



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AR5  
Title : Calcium pump crystal structure with bound TNP-AMP and TG  
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Deposited on : 2010-11-24  
Resolution : 2.20 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

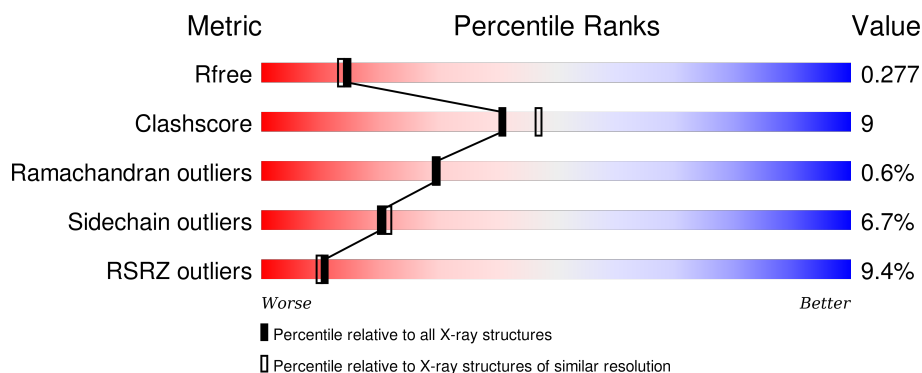
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	995	<div> <div>9%</div> <div>79%</div> <div>19%</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
5	PTY	A	1011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PTY	A	1012	-	-	-	X
5	PTY	A	1013	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8028 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
			7674	4878	1287	1452	57			

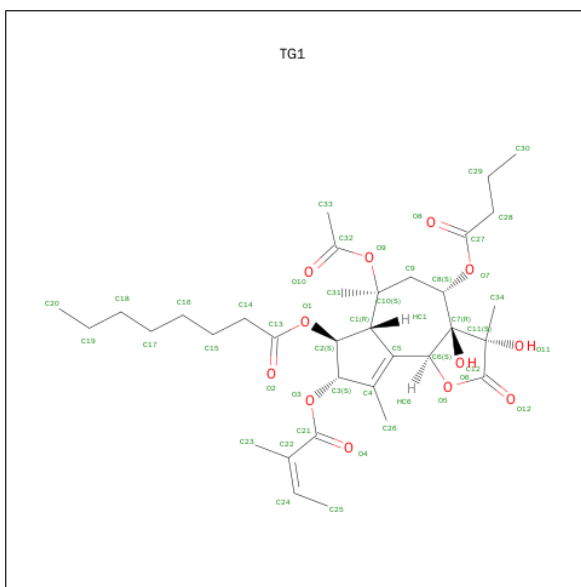
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	ACETYLATION	UNP P04191
A	994	GLY	ASP	SEE REMARK 999	UNP P04191

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

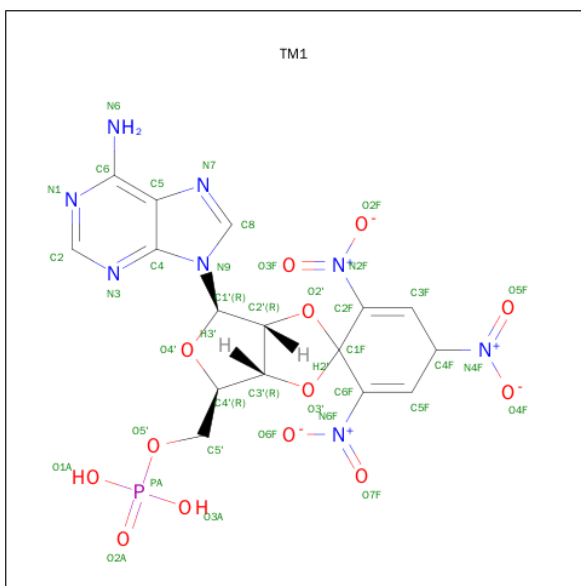
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 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<sub>34</sub>H<sub>50</sub>O<sub>12</sub>).



