



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2017 – 02:06 PM EDT

PDB ID : 3FPB  
Title : The Structure of Sarcoplasmic Reticulum Ca<sup>2+</sup>-ATPase Bound To Cyclopiazonic acid with ATP  
Authors : Moncoq, K.; Morth, J.P.; Bublitz, M.; Laursen, M.; Nissen, P.; Young, H.S.  
Deposited on : unknown  
Resolution : 2.55 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
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) : rb-20029824

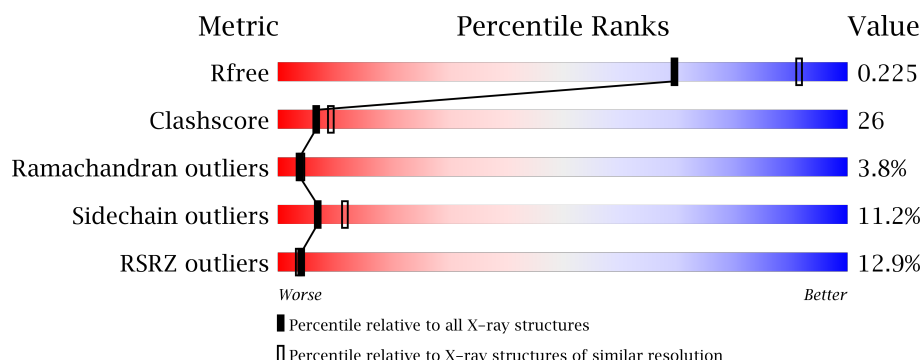
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (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  $\geq 3$ , 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	994	<div> <div>13%</div> <div>51%</div> <div>40%</div> <div>9%</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
6	ATP	A	1002	X	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7930 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	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

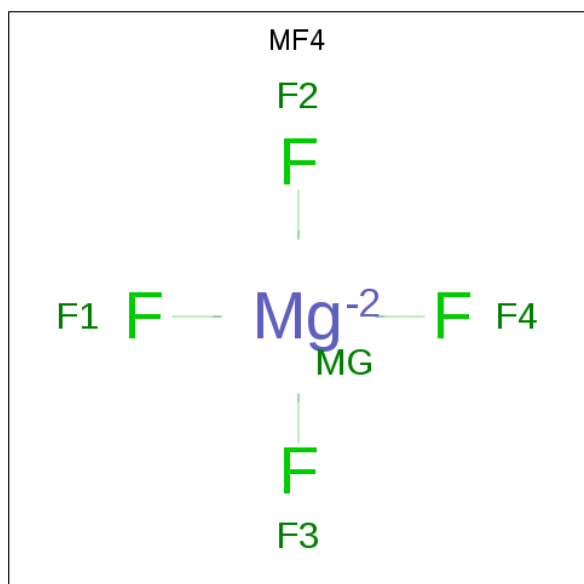
There is a discrepancy between the modelled and reference sequences:

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: F<sub>4</sub>Mg).

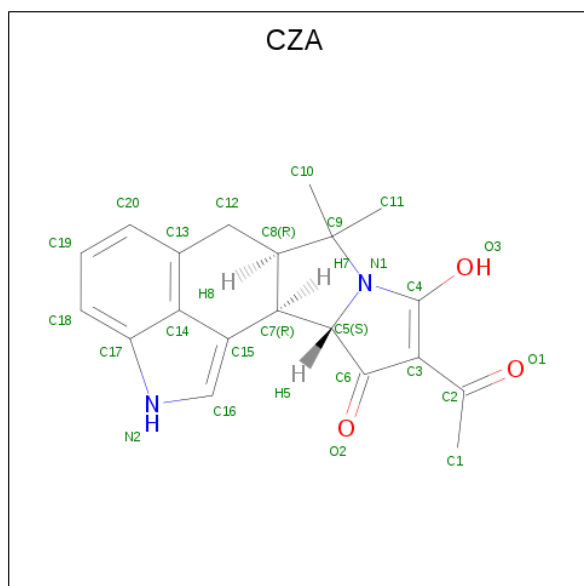


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	F	Mg	0	0
			5	4	1		

- 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: C<sub>20</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).



