



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:46 AM GMT

PDB ID : 2EAT  
Title : Crystal structure of the SR CA2+-ATPASE with bound CPA and TG  
Authors : Takahashi, M.; Kondou, Y.; Toyoshima, C.  
Deposited on : 2007-02-02  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

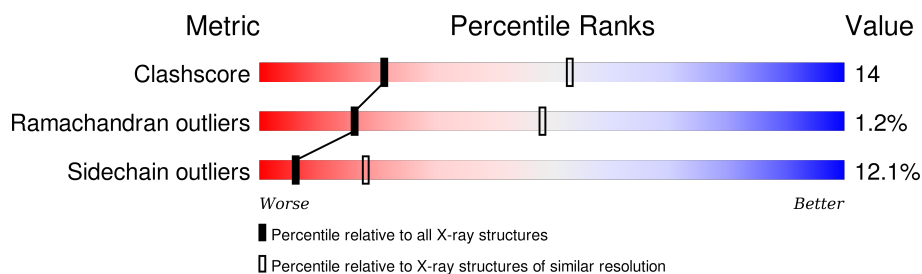
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

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
3	CZA	A	1005	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7744 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

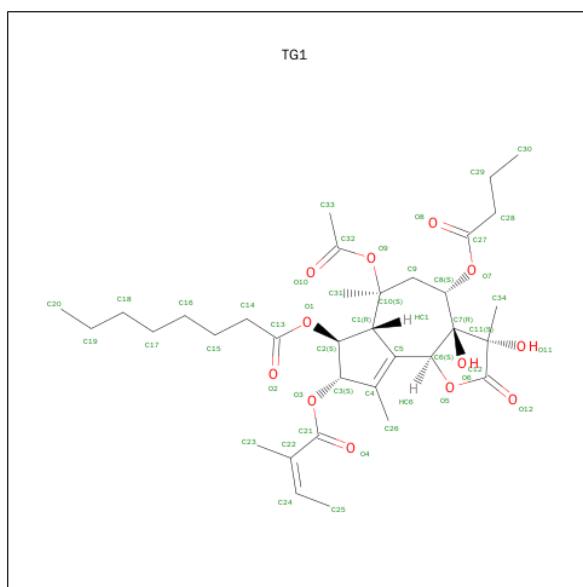
- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	995	Total	C	N	O	S	0	0	0
			7673	4878	1287	1451	57			

There is a discrepancy between the modelled and reference sequences:

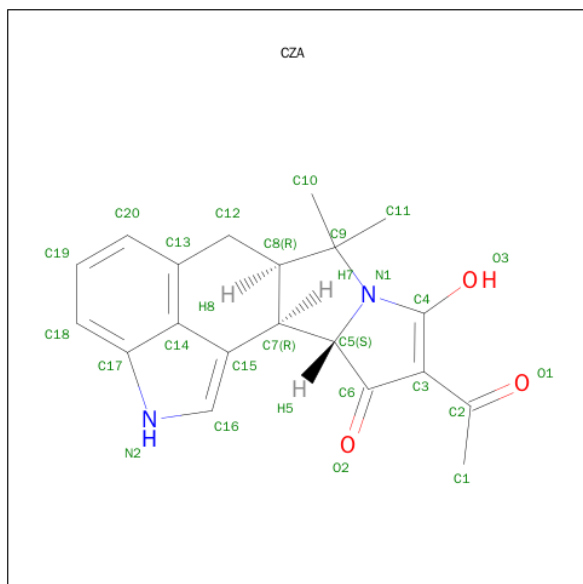
Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9B ALPHA]]-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<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



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

- Molecule 3 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).