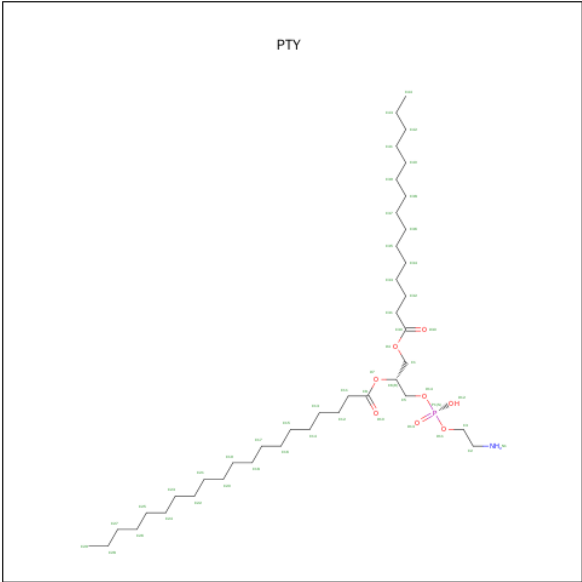
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			46	34	12		

- Molecule 4 is 2',3'-O-[(1R)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE-1,1-DIYL]ADENOSINE 5'-(DIHYDROGEN PHOSPHATE) (three-letter code: TM1) (formula:  $C_{16}H_{15}N_8O_{13}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			38	16	8	13	1		

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



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

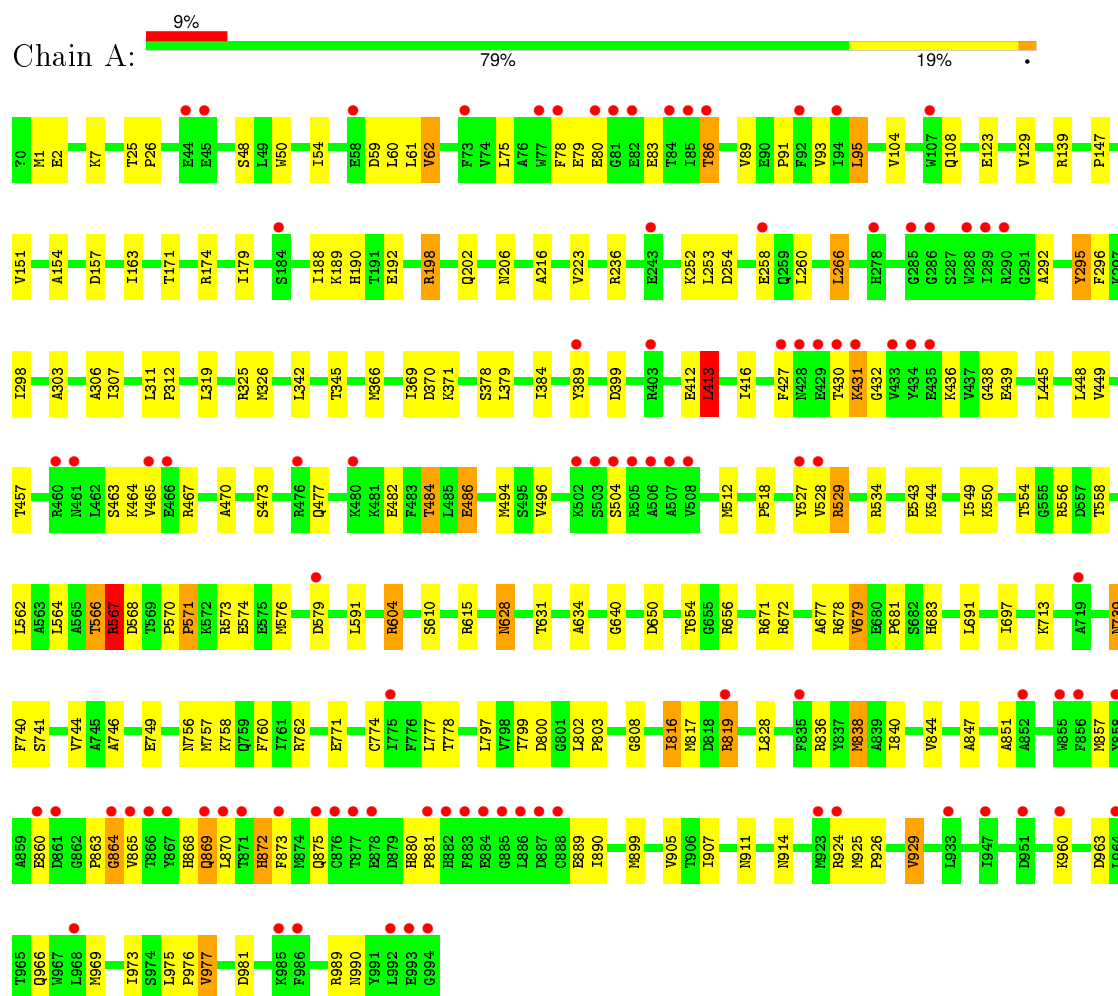
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	212	Total	O	0	0
			212	212		

