101	PCW	O2-C31-C32	5.16	120.79	111.10
5	A	1996	ACP	PA-O3A-PB	7.28	155.85	132.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

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%)	-0.15	12 (1%)	79	72	47, 86, 146, 213	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	GLU	4.8
1	A	505	ARG	4.0
1	A	506	ALA	3.8
1	A	867	TYR	3.5
1	A	182	GLY	3.4
1	A	184	SER	3.3
1	A	507	ALA	3.3
1	A	993	GLU	2.8
1	A	680	GLU	2.7
1	A	181	THR	2.5
1	A	427	PHE	2.2
1	A	285	GLY	2.2

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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å²)	Q<0.9
5	ACP	A	1996	31/31	0.83	0.48	5.92	50,94,129,172	31
3	PCW	A	1101	22/54	0.76	0.53	4.59	96,129,186,189	0
2	TG1	A	1003	46/46	0.97	0.28	2.24	60,90,111,114	0
4	GOL	A	1302	6/6	0.78	0.40	0.66	62,86,87,92	6
3	PCW	A	1103	24/54	0.88	0.21	0.31	59,123,150,150	0
3	PCW	A	1102	23/54	0.80	0.17	-0.44	70,134,142,165	0
4	GOL	A	1301	6/6	0.94	0.14	-0.92	81,86,102,116	0
6	K	A	2001	1/1	0.93	0.10	-1.68	90,90,90,90	0
7	MG	A	2002	1/1	0.89	0.63	-	159,159,159,159	0

6.5 Other polymers ⓘ

There are no such residues in this entry.