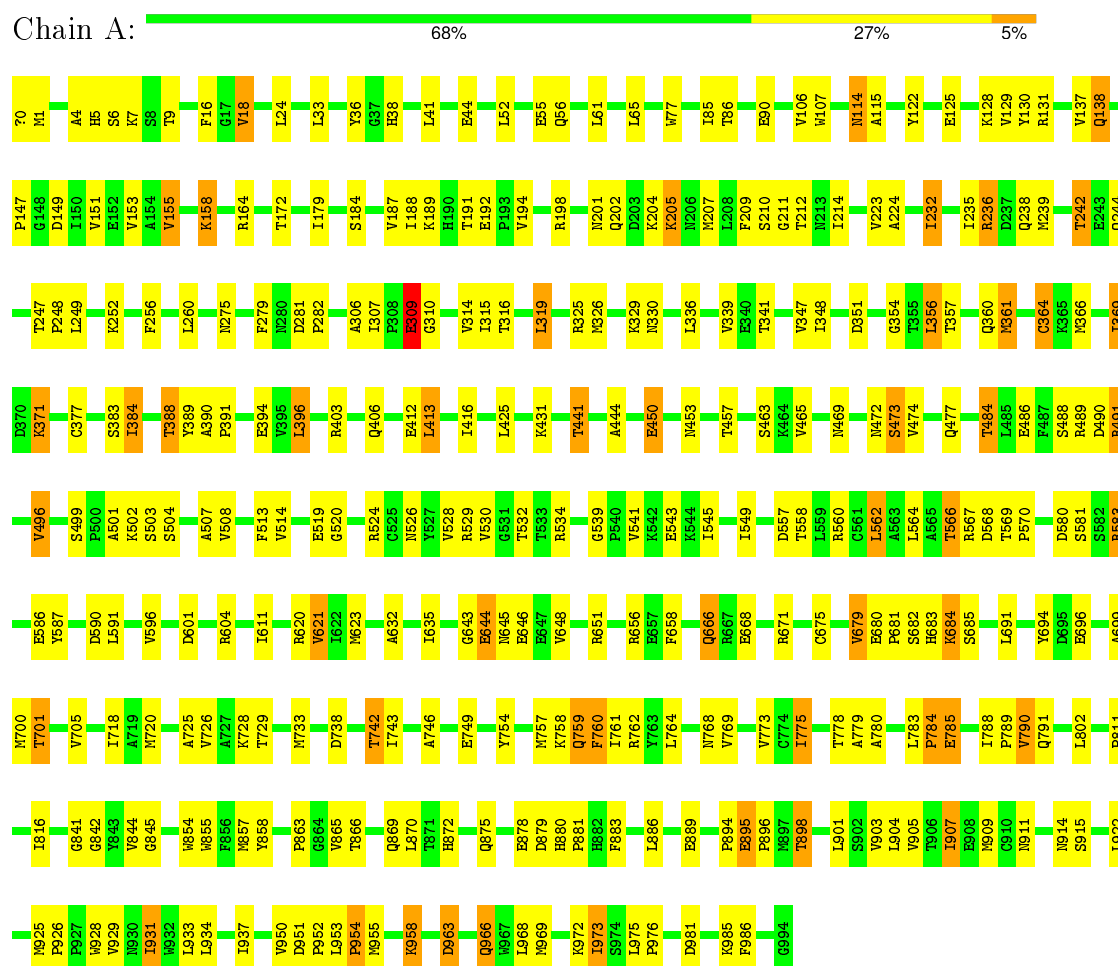
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	25	20	2	3	0	0

### 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 errors 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.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.90 Å 95.64 Å 155.10 Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (15.00-2.90)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.244 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	1/7812 (0.0%)	0.65	0/10594

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	364	CYS	CB-SG	-6.07	1.72	1.82

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	557	ASP	Peptide

### 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	7673	0	7765	221	0
2	A	46	0	50	3	0
3	A	25	0	19	5	0
All	All	7744	0	7834	221	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 14.