### 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.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.68Å 71.68Å 589.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 14.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.20) 99.7 (14.98-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.260 , 0.288 0.242 , 0.277	Depositor DCC
$R_{free}$ test set	4018 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 79796 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TM1, TG1, PTY, ACE, NA

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	0.61	0/7813	0.67	4/10594 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	529	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	413	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	567	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	567	ARG	NE-CZ-NH2	-6.24	117.18	120.30

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	134	0
2	A	1	0	0	0	0
3	A	46	0	50	1	0
4	A	38	0	10	1	0
5	A	57	0	33	3	0
6	A	212	0	0	8	0
All	All	8028	0	7858	134	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 (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HE1	1:A:448:LEU:HD11	1.53	0.90
1:A:628:ASN:HD22	1:A:628:ASN:C	1.76	0.88
1:A:758:LYS:O	1:A:762:ARG:HG3	1.77	0.85
1:A:963:ASP:H	1:A:966:GLN:HE21	1.26	0.84
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.62	0.81
1:A:556:ARG:NH1	6:A:4294:HOH:O	2.14	0.80
1:A:857:MET:O	1:A:864:GLY:HA2	1.80	0.80
1:A:880:HIS:HB2	1:A:881:PRO:HD3	1.66	0.77
1:A:628:ASN:ND2	1:A:631:THR:H	1.82	0.77
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.66	0.76
1:A:615:ARG:NH1	1:A:640:GLY:O	2.19	0.76
1:A:366:MET:CE	1:A:448:LEU:HD11	2.16	0.76
1:A:819:ARG:HG2	1:A:819:ARG:HH11	1.53	0.73
1:A:628:ASN:HD21	1:A:631:THR:H	1.35	0.73
1:A:838:MET:HA	1:A:838:MET:HE3	1.73	0.70
1:A:260:LEU:HD13	3:A:1003:TG1:H252	1.74	0.69
1:A:739:ASN:ND2	1:A:741:SER:H	1.92	0.68
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.74	0.68
1:A:254:ASP:O	1:A:258:GLU:HG2	1.94	0.67
1:A:2:GLU:H	1:A:2:GLU:CD	1.96	0.67
1:A:863:PRO:O	1:A:865:VAL:N	2.26	0.67
1:A:83:GLU:HB2	1:A:86:THR:HG22	1.74	0.67
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.96	0.64
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.28	0.63
1:A:868:HIS:O	1:A:872:HIS:HD2	1.82	0.63
1:A:865:VAL:HB	1:A:868:HIS:CB	2.30	0.62
1:A:863:PRO:HG3	1:A:890:ILE:HD13	1.82	0.62
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.99	0.62
1:A:969:MET:O	1:A:973:ILE:HG22	2.00	0.62
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.82	0.61
1:A:679:VAL:HG22	1:A:683:HIS:ND1	2.15	0.61
1:A:345:THR:HA	1:A:697:ILE:HG22	1.83	0.60
1:A:628:ASN:C	1:A:628:ASN:ND2	2.51	0.60
1:A:467:ARG:HH21	1:A:470:ALA:HB3	1.64	0.60
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.83	0.60
1:A:679:VAL:HG22	1:A:683:HIS:CG	2.37	0.59
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:ASN:ND2	1:A:808:GLY:O	2.32	0.59
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.39	0.57
1:A:427:PHE:HE1	1:A:432:GLY:O	1.88	0.57
1:A:990:ASN:HD21	5:A:1012:PTY:HC31	1.70	0.57
1:A:739:ASN:HD22	1:A:740:PHE:N	2.02	0.57
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.88	0.56
1:A:188:ILE:HD13	1:A:486:GLU:CG	2.35	0.55
1:A:198:ARG:HD3	1:A:198:ARG:O	2.06	0.55
1:A:342:LEU:HD21	1:A:746:ALA:HB1	1.88	0.54
1:A:91:PRO:O	1:A:95:LEU:HB2	2.07	0.54
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.88	0.54
1:A:89:VAL:O	1:A:93:VAL:HG23	2.08	0.54
1:A:800:ASP:C	1:A:803:PRO:HD2	2.28	0.53
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.90	0.53
1:A:739:ASN:HD22	1:A:741:SER:H	1.55	0.53
1:A:292:ALA:O	1:A:296:PHE:HD1	1.92	0.53
1:A:963:ASP:H	1:A:966:GLN:NE2	2.00	0.53
1:A:295:TYR:HD1	1:A:295:TYR:N	2.06	0.52
1:A:757:MET:HA	1:A:760:PHE:CE2	2.44	0.52
1:A:389:TYR:N	6:A:4239:HOH:O	2.42	0.52
