



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2014 – 10:00 AM EDT

PDB ID : 3FPB
Title : The Structure of Sarcoplasmic Reticulum Ca²⁺-ATPase Bound To Cyclopiazonic acid with ATP
Authors : Moncoq, K.; Morth, J.P.; Bublitz, M.; Laursen, M.; Nissen, P.; Young, H.S.
Deposited on : 2009-01-05
Resolution : 2.55 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

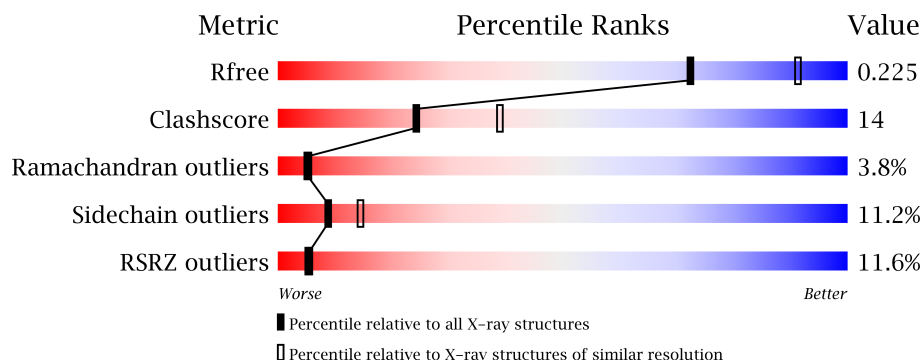
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	994	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	995	-	X
3	MF4	A	996	-	X
6	ATP	A	1002	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 7930 atoms, of which 0 are hydrogen and 0 are deuterium.

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/endoplasmicreticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

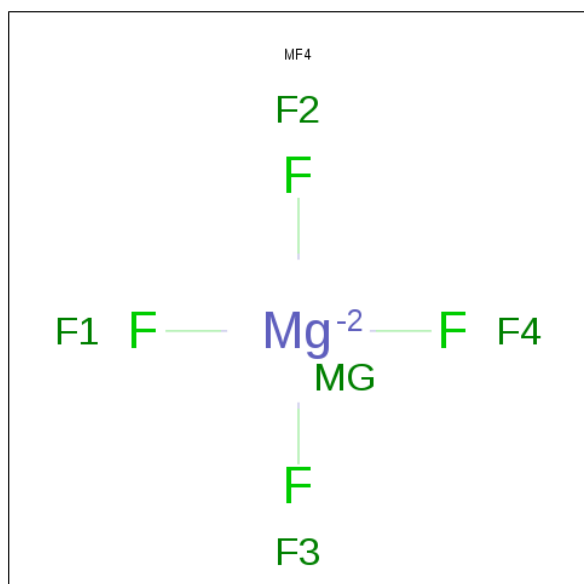
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F₄Mg).

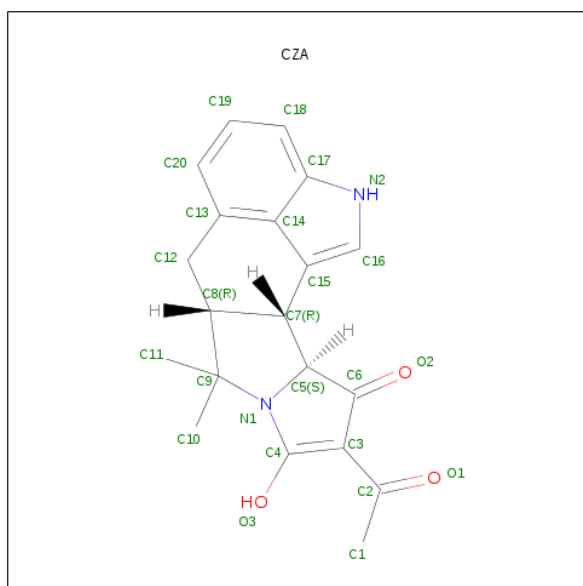


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	F	Mg	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

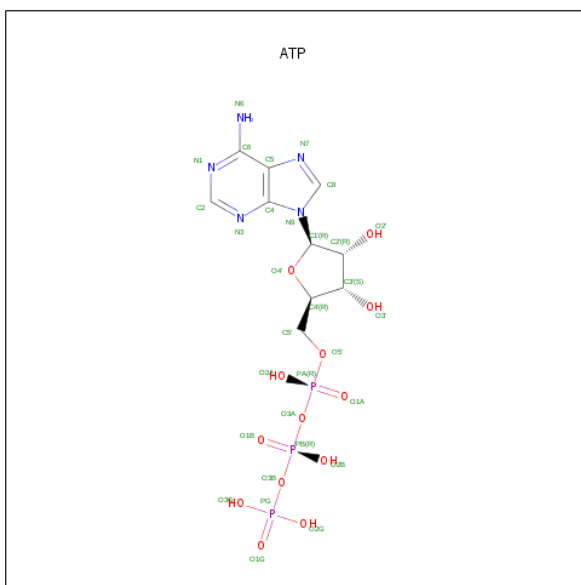
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	K		0	0
			1	1			

- Molecule 5 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: C₂₀H₂₀N₂O₃).