All (221) 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:0:ACE:H1	1:A:16:PHE:CE2	1.84	1.13
1:A:0:ACE:C	1:A:147:PRO:HB2	1.77	1.04
1:A:232:ILE:H	1:A:232:ILE:HD12	1.27	1.00
1:A:0:ACE:CH3	1:A:147:PRO:HB2	1.93	0.99
1:A:558:THR:O	1:A:558:THR:HG22	1.62	0.97
1:A:0:ACE:CH3	1:A:16:PHE:HE2	1.80	0.94
1:A:0:ACE:CH3	1:A:16:PHE:CE2	2.53	0.90
1:A:539:GLY:O	1:A:543:GLU:HG2	1.72	0.89
1:A:0:ACE:O	1:A:147:PRO:CB	2.20	0.89
1:A:0:ACE:O	1:A:147:PRO:HG2	1.73	0.88
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.55	0.88
1:A:164:ARG:HD3	1:A:207:MET:HE2	1.56	0.87
1:A:383:SER:HB2	1:A:396:LEU:HD11	1.58	0.86
1:A:0:ACE:C	1:A:147:PRO:CB	2.43	0.86
1:A:4:ALA:HB1	1:A:7:LYS:HG2	1.56	0.85
1:A:164:ARG:HD3	1:A:207:MET:CE	2.06	0.85
1:A:383:SER:HB2	1:A:396:LEU:CD1	2.07	0.84
1:A:281:ASP:HB2	1:A:282:PRO:HD3	1.60	0.84
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.61	0.83
1:A:351:ASP:H	1:A:701:THR:HG21	1.43	0.83
1:A:5:HIS:HA	1:A:207:MET:HE3	1.61	0.82
1:A:153:VAL:HB	1:A:214:ILE:HD11	1.62	0.81
1:A:232:ILE:H	1:A:232:ILE:CD1	1.93	0.81
1:A:0:ACE:O	1:A:147:PRO:CG	2.29	0.80
1:A:388:THR:HG23	1:A:390:ALA:H	1.46	0.80
1:A:0:ACE:O	1:A:147:PRO:HB2	1.80	0.77
1:A:351:ASP:OD2	1:A:701:THR:HG23	1.85	0.77
1:A:153:VAL:HB	1:A:214:ILE:CD1	2.15	0.75
1:A:202:GLN:NE2	1:A:489:ARG:HD2	2.02	0.75
1:A:720:MET:HE3	1:A:738:ASP:HA	1.70	0.74
1:A:788:ILE:CG1	1:A:789:PRO:HD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:ACE:H3	1:A:36:TYR:CE1	2.23	0.73
1:A:122:TYR:HE1	1:A:726:VAL:HG21	1.54	0.72
1:A:486:GLU:O	1:A:491:ARG:NH2	2.22	0.72
1:A:232:ILE:N	1:A:232:ILE:HD12	2.04	0.72
1:A:351:ASP:H	1:A:701:THR:CG2	2.02	0.72
1:A:783:LEU:N	1:A:784:PRO:HD2	2.04	0.72
1:A:788:ILE:HG12	1:A:789:PRO:HD2	1.72	0.71
1:A:56:GLN:HG3	3:A:1005:CZA:H18	1.72	0.71
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.71	0.71
1:A:202:GLN:HE22	1:A:489:ARG:HD2	1.57	0.70
1:A:209:PHE:O	1:A:212:THR:HB	1.90	0.70
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.73	0.69
1:A:52:LEU:HB3	1:A:106:VAL:HG21	1.74	0.69
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.75	0.69
1:A:4:ALA:HB1	1:A:7:LYS:CG	2.24	0.68
1:A:0:ACE:CH3	1:A:36:TYR:CE1	2.77	0.67
1:A:558:THR:CG2	1:A:558:THR:O	2.37	0.67
1:A:880:HIS:H	1:A:881:PRO:HD2	1.60	0.67
1:A:758:LYS:O	1:A:762:ARG:HG3	1.96	0.65
1:A:210:SER:HB3	1:A:232:ILE:HD13	1.78	0.65
1:A:65:LEU:HD13	1:A:307:ILE:HG13	1.77	0.65
1:A:351:ASP:OD2	1:A:701:THR:CG2	2.46	0.63
1:A:469:ASN:O	1:A:473:SER:OG	2.16	0.63
1:A:202:GLN:NE2	1:A:489:ARG:CD	2.61	0.63