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: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

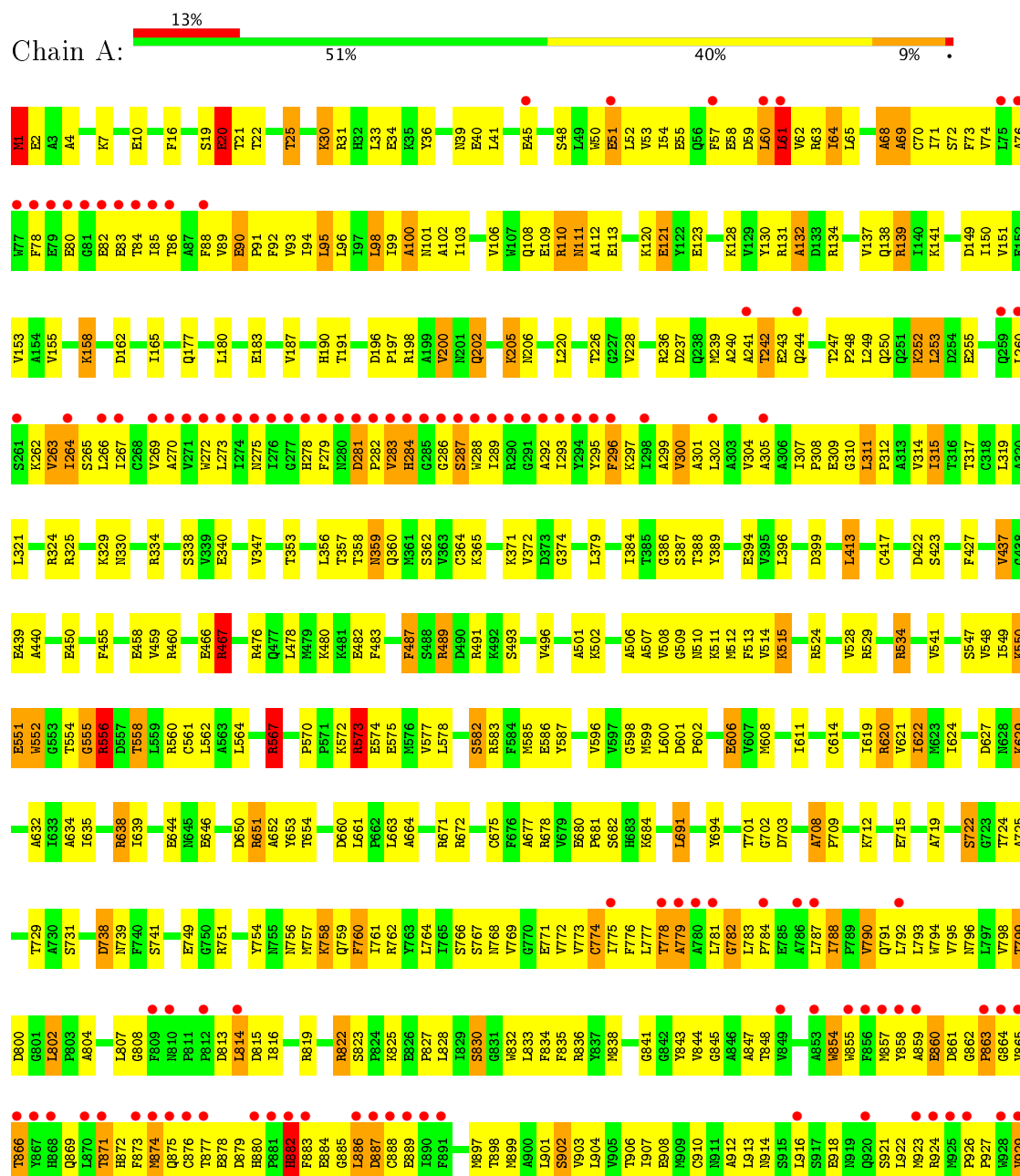
- Molecule 7 is water.

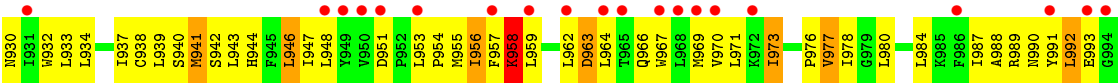
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	195	Total	O	0	0
			195	195		

### 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 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 73.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.333 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: 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 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	7671	0	7764	400	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	19	5	0
6	A	31	0	11	6	0
7	A	195	0	0	6	0
All	All	7930	0	7794	404	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 26.