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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

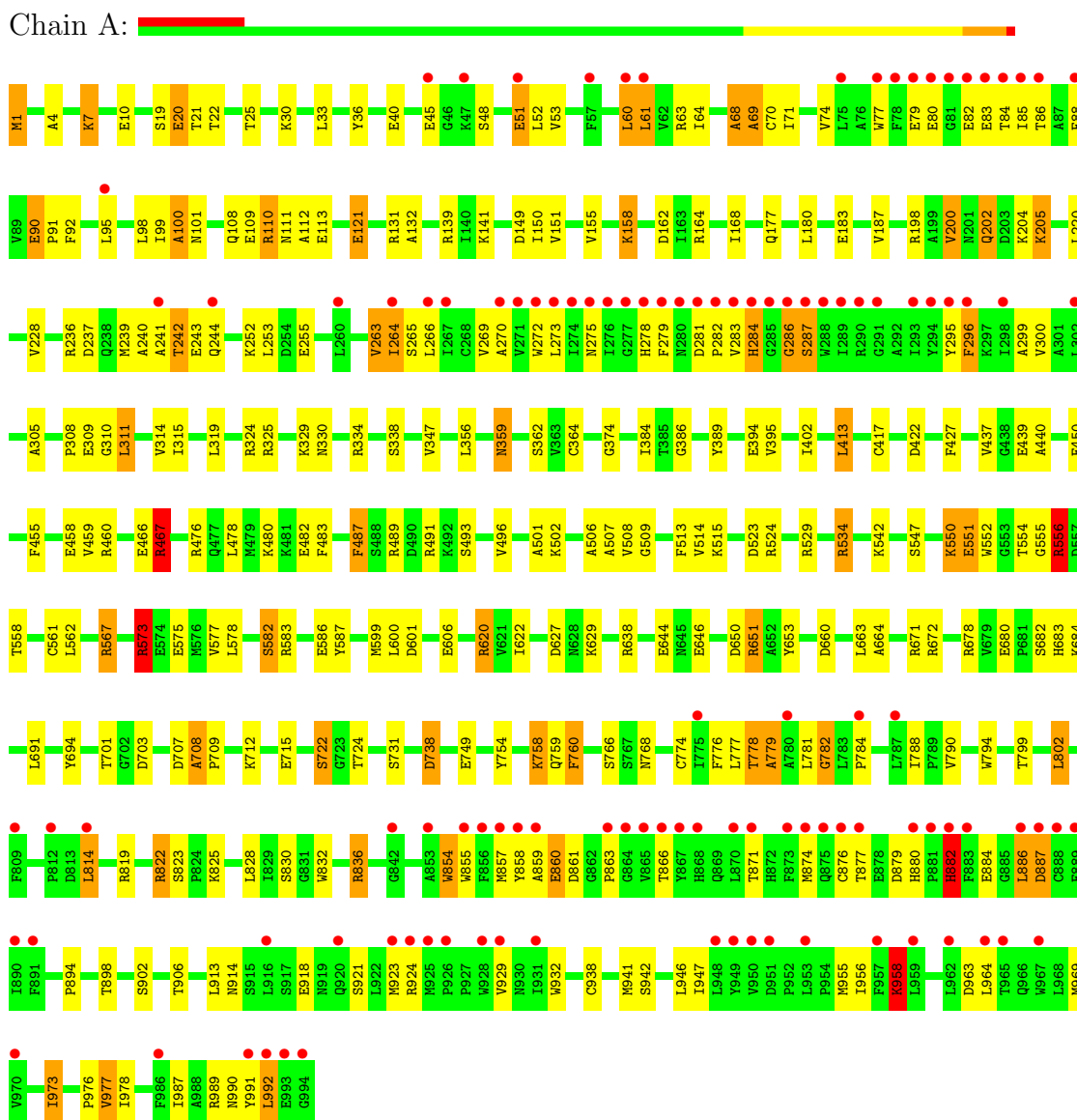
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	195	Total O 195 195	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.