1:A:895:GLU:O	1:A:898:THR:HG22	1.99	0.62
1:A:963:ASP:HB2	1:A:966:GLN:HB2	1.81	0.61
1:A:369:ILE:HG21	1:A:530:VAL:HG22	1.83	0.61
1:A:122:TYR:O	1:A:211:GLY:HA2	2.01	0.61
1:A:122:TYR:HE1	1:A:726:VAL:CG2	2.14	0.61
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.82	0.60
1:A:773:VAL:HG11	1:A:842:GLY:HA2	1.83	0.60
1:A:758:LYS:HG2	1:A:762:ARG:CZ	2.31	0.60
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.83	0.60
1:A:4:ALA:CB	1:A:7:LYS:HG2	2.29	0.60
1:A:783:LEU:N	1:A:784:PRO:CD	2.66	0.59
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.84	0.59
1:A:0:ACE:H2	1:A:16:PHE:HE2	1.66	0.59
1:A:330:ASN:HB2	1:A:742:THR:HG21	1.84	0.59
1:A:1:MET:HA	1:A:224:ALA:O	2.03	0.59
1:A:129:VAL:HG12	1:A:131:ARG:HG2	1.83	0.59
1:A:361:MET:SD	1:A:601:ASP:HB2	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.03	0.58
1:A:484:THR:HB	1:A:496:VAL:HG22	1.86	0.58
1:A:880:HIS:N	1:A:881:PRO:HD2	2.18	0.57
1:A:52:LEU:HB3	1:A:106:VAL:CG2	2.35	0.57
1:A:545:ILE:O	1:A:549:ILE:HG12	2.05	0.57
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.87	0.57
1:A:319:LEU:HB3	1:A:336:LEU:HG	1.87	0.57
1:A:473:SER:O	1:A:477:GLN:HG2	2.06	0.56
1:A:130:TYR:CZ	1:A:137:VAL:HG12	2.40	0.56
1:A:90:GLU:OE1	1:A:790:VAL:HG22	2.05	0.56
1:A:0:ACE:H3	1:A:147:PRO:HB2	1.86	0.56
1:A:950:VAL:O	1:A:954:PRO:HD2	2.04	0.56
1:A:720:MET:HE3	1:A:738:ASP:CA	2.35	0.56
1:A:520:GLY:O	1:A:524:ARG:HG3	2.06	0.56
1:A:733:MET:HE1	1:A:746:ALA:HB1	1.88	0.56
1:A:205:LYS:HE3	1:A:488:SER:OG	2.06	0.56
1:A:326:MET:HG3	1:A:749:GLU:HG2	1.87	0.56
1:A:911:ASN:HA	1:A:914:ASN:HB2	1.88	0.56
1:A:754:TYR:HA	1:A:757:MET:HE2	1.87	0.56
1:A:383:SER:HB2	1:A:396:LEU:HD12	1.87	0.55
1:A:549:ILE:CD1	1:A:596:VAL:HG21	2.37	0.55
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.88	0.55
1:A:309:GLU:HA	3:A:1005:CZA:H101	1.87	0.55
1:A:519:GLU:HG2	1:A:520:GLY:H	1.70	0.55
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.87	0.55
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.89	0.54
1:A:307:ILE:HG23	3:A:1005:CZA:C11	2.37	0.54
1:A:412:GLU:OE2	1:A:566:THR:HG21	2.06	0.54
1:A:307:ILE:HG23	3:A:1005:CZA:H111	1.88	0.54
1:A:18:VAL:HG13	1:A:24:LEU:HD23	1.89	0.54
1:A:725:ALA:O	1:A:729:THR:HG23	2.08	0.54
1:A:56:GLN:OE1	3:A:1005:CZA:N2	2.31	0.54
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.36	0.53
1:A:501:ALA:O	1:A:503:SER:N	2.35	0.53
1:A:783:LEU:H	1:A:784:PRO:HD2	1.70	0.53
1:A:106:VAL:O	1:A:106:VAL:HG13	2.09	0.53
1:A:894:PRO:HA	1:A:958:LYS:HG3	1.89	0.53
1:A:153:VAL:CB	1:A:214:ILE:HD11	2.36	0.53