1:A:869:GLN:HB2	1:A:872:HIS:CD2	2.45	0.52
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.33	0.51
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.91	0.51
1:A:650:ASP:HB2	1:A:672:ARG:NH1	2.25	0.51
1:A:295:TYR:CD1	1:A:295:TYR:N	2.78	0.51
1:A:473:SER:O	1:A:477:GLN:HG2	2.11	0.51
1:A:869:GLN:OE1	1:A:872:HIS:NE2	2.44	0.51
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.47	0.50
1:A:604:ARG:CG	1:A:604:ARG:HH11	2.24	0.50
1:A:550:LYS:O	1:A:554:THR:HB	2.12	0.50
1:A:1:MET:CE	1:A:7:LYS:HG3	2.42	0.50
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.76	0.49
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.93	0.49
1:A:484:THR:HB	1:A:496:VAL:HG12	1.95	0.49
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.94	0.49
1:A:873:PHE:HD2	1:A:875:GLN:H	1.60	0.48
1:A:147:PRO:HA	1:A:223:VAL:HG12	1.94	0.48
1:A:427:PHE:CE1	1:A:432:GLY:O	2.65	0.48
1:A:369:ILE:HD13	1:A:379:LEU:HD22	1.96	0.48
1:A:865:VAL:HB	1:A:868:HIS:HB3	1.93	0.48
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:O	1:A:307:ILE:HG12	2.14	0.48
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.61	0.48
1:A:739:ASN:C	1:A:739:ASN:HD22	2.17	0.47
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.14	0.47
1:A:25:THR:HB	1:A:26:PRO:HD2	1.96	0.47
1:A:872:HIS:HA	6:A:4448:HOH:O	2.14	0.47
1:A:800:ASP:O	1:A:803:PRO:HD2	2.15	0.47
1:A:880:HIS:CB	1:A:881:PRO:HD3	2.40	0.47
1:A:926:PRO:O	1:A:929:VAL:HB	2.15	0.46
1:A:543:GLU:OE1	1:A:543:GLU:HA	2.14	0.46
1:A:79:GLU:HG2	1:A:80:GLU:H	1.80	0.46
1:A:571:PRO:HG2	1:A:576:MET:SD	2.56	0.46
1:A:61:LEU:HD13	1:A:307:ILE:HG23	1.98	0.45
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.45
1:A:819:ARG:CG	1:A:819:ARG:HH11	2.25	0.45
1:A:427:PHE:CZ	1:A:464:LYS:HG2	2.51	0.45
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.98	0.45
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.98	0.45
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.20	0.45
1:A:975:LEU:N	1:A:976:PRO:CD	2.80	0.45
1:A:370:ASP:HB3	1:A:378:SER:OG	2.17	0.45
1:A:681:PRO:HD2	6:A:4328:HOH:O	2.16	0.45
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.82	0.44
1:A:650:ASP:O	1:A:672:ARG:NH1	2.50	0.44
1:A:266:LEU:HD13	1:A:266:LEU:HA	1.86	0.44
1:A:678:ARG:HD3	4:A:1002:TM1:C6	2.48	0.44
1:A:104:VAL:HG12	1:A:108:GLN:HE21	1.82	0.44
1:A:436:LYS:HE2	1:A:438:GLY:O	2.18	0.44
1:A:179:ILE:HG12	6:A:2101:HOH:O	2.18	0.43
1:A:567:ARG:HG3	1:A:591:LEU:HD23	2.01	0.43
1:A:558:THR:HG22	1:A:634:ALA:HB1	2.00	0.43
1:A:192:GLU:HG2	6:A:2063:HOH:O	2.18	0.43
1:A:851:ALA:HB1	1:A:899:MET:HB3	2.00	0.43
1:A:61:LEU:HD22	1:A:307:ILE:HD12	2.00	0.42
1:A:816:ILE:HG22	1:A:817:MET:HG2	2.00	0.42
1:A:654:THR:HA	1:A:677:ALA:O	2.19	0.42
1:A:713:LYS:HB2	1:A:713:LYS:HE3	1.78	0.42
1:A:59:ASP:HB3	1:A:62:VAL:HG13	2.02	0.42
1:A:604:ARG:NH1	1:A:604:ARG:CG	2.81	0.42
1:A:925:MET:HB3	6:A:4438:HOH:O	2.20	0.42
1:A:482:GLU:OE2	1:A:573:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLU:O	1:A:774:CYS:HB3	2.19	0.41
1:A:484:THR:HG21	6:A:2038:HOH:O	2.19	0.41
1:A:427:PHE:HD2	1:A:465:VAL:HG22	1.85	0.41
1:A:989:ARG:NH2	5:A:1012:PTY:HC51	2.35	0.41
1:A:430:THR:HB	1:A:431:LYS:HD2	2.02	0.41
1:A:990:ASN:ND2	5:A:1012:PTY:HC31	2.36	0.41
1:A:366:MET:CE	1:A:384:ILE:HD11	2.51	0.41
1:A:154:ALA:O	1:A:157:ASP:HB2	2.21	0.41
1:A:836:ARG:O	1:A:840:ILE:HG12	2.20	0.41
1:A:777:LEU:HA	1:A:777:LEU:HD23	1.91	0.41
1:A:252:LYS:HD3	1:A:828:LEU:HD12	2.03	0.41
1:A:190:HIS:O	1:A:206:ASN:HA	2.21	0.41
1:A:907:ILE:HG23	1:A:977:VAL:HG11	2.03	0.40
1:A:311:LEU:HB3	1:A:312:PRO:HD3	2.02	0.40
1:A:1:MET:HE1	1:A:7:LYS:HG3	2.03	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%)	940 (95%)	47 (5%)	6 (1%)	30	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	A	864	GLY
1	A	869	GLN
1	A	872	HIS
1	A	463	SER
1	A	889	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%)	784 (93%)	56 (7%)	20	21