- Molecule 1: Sarcoplasmic/endoplasmicreticulum calcium ATPase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.36Å 69.87Å 143.50Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	24.94 – 2.55 46.73 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.94-2.55) 99.8 (46.73-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.183 , 0.231 0.175 , 0.225	Depositor DCC
R_{free} test set	2771 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54351 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CZA, MF4, K, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.36	57/7812 (0.7%)	1.24	51/10592 (0.5%)

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	3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	TYR	CD2-CE2	10.50	1.55	1.39
1	A	364	CYS	CB-SG	10.23	1.99	1.82
1	A	439	GLU	CG-CD	9.13	1.65	1.51
1	A	389	TYR	CB-CG	-8.65	1.38	1.51
1	A	694	TYR	CG-CD1	8.61	1.50	1.39
1	A	384	ILE	CA-CB	8.12	1.73	1.54
1	A	586	GLU	CG-CD	8.10	1.64	1.51
1	A	187	VAL	CB-CG1	7.91	1.69	1.52
1	A	606	GLU	CG-CD	7.59	1.63	1.51
1	A	132	ALA	CA-CB	-7.46	1.36	1.52
1	A	586	GLU	CD-OE2	7.36	1.33	1.25
1	A	552	TRP	CG-CD1	-6.91	1.27	1.36
1	A	417	CYS	CB-SG	6.83	1.93	1.82
1	A	524	ARG	CZ-NH1	6.78	1.41	1.33
1	A	200	VAL	CB-CG2	-6.67	1.38	1.52
1	A	606	GLU	CD-OE2	6.65	1.32	1.25
1	A	455	PHE	CE1-CZ	6.46	1.49	1.37
1	A	551	GLU	CG-CD	6.42	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	PHE	CE1-CZ	6.40	1.49	1.37
1	A	487	PHE	CD1-CE1	6.33	1.51	1.39
1	A	347	VAL	CB-CG2	-6.28	1.39	1.52
1	A	708	ALA	CA-CB	6.17	1.65	1.52
1	A	40	GLU	CD-OE1	6.17	1.32	1.25
1	A	437	VAL	CB-CG1	6.15	1.65	1.52
1	A	496	VAL	CB-CG2	-6.08	1.40	1.52
1	A	36	TYR	CD2-CE2	6.06	1.48	1.39
1	A	437	VAL	CB-CG2	5.95	1.65	1.52
1	A	121	GLU	CB-CG	-5.89	1.41	1.52
1	A	506	ALA	CA-CB	5.81	1.64	1.52
1	A	483	PHE	CE1-CZ	5.80	1.48	1.37
1	A	177	GLN	CB-CG	-5.78	1.36	1.52
1	A	606	GLU	CB-CG	-5.66	1.41	1.52
1	A	513	PHE	CE2-CZ	5.63	1.48	1.37
1	A	664	ALA	CA-CB	5.62	1.64	1.52
1	A	440	ALA	CA-CB	-5.61	1.40	1.52
1	A	487	PHE	CD2-CE2	5.60	1.50	1.39
1	A	724	THR	CB-CG2	5.56	1.70	1.52
1	A	389	TYR	CZ-OH	5.52	1.47	1.37
1	A	427	PHE	CE2-CZ	5.44	1.47	1.37
1	A	359	ASN	CB-CG	5.40	1.63	1.51
1	A	187	VAL	CB-CG2	-5.39	1.41	1.52
1	A	715	GLU	CB-CG	5.35	1.62	1.52
1	A	459	VAL	CB-CG2	5.33	1.64	1.52
1	A	458	GLU	CG-CD	5.33	1.59	1.51
1	A	513	PHE	CG-CD2	5.31	1.46	1.38
1	A	582	SER	CA-CB	5.29	1.60	1.52
1	A	10	GLU	CG-CD	5.24	1.59	1.51
1	A	493	SER	CB-OG	5.23	1.49	1.42
1	A	4	ALA	CA-CB	-5.23	1.41	1.52
1	A	694	TYR	CE1-CZ	5.18	1.45	1.38
1	A	439	GLU	CD-OE2	5.17	1.31	1.25
1	A	514	VAL	CB-CG1	5.17	1.63	1.52
1	A	575	GLU	CG-CD	5.16	1.59	1.51
1	A	575	GLU	CD-OE1	5.13	1.31	1.25
1	A	515	LYS	CB-CG	-5.04	1.39	1.52
1	A	162	ASP	CB-CG	5.01	1.62	1.51
1	A	587	TYR	CD2-CE2	5.01	1.46	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ARG	NE-CZ-NH1	-15.83	112.38	120.30
1	A	476	ARG	NE-CZ-NH1	-13.42	113.59	120.30
1	A	467	ARG	NE-CZ-NH2	12.11	126.35	120.30
1	A	534	ARG	NE-CZ-NH1	-11.14	114.73	120.30
1	A	620	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	A	491	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	A	678	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	A	476	ARG	NE-CZ-NH2	9.09	124.84	120.30
1	A	638	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	A	413	LEU	CA-CB-CG	8.93	135.84	115.30
1	A	529	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	A	567	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	534	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	A	33	LEU	CB-CG-CD2	-7.72	97.87	111.00