All (404) 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:794:TRP:HH2	1:A:943:LEU:HB3	1.29	0.98
1:A:57:PHE:HA	1:A:62:VAL:HG21	1.46	0.98
1:A:875:GLN:HA	1:A:878:GLU:HB3	1.44	0.96
1:A:202:GLN:H	1:A:202:GLN:HE21	0.95	0.95
6:A:1002:ATP:H5'1	6:A:1002:ATP:H8	1.33	0.93
1:A:311:LEU:HD22	1:A:315:ILE:HG13	1.48	0.93
1:A:247:THR:H	1:A:250:GLN:HE21	1.20	0.90
1:A:202:GLN:HE21	1:A:202:GLN:N	1.70	0.89
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.54	0.89
1:A:783:LEU:HD23	1:A:784:PRO:HD2	1.55	0.88
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.60	0.82
1:A:794:TRP:CH2	1:A:943:LEU:HB3	2.15	0.81
1:A:57:PHE:HE1	1:A:98:LEU:HG	1.46	0.80
1:A:501:ALA:O	1:A:502:LYS:HB2	1.80	0.80
1:A:880:HIS:O	1:A:884:GLU:HG3	1.81	0.80
1:A:903:VAL:HG11	1:A:973:ILE:HD11	1.64	0.80
1:A:85:ILE:O	1:A:86:THR:HG23	1.82	0.79
1:A:50:TRP:NE1	1:A:54:ILE:HD11	2.01	0.76
1:A:756:ASN:ND2	1:A:808:GLY:HA2	2.00	0.76
1:A:600:LEU:HD23	1:A:600:LEU:O	1.87	0.75
1:A:934:LEU:HA	1:A:937:ILE:HD12	1.69	0.75
1:A:903:VAL:HG22	1:A:970:VAL:HG13	1.68	0.73
1:A:202:GLN:H	1:A:202:GLN:NE2	1.79	0.73
1:A:284:HIS:CD2	1:A:288:TRP:HE1	2.06	0.73
1:A:556:ARG:O	1:A:556:ARG:HG2	1.87	0.73
1:A:969:MET:O	1:A:973:ILE:HG22	1.88	0.73
6:A:1002:ATP:C8	6:A:1002:ATP:H5'1	2.23	0.73
1:A:754:TYR:CE1	1:A:758:LYS:HD2	2.22	0.73
1:A:450:GLU:OE2	1:A:467:ARG:NH1	2.21	0.73
1:A:30:LYS:O	1:A:34:GLU:HG3	1.90	0.71
1:A:88:PHE:CD2	1:A:92:PHE:HE1	2.08	0.71
1:A:423:SER:HB3	1:A:437:VAL:O	1.89	0.71
1:A:795:VAL:HA	1:A:799:THR:OG1	1.89	0.71
1:A:865:VAL:HB	1:A:869:GLN:HB2	1.70	0.71
1:A:941:MET:CE	1:A:941:MET:HA	2.20	0.71
1:A:958:LYS:NZ	1:A:958:LYS:HB3	2.06	0.71
1:A:886:LEU:CD1	1:A:887:ASP:H	2.04	0.70
1:A:263:VAL:O	1:A:265:SER:N	2.25	0.69
1:A:783:LEU:HD23	1:A:784:PRO:CD	2.22	0.69
1:A:120:LYS:HE2	1:A:123:GLU:OE2	1.93	0.69
1:A:88:PHE:HD2	1:A:92:PHE:HE1	1.41	0.69
1:A:886:LEU:HD12	1:A:887:ASP:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:TRP:HD1	1:A:295:TYR:CE2	2.11	0.68
1:A:72:SER:HB2	1:A:90:GLU:HG2	1.76	0.68
1:A:963:ASP:H	1:A:966:GLN:HG3	1.58	0.67
1:A:30:LYS:N	1:A:30:LYS:HD2	2.09	0.67
1:A:855:TRP:NE1	1:A:861:ASP:HB2	2.10	0.67
1:A:311:LEU:HD22	1:A:315:ILE:CG1	2.24	0.67
1:A:31:ARG:O	1:A:31:ARG:HD2	1.94	0.67
1:A:650:ASP:O	1:A:672:ARG:HD2	1.95	0.67
1:A:95:LEU:HD13	1:A:98:LEU:HD23	1.76	0.67
1:A:329:LYS:O	1:A:330:ASN:HB2	1.92	0.66
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.75	0.66
1:A:247:THR:H	1:A:250:GLN:NE2	1.93	0.66
1:A:263:VAL:HG12	1:A:264:ILE:N	2.11	0.66
1:A:769:VAL:O	1:A:773:VAL:HG23	1.96	0.66
1:A:64:ILE:HD11	1:A:264:ILE:HG21	1.78	0.65
1:A:879:ASP:O	1:A:882:HIS:HB2	1.96	0.65
1:A:783:LEU:CD2	1:A:784:PRO:HD2	2.25	0.65
1:A:756:ASN:HD22	1:A:808:GLY:HA2	1.61	0.64
1:A:879:ASP:HB3	1:A:882:HIS:CG	2.31	0.64
1:A:90:GLU:HB3	1:A:91:PRO:CD	2.27	0.64
1:A:751:ARG:HB3	1:A:816:ILE:HG12	1.79	0.64