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	60	LEU
1	A	62	VAL
1	A	75	LEU
1	A	78	PHE
1	A	86	THR
1	A	95	LEU
1	A	123	GLU
1	A	139	ARG
1	A	171	THR
1	A	189	LYS
1	A	198	ARG
1	A	202	GLN
1	A	236	ARG
1	A	253	LEU
1	A	266	LEU
1	A	295	TYR
1	A	298	ILE
1	A	319	LEU
1	A	371	LYS
1	A	399	ASP
1	A	413	LEU
1	A	431	LYS
1	A	439	GLU
1	A	445	LEU
1	A	449	VAL
1	A	457	THR
1	A	484	THR
1	A	486	GLU
1	A	494	MET

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Mol	Chain	Res	Type
1	A	544	LYS
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	571	PRO
1	A	574	GLU
1	A	579	ASP
1	A	604	ARG
1	A	628	ASN
1	A	656	ARG
1	A	671	ARG
1	A	679	VAL
1	A	691	LEU
1	A	739	ASN
1	A	778	THR
1	A	797	LEU
1	A	802	LEU
1	A	816	ILE
1	A	819	ARG
1	A	838	MET
1	A	860	GLU
1	A	870	LEU
1	A	924	ARG
1	A	929	VAL
1	A	960	LYS
1	A	977	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	202	GLN
1	A	250	GLN
1	A	275	ASN
1	A	359	ASN
1	A	510	ASN
1	A	628	ASN
1	A	739	ASN
1	A	872	HIS
1	A	875	GLN
1	A	911	ASN
1	A	914	ASN