1:A:508:VAL:HG12	1:A:508:VAL:O	2.09	0.53
1:A:658:PHE:CZ	1:A:666:GLN:HG2	2.44	0.53
1:A:878:GLU:HB2	1:A:880:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:THR:HG21	1:A:635:ILE:HG12	1.90	0.52
1:A:129:VAL:CG1	1:A:131:ARG:HG2	2.40	0.52
1:A:41:LEU:HD13	1:A:236:ARG:HG3	1.91	0.51
1:A:904:LEU:HA	1:A:907:ILE:HD11	1.92	0.51
1:A:933:LEU:O	1:A:937:ILE:HG12	2.11	0.51
1:A:137:VAL:O	1:A:137:VAL:HG23	2.11	0.51
1:A:232:ILE:N	1:A:232:ILE:CD1	2.70	0.51
1:A:0:ACE:CH3	1:A:36:TYR:CZ	2.94	0.50
1:A:878:GLU:HB2	1:A:880:HIS:HD2	1.76	0.50
1:A:129:VAL:CG1	1:A:130:TYR:N	2.75	0.50
1:A:122:TYR:CE1	1:A:726:VAL:CG2	2.94	0.50
1:A:463:SER:C	1:A:465:VAL:H	2.15	0.50
1:A:122:TYR:HA	1:A:158:LYS:HE3	1.93	0.50
1:A:857:MET:HA	1:A:866:THR:HA	1.94	0.49
1:A:354:GLY:O	1:A:604:ARG:NH2	2.45	0.49
1:A:671:ARG:HB3	1:A:694:TYR:CE1	2.47	0.49
1:A:855:TRP:CD1	1:A:896:PRO:HB3	2.47	0.49
1:A:783:LEU:H	1:A:784:PRO:CD	2.24	0.49
1:A:684:LYS:HG3	1:A:700:MET:SD	2.53	0.49
1:A:4:ALA:CB	1:A:7:LYS:CG	2.89	0.48
1:A:922:LEU:O	1:A:926:PRO:HA	2.12	0.48
1:A:122:TYR:CE1	1:A:726:VAL:HG21	2.42	0.48
1:A:450:GLU:OE1	1:A:472:ASN:ND2	2.43	0.48
1:A:504:SER:HA	1:A:507:ALA:HB2	1.95	0.48
1:A:347:VAL:HG22	1:A:620:ARG:HB2	1.95	0.48
1:A:953:LEU:C	1:A:955:MET:H	2.16	0.48
1:A:611:ILE:HG23	1:A:621:VAL:HG11	1.95	0.48
1:A:281:ASP:CB	1:A:282:PRO:HD3	2.39	0.48
1:A:425:LEU:O	1:A:469:ASN:ND2	2.45	0.48
1:A:248:PRO:O	1:A:252:LYS:HG2	2.14	0.48
1:A:164:ARG:HA	1:A:207:MET:HE2	1.96	0.47
1:A:844:VAL:HB	1:A:907:ILE:HD12	1.96	0.47
1:A:768:ASN:HB3	2:A:1003:TG1:H251	1.97	0.47
1:A:895:GLU:H	1:A:896:PRO:HD2	1.79	0.47
1:A:560:ARG:NH1	1:A:562:LEU:HD11	2.28	0.47
1:A:583:ARG:NH1	1:A:587:TYR:OH	2.47	0.47
1:A:369:ILE:CG2	1:A:530:VAL:HG22	2.44	0.47
1:A:356:LEU:HD23	1:A:623:MET:HG3	1.95	0.47
1:A:903:VAL:HG12	1:A:907:ILE:HD13	1.96	0.47
1:A:632:ALA:HB1	1:A:675:CYS:SG	2.54	0.47
1:A:329:LYS:O	1:A:742:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.97	0.47
1:A:981:ASP:O	1:A:985:LYS:N	2.36	0.46
1:A:951:ASP:O	1:A:952:PRO:C	2.52	0.46
1:A:6:SER:HA	1:A:194:VAL:O	2.15	0.46
1:A:733:MET:HE1	1:A:746:ALA:CB	2.45	0.46
1:A:238:GLN:O	1:A:242:THR:HG23	2.15	0.46
1:A:769:VAL:HG12	1:A:841:GLY:HA3	1.97	0.46
1:A:769:VAL:HA	2:A:1003:TG1:H24	1.97	0.46
1:A:238:GLN:O	1:A:242:THR:CG2	2.63	0.46
1:A:791:GLN:HB3	1:A:901:LEU:HD13	1.98	0.46
1:A:164:ARG:CD	1:A:207:MET:HE2	2.38	0.45
1:A:348:ILE:HD12	1:A:743:ILE:HG21	1.98	0.45
1:A:114:ASN:HD22	1:A:115:ALA:H	1.62	0.45
1:A:256:PHE:HD1	2:A:1003:TG1:HC6	1.82	0.44
1:A:788:ILE:HG13	1:A:789:PRO:HD2	1.99	0.44