1	A	567	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	629	LYS	CD-CE-NZ	-7.42	94.64	111.70
1	A	491	ARG	NE-CZ-NH1	-6.95	116.82	120.30
1	A	703	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	467	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	524	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	1	MET	N-CA-C	6.27	127.93	111.00
1	A	476	ARG	CG-CD-NE	-6.14	98.91	111.80
1	A	180	LEU	CB-CG-CD2	-6.09	100.65	111.00
1	A	738	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	561	CYS	CA-CB-SG	-5.71	103.71	114.00
1	A	139	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	701	THR	CB-CA-C	-5.67	96.28	111.60
1	A	467	ARG	CG-CD-NE	-5.66	99.92	111.80
1	A	239	MET	CB-CG-SD	-5.65	95.46	112.40
1	A	1	MET	N-CA-CB	5.63	120.74	110.60
1	A	20	GLU	N-CA-CB	-5.62	100.48	110.60
1	A	220	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	A	738	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	534	ARG	CG-CD-NE	-5.49	100.28	111.80
1	A	578	LEU	CA-CB-CG	-5.49	102.69	115.30
1	A	200	VAL	N-CA-CB	-5.46	99.50	111.50
1	A	651	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	622	ILE	CG1-CB-CG2	-5.35	99.64	111.40
1	A	627	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	573	ARG	CG-CD-NE	-5.29	100.69	111.80
1	A	183	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	A	158	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	25	THR	C-N-CD	5.18	139.28	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	ARG	N-CA-C	-5.18	97.00	111.00
1	A	220	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	671	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	386	GLY	N-CA-C	-5.09	100.38	113.10
1	A	422	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	822	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	460	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	682	SER	CA-CB-OG	-5.06	97.55	111.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	555	GLY	Peptide
1	A	556	ARG	Peptide
1	A	830	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	0	108	0
2	A	2	0	0	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	25	0	0	1	0
6	A	31	0	0	2	0
7	A	195	0	0	4	0
All	All	7930	0	0	109	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (109) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:450:GLU:OE2	1:A:467:ARG:NH1	2.21	0.73
1:A:263:VAL:O	1:A:265:SER:N	2.25	0.69
1:A:482:GLU:OE2	1:A:573:ARG:NE	2.31	0.64
1:A:854:TRP:CE3	1:A:854:TRP:O	2.52	0.63
1:A:650:ASP:OD1	1:A:650:ASP:N	2.32	0.63
1:A:854:TRP:CD2	1:A:854:TRP:O	2.51	0.62
1:A:272:TRP:CD1	1:A:295:TYR:CE2	2.87	0.62
1:A:583:ARG:NH1	7:A:1139:HOH:O	2.32	0.62
1:A:310:GLY:O	1:A:311:LEU:C	2.37	0.61
1:A:501:ALA:O	1:A:502:LYS:CB	2.45	0.61
1:A:325:ARG:NH1	1:A:749:GLU:OE1	2.33	0.61
1:A:990:ASN:O	1:A:992:LEU:N	2.34	0.60
1:A:754:TYR:CE1	1:A:758:LYS:CD	2.85	0.60
1:A:781:LEU:O	1:A:782:GLY:C	2.41	0.59
1:A:802:LEU:N	1:A:802:LEU:CD2	2.66	0.58
1:A:296:PHE:CD1	1:A:296:PHE:N	2.71	0.58
1:A:240:ALA:O	1:A:242:THR:N	2.36	0.58
1:A:977:VAL:CG1	1:A:978:ILE:N	2.67	0.57
1:A:886:LEU:CD1	1:A:887:ASP:N	2.67	0.57
1:A:198:ARG:NH1	1:A:660:ASP:OD1	2.37	0.57
1:A:279:PHE:O	1:A:279:PHE:CG	2.57	0.57
1:A:776:PHE:O	1:A:776:PHE:CD2	2.58	0.56
1:A:82:GLU:O	1:A:84:THR:N	2.38	0.56
1:A:202:GLN:NE2	1:A:202:GLN:N	2.54	0.55
1:A:295:TYR:O	1:A:299:ALA:N	2.41	0.54
1:A:722:SER:OG	1:A:738:ASP:OD2	2.24	0.54
6:A:1002:ATP:C8	6:A:1002:ATP:C5'	2.91	0.54
1:A:68:ALA:O	1:A:71:ILE:N	2.41	0.54