1:A:903:VAL:HG11	1:A:973:ILE:CD1	2.26	0.64
1:A:903:VAL:CG2	1:A:970:VAL:HG13	2.27	0.64
1:A:914:ASN:HD22	1:A:922:LEU:HD11	1.62	0.64
1:A:794:TRP:CZ2	1:A:947:ILE:HD11	2.32	0.64
1:A:606:GLU:HG3	1:A:739:ASN:OD1	1.97	0.63
1:A:360:GLN:NE2	1:A:388:THR:HG22	2.14	0.63
1:A:854:TRP:CE3	1:A:854:TRP:O	2.52	0.63
1:A:634:ALA:O	1:A:638:ARG:HG3	1.99	0.62
1:A:854:TRP:O	1:A:854:TRP:CD2	2.51	0.62
1:A:951:ASP:O	1:A:954:PRO:HD2	1.99	0.62
1:A:272:TRP:CD1	1:A:295:TYR:CE2	2.87	0.62
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.29	0.62
1:A:387:SER:HB2	1:A:602:PRO:HG3	1.82	0.62
1:A:310:GLY:O	1:A:311:LEU:C	2.37	0.61
1:A:958:LYS:O	1:A:958:LYS:HG3	2.00	0.61
1:A:977:VAL:O	1:A:980:LEU:HB3	2.00	0.61
1:A:646:GLU:OE2	1:A:651:ARG:HD3	1.99	0.61
1:A:855:TRP:HE1	1:A:861:ASP:HB2	1.66	0.61
1:A:325:ARG:NH1	1:A:749:GLU:OE1	2.33	0.61
1:A:794:TRP:CH2	1:A:947:ILE:HD11	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1002:ATP:H8	6:A:1002:ATP:C5'	2.10	0.61
1:A:85:ILE:HG13	1:A:85:ILE:O	1.99	0.61
1:A:73:PHE:HA	1:A:91:PRO:HG3	1.83	0.61
1:A:362:SER:O	1:A:599:MET:HA	2.01	0.60
1:A:956:ILE:HG13	1:A:957:PHE:CD1	2.36	0.60
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.83	0.60
1:A:353:THR:HA	1:A:357:THR:OG1	2.01	0.60
1:A:57:PHE:HA	1:A:62:VAL:CG2	2.26	0.60
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.83	0.60
1:A:754:TYR:CE1	1:A:758:LYS:CD	2.85	0.60
1:A:773:VAL:O	1:A:777:LEU:HG	2.01	0.60
1:A:792:LEU:O	1:A:796:ASN:HB2	2.02	0.60
1:A:76:ALA:HB2	1:A:91:PRO:HG2	1.84	0.60
1:A:865:VAL:CG1	1:A:869:GLN:HG3	2.32	0.59
1:A:76:ALA:HB2	1:A:91:PRO:CG	2.32	0.59
1:A:781:LEU:O	1:A:782:GLY:C	2.41	0.59
1:A:757:MET:O	1:A:761:ILE:HD12	2.03	0.59
1:A:266:LEU:O	1:A:269:VAL:HG12	2.01	0.59
1:A:551:GLU:HG2	1:A:552:TRP:HD1	1.67	0.59
1:A:767:SER:HA	1:A:908:GLU:OE2	2.03	0.59
1:A:102:ALA:O	1:A:106:VAL:HG23	2.03	0.59
1:A:482:GLU:OE2	1:A:573:ARG:NE	2.31	0.59
1:A:802:LEU:CD2	1:A:802:LEU:N	2.66	0.58
1:A:889:GLU:HG2	1:A:889:GLU:O	2.03	0.58
1:A:296:PHE:CD1	1:A:296:PHE:N	2.71	0.58
1:A:650:ASP:OD1	1:A:650:ASP:N	2.32	0.58
1:A:240:ALA:O	1:A:242:THR:N	2.36	0.58
1:A:41:LEU:O	1:A:120:LYS:HE3	2.03	0.58
1:A:72:SER:O	1:A:91:PRO:HG3	2.03	0.58
1:A:739:ASN:OD1	1:A:741:SER:HB2	2.04	0.58
1:A:61:LEU:O	1:A:64:ILE:HG22	2.03	0.58
1:A:205:LYS:HE3	6:A:1002:ATP:O2G	2.03	0.58
1:A:263:VAL:HG12	1:A:264:ILE:H	1.68	0.58
1:A:929:VAL:HG12	1:A:930:ASN:N	2.17	0.58
1:A:992:LEU:C	1:A:992:LEU:HD12	2.23	0.58
1:A:977:VAL:CG1	1:A:978:ILE:N	2.67	0.57
1:A:293:ILE:O	1:A:293:ILE:HG22	2.05	0.57
1:A:279:PHE:CG	1:A:279:PHE:O	2.57	0.57
1:A:802:LEU:HD12	1:A:939:LEU:HD23	1.87	0.57
1:A:614:CYS:HB3	1:A:619:ILE:HB	1.86	0.57
1:A:288:TRP:O	1:A:292:ALA:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:HB2	1:A:296:PHE:CD1	2.40	0.56
1:A:61:LEU:C	1:A:64:ILE:HG22	2.25	0.56
1:A:776:PHE:CD2	1:A:776:PHE:O	2.58	0.56