1:A:310:GLY:O	1:A:314:VAL:HG23	2.18	0.44
1:A:775:ILE:HA	1:A:778:THR:HG22	2.00	0.44
1:A:759:GLN:HG3	1:A:915:SER:O	2.18	0.44
1:A:129:VAL:HG11	1:A:131:ARG:HE	1.83	0.44
1:A:785:GLU:H	1:A:785:GLU:HG3	1.53	0.44
1:A:189:LYS:HE3	1:A:207:MET:O	2.18	0.44
1:A:413:LEU:HD22	1:A:564:LEU:HD12	2.00	0.44
1:A:526:ASN:ND2	1:A:590:ASP:HA	2.33	0.44
1:A:648:VAL:C	1:A:651:ARG:HG3	2.38	0.44
1:A:931:ILE:HD12	1:A:931:ILE:H	1.83	0.43
1:A:366:MET:HG2	1:A:384:ILE:HD11	1.99	0.43
1:A:179:ILE:O	1:A:705:VAL:HG13	2.17	0.43
1:A:235:ILE:O	1:A:239:MET:HG3	2.19	0.43
1:A:192:GLU:OE2	1:A:580:ASP:HB3	2.18	0.43
1:A:315:ILE:HG13	1:A:316:THR:N	2.34	0.43
1:A:975:LEU:N	1:A:976:PRO:CD	2.81	0.43
1:A:760:PHE:C	1:A:760:PHE:CD1	2.92	0.43
1:A:147:PRO:HA	1:A:223:VAL:HG12	2.01	0.43
1:A:65:LEU:HD22	1:A:307:ILE:HG21	2.00	0.43
1:A:391:PRO:HB3	1:A:450:GLU:HB3	2.01	0.43
1:A:361:MET:HG2	1:A:441:THR:HA	2.00	0.42
1:A:61:LEU:HD21	1:A:260:LEU:HB3	2.01	0.42
1:A:403:ARG:CZ	1:A:406:GLN:HG3	2.49	0.42
1:A:854:TRP:CZ2	1:A:858:TYR:CD2	3.07	0.42
1:A:453:ASN:ND2	1:A:457:THR:O	2.49	0.42
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:VAL:HA	1:A:651:ARG:HG3	2.01	0.42
1:A:514:VAL:HG21	1:A:591:LEU:HD22	2.01	0.42
1:A:416:ILE:HG21	1:A:564:LEU:HB3	2.01	0.41
1:A:348:ILE:HA	1:A:699:ALA:HB3	2.02	0.41
1:A:718:ILE:HD13	1:A:743:ILE:HG12	2.02	0.41
1:A:388:THR:HG23	1:A:390:ALA:N	2.23	0.41
1:A:137:VAL:O	1:A:138:GLN:C	2.57	0.41
1:A:357:THR:HA	1:A:604:ARG:H	1.85	0.41
1:A:33:LEU:HD11	1:A:38:HIS:ND1	2.35	0.41
1:A:416:ILE:HD11	1:A:566:THR:HG22	2.03	0.41
1:A:754:TYR:HA	1:A:757:MET:CE	2.49	0.41
1:A:869:GLN:O	1:A:872:HIS:HB2	2.19	0.41
1:A:643:GLY:N	1:A:646:GLU:HG2	2.36	0.41
1:A:138:GLN:HG2	1:A:138:GLN:H	1.68	0.41
1:A:894:PRO:CA	1:A:958:LYS:HG3	2.51	0.41
1:A:513:PHE:CD1	1:A:566:THR:HB	2.56	0.41
1:A:457:THR:OG1	1:A:474:VAL:HG21	2.21	0.41
1:A:371:LYS:HE3	1:A:371:LYS:HB2	1.76	0.40
1:A:153:VAL:CG2	1:A:214:ILE:HD11	2.51	0.40
1:A:878:GLU:HG3	1:A:879:ASP:N	2.37	0.40
1:A:364:CYS:O	1:A:383:SER:HA	2.22	0.40
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.56	0.40
1:A:356:LEU:HA	1:A:356:LEU:HD12	1.97	0.40
1:A:513:PHE:HD1	1:A:566:THR:HB	1.87	0.40
1:A:969:MET:O	1:A:973:ILE:HB	2.20	0.40
1:A:905:VAL:O	1:A:909:MET:HG2	2.21	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	993/995 (100%)	876 (88%)	105 (11%)	12 (1%)	16	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LYS
1	A	644	GLU
1	A	77	TRP
1	A	184	SER
1	A	780	ALA
1	A	863	PRO
1	A	895	GLU
1	A	954	PRO
1	A	309	GLU
1	A	779	ALA
1	A	155	VAL
1	A	784	PRO