1:A:969:MET:O	1:A:973:ILE:CG2	2.56	0.54
1:A:113:GLU:N	1:A:113:GLU:OE1	2.41	0.54
1:A:487:PHE:CD1	1:A:487:PHE:C	2.82	0.53
1:A:879:ASP:O	1:A:882:HIS:N	2.41	0.53
1:A:508:VAL:CG1	1:A:509:GLY:N	2.71	0.53
1:A:263:VAL:O	1:A:266:LEU:N	2.41	0.53
1:A:205:LYS:CE	6:A:1002:ATP:O2G	2.57	0.52
1:A:646:GLU:OE2	1:A:651:ARG:NH1	2.43	0.52
1:A:85:ILE:O	1:A:86:THR:CG2	2.57	0.52
1:A:109:GLU:O	1:A:110:ARG:O	2.27	0.52
1:A:976:PRO:O	1:A:977:VAL:C	2.49	0.51
1:A:237:ASP:OD1	7:A:1162:HOH:O	2.19	0.51
1:A:880:HIS:O	1:A:884:GLU:CG	2.58	0.51
1:A:859:ALA:O	1:A:861:ASP:N	2.44	0.51
1:A:556:ARG:O	1:A:556:ARG:CG	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88:PHE:CD2	1:A:92:PHE:CE1	2.99	0.50
1:A:269:VAL:O	1:A:273:LEU:N	2.43	0.50
1:A:832:TRP:CZ2	1:A:987:ILE:CG2	2.94	0.50
1:A:7:LYS:O	1:A:164:ARG:NH2	2.45	0.49
1:A:80:GLU:O	1:A:82:GLU:N	2.46	0.48
1:A:836:ARG:NH1	1:A:918:GLU:O	2.47	0.48
1:A:325:ARG:NH1	1:A:749:GLU:OE2	2.46	0.48
1:A:855:TRP:CD2	1:A:855:TRP:O	2.67	0.48
1:A:70:CYS:O	1:A:74:VAL:N	2.47	0.48
1:A:272:TRP:O	1:A:272:TRP:CD2	2.67	0.48
1:A:754:TYR:CD2	1:A:822:ARG:NH2	2.82	0.47
1:A:894:PRO:O	1:A:898:THR:N	2.47	0.47
1:A:305:ALA:O	1:A:768:ASN:ND2	2.48	0.47
1:A:68:ALA:O	1:A:69:ALA:C	2.53	0.47
1:A:760:PHE:CD1	1:A:760:PHE:C	2.88	0.47
1:A:113:GLU:OE2	1:A:334:ARG:NH1	2.47	0.47
1:A:131:ARG:NH2	1:A:149:ASP:OD2	2.48	0.46
1:A:68:ALA:O	1:A:70:CYS:N	2.48	0.46
1:A:857:MET:O	1:A:859:ALA:N	2.48	0.46
1:A:556:ARG:NH2	1:A:644:GLU:OE2	2.48	0.46
1:A:263:VAL:O	1:A:264:ILE:C	2.54	0.46
1:A:938:CYS:O	1:A:942:SER:OG	2.34	0.46
1:A:269:VAL:CG1	1:A:270:ALA:N	2.80	0.45
1:A:550:LYS:O	1:A:551:GLU:C	2.53	0.45
1:A:359:ASN:N	1:A:601:ASP:OD1	2.50	0.45
1:A:855:TRP:CE3	1:A:855:TRP:O	2.70	0.45
1:A:263:VAL:CG1	1:A:264:ILE:N	2.80	0.45
1:A:168:ILE:N	7:A:1008:HOH:O	2.50	0.44
1:A:958:LYS:CB	1:A:958:LYS:NZ	2.78	0.44
1:A:708:ALA:N	1:A:709:PRO:CD	2.81	0.44
1:A:778:THR:OG1	1:A:784:PRO:O	2.35	0.44
1:A:680:GLU:N	1:A:683:HIS:ND1	2.66	0.44
1:A:329:LYS:O	1:A:330:ASN:CB	2.66	0.44
1:A:272:TRP:CG	1:A:272:TRP:O	2.70	0.43
1:A:794:TRP:CH2	1:A:947:ILE:CD1	3.00	0.43
1:A:282:PRO:C	1:A:284:HIS:N	2.71	0.43
1:A:684:LYS:NZ	1:A:707:ASP:OD1	2.52	0.43
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.43
1:A:275:ASN:ND2	1:A:295:TYR:CE1	2.87	0.43
1:A:777:LEU:C	1:A:779:ALA:N	2.72	0.43
1:A:308:PRO:C	1:A:309:GLU:O	2.53	0.43
1:A:653:TYR:OH	1:A:672:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:LYS:NZ	7:A:1086:HOH:O	2.53	0.42
1:A:362:SER:O	1:A:599:MET:CA	2.68	0.42
1:A:777:LEU:O	1:A:779:ALA:N	2.53	0.42
1:A:77:TRP:O	1:A:79:GLU:N	2.53	0.42
1:A:60:LEU:O	1:A:63:ARG:N	2.53	0.42
1:A:973:ILE:CG1	1:A:973:ILE:O	2.68	0.42
1:A:112:ALA:O	1:A:113:GLU:C	2.58	0.42
1:A:325:ARG:NH1	1:A:749:GLU:CD	2.73	0.42
1:A:523:ASP:OD1	1:A:542:LYS:NZ	2.53	0.41
1:A:854:TRP:CG	1:A:854:TRP:O	2.73	0.41
1:A:913:LEU:O	1:A:914:ASN:C	2.57	0.41
1:A:99:ILE:O	1:A:100:ALA:C	2.57	0.41
1:A:101:ASN:CB	5:A:1001:CZA:O3	2.69	0.41
1:A:286:GLY:O	1:A:287:SER:OG	2.39	0.41
1:A:48:SER:N	1:A:51:GLU:OE2	2.53	0.41
1:A:395:VAL:O	1:A:402:ILE:N	2.53	0.41
1:A:924:ARG:NH2	1:A:989:ARG:NH2	2.69	0.41
1:A:52:LEU:O	1:A:53:VAL:C	2.60	0.41
1:A:90:GLU:CB	1:A:91:PRO:CD	2.99	0.41
1:A:794:TRP:CZ3	1:A:947:ILE:CD1	3.03	0.40
1:A:90:GLU:O	1:A:91:PRO:C	2.59	0.40
1:A:814:LEU:CD1	1:A:814:LEU:N	2.84	0.40
1:A:921:SER:C	1:A:923:MET:N	2.75	0.40
1:A:600:LEU:CD2	1:A:600:LEU:O	2.70	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	992/994 (100%)	865 (87%)	89 (9%)	38 (4%)	5 5