1:A:886:LEU:CD1	1:A:887:ASP:N	2.67	0.56
1:A:937:ILE:O	1:A:941:MET:HB2	2.06	0.56
1:A:70:CYS:O	1:A:74:VAL:HG23	2.06	0.56
1:A:88:PHE:HD2	1:A:92:PHE:CE1	2.24	0.56
1:A:832:TRP:CZ2	1:A:987:ILE:HG23	2.41	0.56
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.88	0.56
1:A:82:GLU:O	1:A:84:THR:N	2.38	0.56
1:A:764:LEU:CD2	1:A:800:ASP:HB3	2.36	0.55
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.88	0.55
1:A:61:LEU:HD12	5:A:1001:CZA:H8	1.89	0.55
1:A:260:LEU:O	1:A:263:VAL:HB	2.06	0.55
1:A:272:TRP:CD1	1:A:295:TYR:HE2	2.24	0.55
1:A:879:ASP:HB3	1:A:882:HIS:ND1	2.22	0.55
1:A:71:ILE:HA	1:A:74:VAL:HG23	1.88	0.55
1:A:958:LYS:HZ2	1:A:958:LYS:HB3	1.70	0.55
1:A:1:MET:HB2	1:A:16:PHE:CZ	2.42	0.55
1:A:864:GLY:O	1:A:866:THR:HG22	2.06	0.55
1:A:296:PHE:H	1:A:296:PHE:HD1	1.55	0.54
1:A:198:ARG:NH1	1:A:660:ASP:OD1	2.37	0.54
1:A:360:GLN:HE21	1:A:388:THR:HG22	1.72	0.54
1:A:304:VAL:HG13	1:A:793:LEU:HD21	1.88	0.54
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.34	0.54
1:A:722:SER:OG	1:A:738:ASP:OD2	2.24	0.54
1:A:834:PHE:CE1	1:A:838:MET:HE2	2.42	0.54
1:A:989:ARG:HG3	1:A:990:ASN:ND2	2.22	0.54
1:A:68:ALA:O	1:A:71:ILE:N	2.41	0.54
1:A:611:ILE:CD1	1:A:621:VAL:HG11	2.38	0.54
1:A:76:ALA:CB	1:A:91:PRO:HG2	2.38	0.54
1:A:487:PHE:C	1:A:487:PHE:CD1	2.82	0.53
1:A:910:CYS:HB2	1:A:977:VAL:HG11	1.89	0.53
1:A:775:ILE:HA	1:A:778:THR:HG22	1.91	0.53
1:A:508:VAL:CG1	1:A:509:GLY:N	2.71	0.53
1:A:830:SER:O	1:A:833:LEU:HD13	2.09	0.53
1:A:90:GLU:O	1:A:94:ILE:HG13	2.08	0.53
1:A:914:ASN:ND2	1:A:922:LEU:HD11	2.24	0.53
1:A:777:LEU:C	1:A:779:ALA:H	2.11	0.53
1:A:629:LYS:HE3	1:A:654:THR:HG23	1.91	0.53
1:A:95:LEU:O	1:A:99:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:CE	6:A:1002:ATP:O2G	2.57	0.52
1:A:307:ILE:HG22	1:A:309:GLU:N	2.24	0.52
1:A:64:ILE:HG23	1:A:65:LEU:HD12	1.91	0.52
1:A:855:TRP:HA	1:A:859:ALA:CB	2.39	0.52
1:A:281:ASP:N	1:A:282:PRO:HD3	2.25	0.52
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.40	0.52
1:A:59:ASP:O	1:A:62:VAL:HG22	2.09	0.52
1:A:95:LEU:CD1	1:A:98:LEU:HD23	2.38	0.52
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.92	0.52
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.92	0.52
1:A:113:GLU:OE1	1:A:113:GLU:N	2.41	0.52
1:A:74:VAL:O	1:A:78:PHE:HD1	1.92	0.52
1:A:20:GLU:HB3	7:A:1003:HOH:O	2.10	0.52
1:A:947:ILE:O	1:A:947:ILE:HG22	2.10	0.52
1:A:109:GLU:O	1:A:110:ARG:O	2.27	0.52
1:A:263:VAL:O	1:A:266:LEU:N	2.41	0.52
1:A:102:ALA:HB2	5:A:1001:CZA:H11	1.92	0.51
1:A:510:ASN:O	1:A:511:LYS:HD3	2.10	0.51
1:A:992:LEU:O	1:A:993:GLU:HG2	2.10	0.51
1:A:101:ASN:HB3	5:A:1001:CZA:C4	2.41	0.51
1:A:969:MET:O	1:A:973:ILE:CG2	2.56	0.51
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:311:LEU:CD2	1:A:315:ILE:HG13	2.32	0.51
1:A:832:TRP:HZ2	1:A:987:ILE:CG2	2.24	0.51
1:A:62:VAL:HG12	5:A:1001:CZA:H103	1.93	0.51