### 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%)	738 (88%)	102 (12%)	6	18

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	18	VAL
1	A	44	GLU
1	A	55	GLU
1	A	85	ILE
1	A	86	THR
1	A	107	TRP
1	A	114	ASN
1	A	125	GLU

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Mol	Chain	Res	Type
1	A	128	LYS
1	A	138	GLN
1	A	151	VAL
1	A	155	VAL
1	A	158	LYS
1	A	172	THR
1	A	187	VAL
1	A	188	ILE
1	A	191	THR
1	A	198	ARG
1	A	205	LYS
1	A	232	ILE
1	A	236	ARG
1	A	242	THR
1	A	244	GLN
1	A	247	THR
1	A	249	LEU
1	A	275	ASN
1	A	279	PHE
1	A	309	GLU
1	A	319	LEU
1	A	325	ARG
1	A	339	VAL
1	A	341	THR
1	A	356	LEU
1	A	360	GLN
1	A	361	MET
1	A	369	ILE
1	A	371	LYS
1	A	377	CYS
1	A	384	ILE
1	A	388	THR
1	A	394	GLU
1	A	396	LEU
1	A	413	LEU
1	A	431	LYS
1	A	441	THR
1	A	450	GLU
1	A	473	SER
1	A	484	THR
1	A	490	ASP
1	A	491	ARG