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ARG
1	A	241	ALA
1	A	264	ILE
1	A	819	ARG
1	A	882	HIS
1	A	61	LEU
1	A	68	ALA
1	A	83	GLU
1	A	100	ALA
1	A	243	GLU
1	A	284	HIS
1	A	507	ALA
1	A	782	GLY
1	A	858	TYR
1	A	860	GLU
1	A	876	CYS
1	A	886	LEU
1	A	887	ASP
1	A	991	TYR
1	A	69	ALA
1	A	286	GLY
1	A	778	THR
1	A	863	PRO
1	A	60	LEU
1	A	263	VAL
1	A	287	SER
1	A	550	LYS
1	A	554	THR
1	A	558	THR
1	A	111	ASN
1	A	958	LYS
1	A	779	ALA
1	A	90	GLU
1	A	155	VAL
1	A	283	VAL
1	A	374	GLY
1	A	929	VAL
1	A	281	ASP

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%)	746 (89%)	94 (11%)	9	14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LYS
1	A	19	SER
1	A	20	GLU
1	A	21	THR
1	A	22	THR
1	A	30	LYS
1	A	45	GLU
1	A	51	GLU
1	A	61	LEU
1	A	64	ILE
1	A	95	LEU
1	A	98	LEU
1	A	108	GLN
1	A	121	GLU
1	A	141	LYS
1	A	150	ILE
1	A	151	VAL
1	A	158	LYS
1	A	200	VAL
1	A	202	GLN
1	A	205	LYS
1	A	228	VAL
1	A	236	ARG
1	A	242	THR
1	A	244	GLN
1	A	252	LYS
1	A	253	LEU
1	A	255	GLU
1	A	278	HIS
1	A	296	PHE
1	A	300	VAL
1	A	311	LEU
1	A	314	VAL
1	A	315	ILE

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Mol	Chain	Res	Type
1	A	319	LEU
1	A	324	ARG
1	A	338	SER
1	A	356	LEU
1	A	394	GLU
1	A	413	LEU
1	A	466	GLU
1	A	467	ARG
1	A	478	LEU
1	A	480	LYS
1	A	489	ARG
1	A	534	ARG
1	A	547	SER
1	A	556	ARG
1	A	562	LEU
1	A	567	ARG
1	A	573	ARG
1	A	577	VAL
1	A	582	SER
1	A	620	ARG
1	A	663	LEU
1	A	691	LEU
1	A	712	LYS
1	A	722	SER
1	A	731	SER
1	A	758	LYS
1	A	759	GLN
1	A	760	PHE
1	A	766	SER
1	A	774	CYS
1	A	788	ILE
1	A	790	VAL
1	A	799	THR
1	A	802	LEU
1	A	814	LEU
1	A	823	SER
1	A	825	LYS
1	A	828	LEU
1	A	836	ARG
1	A	854	TRP
1	A	860	GLU
1	A	866	THR

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Mol	Chain	Res	Type
1	A	871	THR
1	A	874	MET
1	A	877	THR
1	A	882	HIS
1	A	902	SER
1	A	906	THR
1	A	932	TRP
1	A	941	MET
1	A	946	LEU
1	A	955	MET
1	A	956	ILE
1	A	958	LYS
1	A	963	ASP
1	A	964	LEU
1	A	973	ILE
1	A	977	VAL
1	A	992	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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, 3 are monoatomic - leaving 3 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
5	CZA	A	1001	2	29,29,29	1.73	8 (27%)	47,48,48	3.11	14 (29%)
6	ATP	A	1002	-	33,33,33	2.82	17 (51%)	52,52,52	2.89	18 (34%)
3	MF4	A	996	1	0,4,4	0.00	-	0,6,6	0.00	-