1:A:110:ARG:HG2	1:A:111:ASN:H	1.76	0.51
1:A:774:CYS:SG	1:A:787:LEU:HD12	2.51	0.51
1:A:859:ALA:O	1:A:861:ASP:N	2.44	0.51
6:A:1002:ATP:C8	6:A:1002:ATP:C5'	2.91	0.51
1:A:295:TYR:O	1:A:299:ALA:N	2.41	0.51
1:A:556:ARG:O	1:A:556:ARG:CG	2.58	0.51
1:A:583:ARG:NH1	7:A:1139:HOH:O	2.32	0.50
1:A:622:ILE:HD12	1:A:691:LEU:HD21	1.94	0.50
1:A:632:ALA:HB1	1:A:675:CYS:SG	2.51	0.50
1:A:269:VAL:O	1:A:273:LEU:N	2.43	0.50
1:A:899:MET:O	1:A:903:VAL:HG23	2.11	0.50
1:A:788:ILE:HG12	1:A:791:GLN:HG3	1.93	0.50
1:A:865:VAL:HG11	1:A:869:GLN:HG3	1.92	0.50
1:A:898:THR:O	1:A:902:SER:HB2	2.11	0.50
1:A:832:TRP:CZ2	1:A:987:ILE:CG2	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD22	1:A:340:GLU:HG3	1.93	0.50
1:A:944:HIS:CE1	1:A:967:TRP:HH2	2.30	0.50
1:A:865:VAL:HG12	1:A:869:GLN:HG3	1.94	0.49
1:A:287:SER:HB2	1:A:289:ILE:HG22	1.94	0.49
1:A:963:ASP:CB	1:A:966:GLN:HG2	2.43	0.49
1:A:967:TRP:C	1:A:971:LEU:HD12	2.32	0.49
1:A:887:ASP:CG	1:A:888:CYS:H	2.14	0.49
1:A:902:SER:HB3	1:A:970:VAL:HG11	1.94	0.49
1:A:769:VAL:HG12	1:A:841:GLY:HA3	1.95	0.49
1:A:924:ARG:HH22	1:A:989:ARG:NH2	2.10	0.49
1:A:72:SER:C	1:A:91:PRO:HG3	2.33	0.49
1:A:654:THR:HA	1:A:677:ALA:O	2.13	0.48
1:A:85:ILE:O	1:A:86:THR:CG2	2.57	0.48
1:A:25:THR:HA	1:A:132:ALA:HB3	1.95	0.48
1:A:358:THR:O	1:A:359:ASN:HB3	2.13	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:875:GLN:HB3	1:A:879:ASP:HB2	1.94	0.48
1:A:977:VAL:HG12	1:A:978:ILE:N	2.28	0.48
1:A:300:VAL:HG12	1:A:301:ALA:N	2.27	0.48
1:A:39:ASN:OD1	1:A:226:THR:HB	2.14	0.48
1:A:802:LEU:CD1	1:A:939:LEU:HD23	2.44	0.48
1:A:489:ARG:HG3	7:A:1118:HOH:O	2.12	0.48
1:A:304:VAL:HG13	1:A:793:LEU:CD2	2.44	0.48
1:A:751:ARG:HB3	1:A:816:ILE:CG1	2.43	0.48
1:A:272:TRP:CD2	1:A:272:TRP:O	2.67	0.48
1:A:778:THR:HA	1:A:783:LEU:HB2	1.95	0.48
1:A:886:LEU:HD13	1:A:887:ASP:H	1.78	0.48
1:A:52:LEU:HD13	1:A:106:VAL:CG1	2.44	0.47
1:A:813:ASP:HB3	1:A:815:ASP:OD1	2.14	0.47
1:A:754:TYR:CD2	1:A:822:ARG:NH2	2.82	0.47
1:A:762:ARG:HH22	1:A:918:GLU:HA	1.78	0.47
1:A:515:LYS:HB2	1:A:564:LEU:HD23	1.96	0.47
1:A:990:ASN:O	1:A:992:LEU:N	2.34	0.47
1:A:305:ALA:O	1:A:768:ASN:ND2	2.48	0.47
1:A:528:VAL:HG11	1:A:541:VAL:HG11	1.97	0.47
1:A:832:TRP:HZ2	1:A:987:ILE:HG23	1.79	0.47
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.55	0.47
1:A:567:ARG:CD	1:A:570:PRO:HA	2.36	0.47
1:A:795:VAL:HG21	1:A:904:LEU:HD23	1.97	0.47
1:A:622:ILE:CD1	1:A:691:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:MET:SD	1:A:958:LYS:HD2	2.55	0.47
1:A:68:ALA:O	1:A:69:ALA:C	2.53	0.47
1:A:885:GLY:O	1:A:886:LEU:HB3	2.15	0.47
1:A:760:PHE:C	1:A:760:PHE:CD1	2.88	0.47
1:A:912:ALA:O	1:A:933:LEU:HD21	2.14	0.47
1:A:966:GLN:O	1:A:970:VAL:HG23	2.15	0.47
1:A:247:THR:HB	1:A:248:PRO:HD2	1.95	0.47
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.44	0.47
1:A:113:GLU:OE2	1:A:334:ARG:NH1	2.47	0.47