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Mol	Chain	Res	Type
1	A	919	ASN
1	A	966	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 ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	TM1	A	1002	-	26,42,42	1.84	5 (19%)	25,66,66	2.97	7 (28%)
3	TG1	A	1003	-	43,48,48	2.51	8 (18%)	42,72,72	2.09	9 (21%)
5	PTY	A	1011	-	17,18,49	1.52	2 (11%)	18,23,54	1.58	3 (16%)
5	PTY	A	1012	-	17,18,49	1.55	3 (17%)	18,23,54	1.61	3 (16%)
5	PTY	A	1013	-	17,18,49	1.45	2 (11%)	18,23,54	1.41	2 (11%)

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	TM1	A	1002	-	-	0/12/68/68	0/5/5/5
3	TG1	A	1003	-	-	0/33/99/99	0/3/3/3
5	PTY	A	1011	-	-	0/20/20/53	0/0/0/0
5	PTY	A	1012	-	-	0/20/20/53	0/0/0/0
5	PTY	A	1013	-	-	0/20/20/53	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	TM1	C3'-C4'	-5.78	1.36	1.52
3	A	1003	TG1	C33-C32	-4.62	1.32	1.49
4	A	1002	TM1	C4F-C5F	-3.37	1.35	1.49
4	A	1002	TM1	C3'-C2'	-2.49	1.47	1.53
4	A	1002	TM1	C2-N3	2.14	1.36	1.32
5	A	1012	PTY	C1-C6	2.16	1.56	1.50
5	A	1012	PTY	O4-C30	2.39	1.46	1.33
5	A	1013	PTY	O4-C30	2.46	1.46	1.33
5	A	1011	PTY	O4-C30	2.52	1.46	1.33
3	A	1003	TG1	C9-C8	2.74	1.55	1.52
4	A	1002	TM1	O4'-C1'	3.02	1.45	1.41
3	A	1003	TG1	O1-C13	3.81	1.45	1.34
3	A	1003	TG1	O7-C27	3.82	1.45	1.34
3	A	1003	TG1	O3-C21	4.34	1.44	1.34
3	A	1003	TG1	O9-C32	4.39	1.46	1.35
5	A	1013	PTY	O7-C8	4.79	1.46	1.35
5	A	1012	PTY	O7-C8	4.87	1.46	1.35
5	A	1011	PTY	O7-C8	5.15	1.47	1.35
3	A	1003	TG1	O5-C12	6.19	1.45	1.35
3	A	1003	TG1	O4-C21	10.93	1.44	1.21