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
5	CZA	A	1001	2	-	0/4/52/52	0/0/5/5
6	ATP	A	1002	-	1/1/7/7	0/22/38/38	0/1/3/3
3	MF4	A	996	1	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	ATP	C4-N9	5.46	1.45	1.37
6	A	1002	ATP	PB-O3B	5.11	1.69	1.59
6	A	1002	ATP	PA-O3A	4.70	1.68	1.59
6	A	1002	ATP	PG-O1G	4.64	1.66	1.51
6	A	1002	ATP	C8-N7	4.43	1.43	1.34
6	A	1002	ATP	PG-O3B	4.30	1.67	1.60
6	A	1002	ATP	C2-N3	4.24	1.40	1.32
6	A	1002	ATP	PA-O1A	3.95	1.66	1.51
5	A	1001	CZA	C12-C8	3.88	1.58	1.53
6	A	1002	ATP	PB-O3A	3.87	1.66	1.59
6	A	1002	ATP	PB-O1B	3.85	1.66	1.51
5	A	1001	CZA	C19-C18	3.08	1.43	1.36
6	A	1002	ATP	O4'-C1'	2.98	1.45	1.41
5	A	1001	CZA	C1-C2	2.93	1.56	1.50
6	A	1002	ATP	PA-O5'	2.93	1.72	1.59
6	A	1002	ATP	C6-N6	2.79	1.44	1.35
5	A	1001	CZA	C3-C4	-2.75	1.35	1.40
5	A	1001	CZA	C20-C13	2.57	1.42	1.37
6	A	1002	ATP	PG-O2G	2.54	1.64	1.54
5	A	1001	CZA	C13-C14	-2.43	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	CZA	C4-N1	-2.19	1.33	1.38
6	A	1002	ATP	C5-C4	-2.18	1.35	1.40
6	A	1002	ATP	C5'-C4'	2.18	1.58	1.51
6	A	1002	ATP	PG-O3G	-2.06	1.47	1.54
5	A	1001	CZA	C9-C8	2.01	1.57	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	ATP	N3-C2-N1	-12.68	118.11	128.71
5	A	1001	CZA	C7-C15-C14	-11.33	118.82	124.56
5	A	1001	CZA	C16-C15-C7	9.08	136.04	130.45
5	A	1001	CZA	C12-C13-C14	-7.57	114.36	119.33
6	A	1002	ATP	C4'-O4'-C1'	-6.31	102.90	109.75
6	A	1002	ATP	O4'-C1'-N9	5.86	113.89	108.44
6	A	1002	ATP	O3A-PB-O3B	5.06	111.95	101.66
5	A	1001	CZA	C13-C14-C17	5.02	120.76	118.30
5	A	1001	CZA	C15-C14-C17	4.93	112.27	106.73
5	A	1001	CZA	C8-C7-C5	-4.82	94.76	103.24
5	A	1001	CZA	C5-C6-C3	-4.70	102.29	107.12
5	A	1001	CZA	C8-C9-N1	-4.25	95.71	100.97
6	A	1002	ATP	O2'-C2'-C1'	4.06	123.52	111.23
6	A	1002	ATP	O3'-C3'-C4'	3.94	122.69	111.08
6	A	1002	ATP	O5'-C5'-C4'	3.86	123.11	108.94
6	A	1002	ATP	C2-N3-C4	3.86	125.00	114.01
6	A	1002	ATP	N3-C4-N9	3.74	132.19	125.43
6	A	1002	ATP	C5-C4-N3	-3.70	117.64	125.70
6	A	1002	ATP	O2'-C2'-C3'	3.54	123.36	111.83
6	A	1002	ATP	O4'-C4'-C5'	3.34	121.29	109.36
5	A	1001	CZA	C13-C14-C15	3.19	126.96	123.54
6	A	1002	ATP	C8-N9-C4	-2.80	104.77	106.90
6	A	1002	ATP	O2G-PG-O3B	2.53	117.16	105.14
6	A	1002	ATP	PA-O3A-PB	-2.48	124.40	131.68
5	A	1001	CZA	C12-C8-C7	-2.43	106.23	111.30
5	A	1001	CZA	O2-C6-C3	2.32	134.47	128.21
6	A	1002	ATP	O3'-C3'-C2'	2.29	119.27	111.83
5	A	1001	CZA	C9-N1-C5	2.22	115.66	111.75
5	A	1001	CZA	C16-C15-C14	-2.11	105.05	107.30
6	A	1002	ATP	C5-C4-N9	2.07	110.16	107.16
5	A	1001	CZA	C3-C4-N1	-2.05	107.12	111.40
6	A	1002	ATP	O4'-C4'-C3'	-2.02	101.08	105.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1002	ATP	C3'