1:A:73:PHE:CA	1:A:91:PRO:HG3	2.44	0.47
1:A:947:ILE:HG22	1:A:959:LEU:HD12	1.97	0.47
1:A:68:ALA:O	1:A:70:CYS:N	2.48	0.46
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.50	0.46
1:A:190:HIS:O	1:A:206:ASN:HA	2.16	0.46
1:A:857:MET:O	1:A:859:ALA:N	2.48	0.46
1:A:988:ALA:HA	1:A:992:LEU:HD23	1.98	0.46
1:A:556:ARG:NH2	1:A:644:GLU:OE2	2.48	0.46
1:A:799:THR:HG22	1:A:940:SER:HB3	1.96	0.46
1:A:802:LEU:N	1:A:802:LEU:HD22	2.29	0.46
1:A:857:MET:C	1:A:859:ALA:H	2.19	0.46
1:A:939:LEU:HD12	1:A:939:LEU:O	2.15	0.46
1:A:946:LEU:HA	1:A:946:LEU:HD12	1.77	0.46
1:A:267:ILE:HG22	1:A:302:LEU:HD13	1.98	0.46
1:A:501:ALA:O	1:A:502:LYS:CB	2.45	0.46
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.65	0.46
1:A:2:GLU:HA	1:A:2:GLU:OE1	2.15	0.46
1:A:725:ALA:O	1:A:729:THR:HG23	2.16	0.46
1:A:263:VAL:O	1:A:264:ILE:C	2.54	0.46
1:A:622:ILE:HG21	1:A:622:ILE:HD13	1.75	0.46
1:A:768:ASN:O	1:A:772:VAL:HG23	2.16	0.46
1:A:901:LEU:HD12	1:A:901:LEU:O	2.16	0.46
1:A:903:VAL:O	1:A:907:ILE:HG13	2.16	0.46
1:A:73:PHE:CE2	1:A:88:PHE:HE2	2.34	0.45
1:A:788:ILE:HG13	1:A:790:VAL:HG23	1.98	0.45
1:A:269:VAL:CG1	1:A:270:ALA:N	2.80	0.45
1:A:70:CYS:O	1:A:74:VAL:N	2.47	0.45
1:A:99:ILE:O	1:A:103:ILE:HG13	2.17	0.45
1:A:550:LYS:O	1:A:551:GLU:C	2.53	0.45
1:A:61:LEU:HA	1:A:64:ILE:HG22	1.98	0.45
1:A:556:ARG:HG2	1:A:638:ARG:HG2	1.99	0.45
1:A:774:CYS:SG	1:A:775:ILE:HD13	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ASP:HB3	1:A:882:HIS:HB2	1.98	0.45
1:A:295:TYR:C	1:A:297:LYS:H	2.20	0.45
1:A:359:ASN:N	1:A:601:ASP:OD1	2.50	0.45
1:A:69:ALA:HB2	1:A:94:ILE:CG2	2.47	0.45
1:A:916:LEU:HD21	1:A:933:LEU:HD22	1.99	0.45
1:A:635:ILE:O	1:A:639:ILE:HG12	2.16	0.45
1:A:804:ALA:HA	1:A:807:LEU:HD12	1.99	0.45
1:A:855:TRP:CE3	1:A:855:TRP:O	2.70	0.45
1:A:963:ASP:O	1:A:966:GLN:HB2	2.17	0.45
1:A:984:LEU:HA	1:A:987:ILE:HG22	1.98	0.45
1:A:702:GLY:O	1:A:719:ALA:HA	2.17	0.45
1:A:555:GLY:H	1:A:558:THR:H	1.65	0.44
1:A:832:TRP:HA	1:A:832:TRP:CE3	2.52	0.44
1:A:708:ALA:N	1:A:709:PRO:CD	2.81	0.44
1:A:882:HIS:HB3	1:A:883:PHE:H	1.38	0.44
1:A:963:ASP:HB3	1:A:966:GLN:HG2	1.98	0.44
1:A:880:HIS:O	1:A:884:GLU:CG	2.58	0.44
1:A:798:VAL:O	1:A:802:LEU:HD23	2.18	0.44
1:A:88:PHE:O	1:A:92:PHE:HD1	2.01	0.44
1:A:272:TRP:CG	1:A:272:TRP:O	2.70	0.43
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.99	0.43
1:A:371:LYS:HG3	1:A:372:VAL:N	2.33	0.43
1:A:862:GLY:N	1:A:863:PRO:HD3	2.32	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.71	0.43
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.54	0.43
1:A:624:ILE:HG22	1:A:684:LYS:HG2	1.97	0.43
1:A:778:THR:OG1	1:A:784:PRO:O	2.35	0.43
1:A:96:LEU:HD12	1:A:96:LEU:O	2.19	0.43
1:A:252:LYS:HD3	1:A:252:LYS:HA	1.60	0.43
1:A:282:PRO:C	1:A:284:HIS:N	2.71	0.43
1:A:551:GLU:HG2	1:A:552:TRP:N	2.33	0.43
1:A:913:LEU:HD21	1:A:934:LEU:HD21	2.01	0.43