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Mol	Chain	Res	Type
1	A	496	VAL
1	A	499	SER
1	A	532	THR
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	569	THR
1	A	581	SER
1	A	583	ARG
1	A	586	GLU
1	A	621	VAL
1	A	644	GLU
1	A	645	ASN
1	A	656	ARG
1	A	666	GLN
1	A	668	GLU
1	A	679	VAL
1	A	682	SER
1	A	684	LYS
1	A	685	SER
1	A	691	LEU
1	A	696	GLU
1	A	701	THR
1	A	728	LYS
1	A	742	THR
1	A	759	GLN
1	A	760	PHE
1	A	761	ILE
1	A	764	LEU
1	A	775	ILE
1	A	785	GLU
1	A	790	VAL
1	A	802	LEU
1	A	816	ILE
1	A	865	VAL
1	A	870	LEU
1	A	875	GLN
1	A	883	PHE
1	A	886	LEU
1	A	889	GLU
1	A	898	THR
1	A	907	ILE

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Mol	Chain	Res	Type
1	A	925	MET
1	A	931	ILE
1	A	958	LYS
1	A	963	ASP
1	A	966	GLN
1	A	968	LEU
1	A	972	LYS
1	A	973	ILE
1	A	986	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	114	ASN
1	A	202	GLN
1	A	213	ASN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN
1	A	706	ASN
1	A	875	GLN
1	A	880	HIS
1	A	920	GLN

### 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

2 ligands are modelled in this entry.

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	2.39	8 (18%)	42,72,72	1.93	9 (21%)
3	CZA	A	1005	-	25,29,29	2.70	9 (36%)	22,48,48	1.97	3 (13%)

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	CZA	A	1005	-	3/3/9/9	0/4/52/52	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005	CZA	C1-C2	-8.23	1.32	1.50
3	A	1005	CZA	C3-C2	-4.08	1.34	1.46
3	A	1005	CZA	C3-C6	-3.45	1.32	1.45
3	A	1005	CZA	C15-C14	-3.29	1.36	1.40
3	A	1005	CZA	O3-C4	-3.21	1.22	1.31
3	A	1005	CZA	C13-C14	-3.10	1.37	1.44
2	A	1003	TG1	O9-C10	-2.27	1.44	1.48
2	A	1003	TG1	C9-C8	2.88	1.55	1.52
3	A	1005	CZA	C4-N1	3.12	1.42	1.39
3	A	1005	CZA	C3-C4	3.28	1.46	1.40
2	A	1003	TG1	O3-C21	3.75	1.43	1.34
2	A	1003	TG1	O7-C27	3.80	1.45	1.34
2	A	1003	TG1	O1-C13	4.17	1.46	1.34
2	A	1003	TG1	O9-C32	4.63	1.46	1.35
3	A	1005	CZA	O1-C2	4.65	1.33	1.23
2	A	1003	TG1	O5-C12	6.22	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	TG1	O4-C21	10.64	1.44	1.21

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	TG1	O3-C21-O4	-6.10	111.12	123.30
3	A	1005	CZA	C12-C13-C14	-5.28	114.89	119.49
2	A	1003	TG1	O4-C21-C22	-4.45	110.58	125.17
2	A	1003	TG1	O12-C12-C11	-3.44	125.10	128.26
3	A	1005	CZA	C11-C9-C8	-2.49	106.31	112.22
2	A	1003	TG1	O7-C8-C9	2.20	111.05	107.03
2	A	1003	TG1	O5-C6-C7	2.39	106.20	104.08
2	A	1003	TG1	O7-C27-C28	2.80	117.62	111.53
2	A	1003	TG1	C10-O9-C32	3.58	129.24	121.90
2	A	1003	TG1	O1-C13-C14	3.67	119.50	111.53
2	A	1003	TG1	O9-C32-C33	3.74	118.81	110.73
3	A	1005	CZA	C13-C14-C15	5.59	128.82	123.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1005	CZA	C5
3	A	1005	CZA	C8
3	A	1005	CZA	C7

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	TG1	3	0
3	A	1005	CZA	5	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.