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	994/994 (100%)	0.62	116 (11%) 5 5	34, 72, 209, 337	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	12.2
1	A	282	PRO	11.6
1	A	279	PHE	10.5
1	A	280	ASN	10.1
1	A	77	TRP	9.8
1	A	287	SER	9.3
1	A	867	TYR	9.0
1	A	890	ILE	9.0
1	A	891	PHE	8.9
1	A	286	GLY	8.9
1	A	288	TRP	8.7
1	A	856	PHE	8.7
1	A	290	ARG	8.6
1	A	85	ILE	8.5
1	A	285	GLY	8.2
1	A	298	ILE	8.0
1	A	991	TYR	7.8
1	A	283	VAL	7.5
1	A	278	HIS	7.4
1	A	289	ILE	7.2
1	A	284	HIS	6.6
1	A	870	LEU	6.4
1	A	84	THR	5.9
1	A	881	PRO	5.8
1	A	873	PHE	5.7
1	A	886	LEU	5.6
1	A	86	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLY	5.4
1	A	294	TYR	5.4
1	A	874	MET	5.4
1	A	858	TYR	5.2
1	A	855	TRP	5.1
1	A	929	VAL	4.9
1	A	302	LEU	4.9
1	A	78	PHE	4.9
1	A	877	THR	4.8
1	A	291	GLY	4.8
1	A	295	TYR	4.7
1	A	889	GLU	4.7
1	A	949	TYR	4.6
1	A	888	CYS	4.5
1	A	925	MET	4.5
1	A	928	TRP	4.5
1	A	274	ILE	4.4
1	A	993	GLU	4.4
1	A	994	GLY	4.3
1	A	967	TRP	4.3
1	A	964	LEU	4.3
1	A	780	ALA	4.3
1	A	75	LEU	4.2
1	A	951	ASP	4.2
1	A	957	PHE	4.1
1	A	887	ASP	4.1
1	A	784	PRO	4.0
1	A	244	GLN	4.0
1	A	953	LEU	4.0
1	A	787	LEU	4.0
1	A	267	ILE	3.9
1	A	276	ILE	3.9
1	A	81	GLY	3.9
1	A	293	ILE	3.9
1	A	876	CYS	3.8
1	A	923	MET	3.8
1	A	863	PRO	3.7
1	A	275	ASN	3.7
1	A	271	VAL	3.7
1	A	853	ALA	3.5
1	A	864	GLY	3.4
1	A	950	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	866	THR	3.3
1	A	924	ARG	3.3
1	A	965	THR	3.2
1	A	920	GLN	3.1
1	A	948	LEU	3.1
1	A	986	PHE	3.1
1	A	57	PHE	3.1
1	A	883	PHE	3.1
1	A	83	GLU	3.0
1	A	857	MET	3.0
1	A	868	HIS	3.0
1	A	812	PRO	2.9
1	A	875	GLN	2.9
1	A	775	ILE	2.9
1	A	88	PHE	2.9
1	A	865	VAL	2.8
1	A	51	GLU	2.7
1	A	270	ALA	2.7
1	A	95	LEU	2.7
1	A	79	GLU	2.7
1	A	60	LEU	2.7
1	A	809	PHE	2.6
1	A	264	ILE	2.5
1	A	296	PHE	2.5
1	A	880	HIS	2.5
1	A	859	ALA	2.4
1	A	916	LEU	2.4
1	A	970	VAL	2.4
1	A	926	PRO	2.4
1	A	959	LEU	2.4
1	A	266	LEU	2.4
1	A	992	LEU	2.4
1	A	61	LEU	2.4
1	A	272	TRP	2.3
1	A	273	LEU	2.3
1	A	814	LEU	2.3
1	A	47	LYS	2.2
1	A	260	LEU	2.2
1	A	82	GLU	2.2
1	A	962	LEU	2.2
1	A	871	THR	2.2
1	A	931	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	882	HIS	2.1
1	A	842	GLY	2.1
1	A	45	GLU	2.1
1	A	241	ALA	2.1
1	A	80	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ATP	A	1002	31/31	0.27	4.09	42,87,197,402	31
2	MG	A	995	1/1	0.21	2.58	37,37,37,37	0
3	MF4	A	996	5/5	0.22	2.55	34,38,47,58	0
2	MG	A	1000	1/1	0.10	1.22	107,107,107,107	0
4	K	A	997	1/1	0.17	-0.11	107,107,107,107	0
5	CZA	A	1001	25/25	0.13	-0.51	83,103,107,115	0

6.5 Other polymers ⓘ

There are no such residues in this entry.