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	TM1	N3-C2-N1	-9.11	121.92	128.89
3	A	1003	TG1	O3-C21-O4	-6.10	111.12	123.30
3	A	1003	TG1	O4-C21-C22	-5.37	107.58	125.17
3	A	1003	TG1	O12-C12-C11	-3.44	125.10	128.26
3	A	1003	TG1	C23-C22-C24	-2.29	115.00	123.55
5	A	1013	PTY	O7-C8-O10	-2.25	118.43	122.92
5	A	1011	PTY	O7-C8-O10	-2.03	118.87	122.92
5	A	1012	PTY	C1-O4-C30	2.06	122.37	117.14
3	A	1003	TG1	O7-C8-C9	2.07	110.81	107.03
5	A	1011	PTY	C1-O4-C30	2.11	122.47	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	TM1	O5'-C5'-C4'	2.12	116.92	109.12
3	A	1003	TG1	O7-C27-C28	2.77	117.55	111.53
3	A	1003	TG1	O1-C13-C14	3.18	118.43	111.53
5	A	1012	PTY	O7-C8-C11	3.52	117.74	111.10
4	A	1002	TM1	C2'-C3'-C4'	3.60	112.71	103.69
3	A	1003	TG1	C10-O9-C32	3.74	129.57	121.90
5	A	1012	PTY	O4-C1-C6	3.79	118.89	108.69
4	A	1002	TM1	O4'-C4'-C5'	4.02	123.71	109.32
4	A	1002	TM1	C5'-C4'-C3'	4.23	129.54	114.31
5	A	1013	PTY	O7-C8-C11	4.55	119.69	111.10
4	A	1002	TM1	O3'-C3'-C2'	4.75	111.08	103.64
5	A	1011	PTY	O7-C8-C11	4.97	120.47	111.10
3	A	1003	TG1	O9-C32-C33	5.39	122.36	110.73
4	A	1002	TM1	O3'-C3'-C4'	6.82	130.51	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	TM1	1	0
3	A	1003	TG1	1	0
5	A	1012	PTY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	994/995 (99%)	0.44	93 (9%) 11 10	35, 65, 121, 155	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	886	LEU	13.3
1	A	883	PHE	10.7
1	A	504	SER	9.8
1	A	507	ALA	8.3
1	A	506	ALA	8.1
1	A	866	THR	8.1
1	A	85	ILE	8.1
1	A	505	ARG	8.0
1	A	84	THR	7.6
1	A	884	GLU	7.5
1	A	994	GLY	7.2
1	A	993	GLU	6.7
1	A	503	SER	6.3
1	A	885	GLY	6.2
1	A	508	VAL	6.0
1	A	887	ASP	5.6
1	A	873	PHE	5.4
1	A	77	TRP	5.4
1	A	78	PHE	5.3
1	A	45	GLU	5.1
1	A	881	PRO	5.0
1	A	285	GLY	4.8
1	A	867	TYR	4.4
1	A	107	TRP	4.3
1	A	81	GLY	4.3
1	A	877	THR	4.3
1	A	460	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	430	THR	4.2
1	A	992	LEU	4.1
1	A	82	GLU	4.1
1	A	80	GLU	4.0
1	A	289	ILE	4.0
1	A	86	THR	3.7
1	A	875	GLN	3.7
1	A	427	PHE	3.7
1	A	433	VAL	3.5
1	A	856	PHE	3.4
1	A	968	LEU	3.4
1	A	947	ILE	3.3
1	A	882	HIS	3.3
1	A	502	LYS	3.3
1	A	243	GLU	3.3
1	A	466	GLU	3.2
1	A	864	GLY	3.2
1	A	434	TYR	3.2
1	A	876	CYS	3.2
1	A	461	ASN	3.2
1	A	428	ASN	3.1
1	A	278	HIS	3.1
1	A	865	VAL	3.1
1	A	290	ARG	3.1
1	A	480	LYS	3.0
1	A	860	GLU	3.0
1	A	286	GLY	3.0
1	A	92	PHE	2.9
1	A	476	ARG	2.9
1	A	775	ILE	2.8
1	A	431	LYS	2.8
1	A	951	ASP	2.7
1	A	429	GLU	2.7
1	A	73	PHE	2.7
1	A	435	GLU	2.7
1	A	869	GLN	2.6
1	A	58	GLU	2.5
1	A	528	VAL	2.5
1	A	878	GLU	2.5
1	A	579	ASP	2.5
1	A	858	TYR	2.5
1	A	985	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	403	ARG	2.5
1	A	44	GLU	2.4
1	A	924	ARG	2.4
1	A	719	ALA	2.4
1	A	964	LEU	2.4
1	A	94	ILE	2.4
1	A	861	ASP	2.3
1	A	527	TYR	2.3
1	A	855	TRP	2.3
1	A	871	THR	2.3
1	A	852	ALA	2.3
1	A	960	LYS	2.3
1	A	258	GLU	2.3
1	A	819	ARG	2.3
1	A	288	TRP	2.2
1	A	923	MET	2.2
1	A	835	PHE	2.1
1	A	933	LEU	2.1
1	A	870	LEU	2.1
1	A	986	PHE	2.1
1	A	184	SER	2.1
1	A	389	TYR	2.1
1	A	465	VAL	2.1
1	A	888	CYS	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 carbohydrates 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. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	PTY	A	1012	19/50	0.77	0.45	6.59	100,103,106,106	0
5	PTY	A	1011	19/50	0.80	0.39	4.33	107,108,110,110	0
5	PTY	A	1013	19/50	0.85	0.27	2.20	97,101,103,103	0
4	TM1	A	1002	38/38	0.95	0.15	1.45	44,52,70,73	0
2	NA	A	1000	1/1	0.93	0.13	0.31	34,34,34,34	0
3	TG1	A	1003	46/46	0.92	0.15	0.07	43,48,62,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.