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.43
1:A:284:HIS:HD2	1:A:288:TRP:HE1	1.59	0.43
1:A:832:TRP:O	1:A:835:PHE:HB3	2.19	0.43
1:A:73:PHE:HA	1:A:91:PRO:CG	2.48	0.43
1:A:794:TRP:CH2	1:A:947:ILE:CD1	3.00	0.43
1:A:874:MET:H	1:A:874:MET:HG2	1.60	0.43
1:A:275:ASN:ND2	1:A:295:TYR:CE1	2.87	0.43
1:A:827:PRO:CG	1:A:830:SER:HB3	2.48	0.43
1:A:941:MET:HE2	1:A:941:MET:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:TRP:O	1:A:971:LEU:HD12	2.19	0.43
1:A:282:PRO:O	1:A:283:VAL:HG12	2.19	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
1:A:782:GLY:C	1:A:873:PHE:HE2	2.22	0.43
1:A:847:ALA:HB1	1:A:973:ILE:HD11	1.99	0.43
1:A:946:LEU:O	1:A:953:LEU:HD12	2.18	0.42
1:A:65:LEU:HD12	1:A:65:LEU:N	2.34	0.42
1:A:55:GLU:O	1:A:58:GLU:HB2	2.18	0.42
1:A:774:CYS:HB2	1:A:848:THR:OG1	2.20	0.42
1:A:131:ARG:NH2	1:A:149:ASP:OD2	2.48	0.42
1:A:771:GLU:HG2	1:A:904:LEU:CD1	2.50	0.42
1:A:762:ARG:HE	1:A:762:ARG:HB3	1.47	0.42
1:A:777:LEU:C	1:A:779:ALA:N	2.72	0.42
1:A:794:TRP:HZ2	1:A:943:LEU:HD22	1.84	0.42
1:A:865:VAL:CB	1:A:869:GLN:HB2	2.45	0.42
1:A:134:ARG:NE	1:A:138:GLN:HG2	2.34	0.42
1:A:50:TRP:HE1	1:A:54:ILE:HD11	1.80	0.42
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.49	0.42
1:A:89:VAL:HG12	1:A:93:VAL:HG23	2.00	0.42
1:A:908:GLU:OE1	1:A:908:GLU:HA	2.19	0.42
1:A:941:MET:O	1:A:944:HIS:HB3	2.18	0.42
1:A:362:SER:O	1:A:599:MET:CA	2.68	0.42
1:A:101:ASN:OD1	1:A:312:PRO:HB2	2.20	0.42
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.70	0.42
1:A:287:SER:C	1:A:289:ILE:H	2.23	0.42
1:A:60:LEU:O	1:A:63:ARG:N	2.53	0.42
1:A:973:ILE:O	1:A:973:ILE:CG1	2.68	0.42
1:A:112:ALA:O	1:A:113:GLU:C	2.58	0.42
1:A:387:SER:CB	1:A:602:PRO:HG3	2.47	0.42
1:A:661:LEU:HD23	1:A:661:LEU:HA	1.79	0.42
1:A:325:ARG:NH1	1:A:749:GLU:CD	2.73	0.42
1:A:769:VAL:CG1	1:A:841:GLY:HA3	2.50	0.42
1:A:80:GLU:O	1:A:82:GLU:N	2.46	0.42
1:A:834:PHE:CZ	1:A:838:MET:HE3	2.55	0.42
1:A:963:ASP:N	1:A:966:GLN:HG3	2.29	0.42
1:A:854:TRP:CG	1:A:854:TRP:O	2.73	0.41
1:A:86:THR:O	1:A:89:VAL:HG23	2.20	0.41
1:A:153:VAL:HG23	1:A:153:VAL:O	2.20	0.41
1:A:71:ILE:HA	1:A:74:VAL:CG2	2.50	0.41
1:A:984:LEU:HA	1:A:987:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HD13	1:A:399:ASP:HA	2.01	0.41
1:A:317:THR:O	1:A:321:LEU:HG	2.20	0.41
1:A:871:THR:HG22	1:A:872:HIS:CE1	2.56	0.41
1:A:913:LEU:O	1:A:914:ASN:C	2.57	0.41
1:A:198:ARG:HD3	1:A:198:ARG:HH21	1.70	0.41
1:A:608:MET:HB3	7:A:1144:HOH:O	2.20	0.41
1:A:938:CYS:O	1:A:942:SER:OG	2.34	0.41
1:A:944:HIS:O	1:A:948:LEU:HG	2.20	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:48:SER:N	1:A:51:GLU:OE2	2.53	0.41
1:A:64:ILE:CD1	1:A:264:ILE:HD13	2.51	0.41
1:A:992:LEU:O	1:A:992:LEU:HD12	2.21	0.41
1:A:560:ARG:O	1:A:598:GLY:HA2	2.20	0.41
1:A:924:ARG:NH2	1:A:989:ARG:NH2	2.69	0.41
1:A:262:LYS:HA	1:A:262:LYS:HD3	1.92	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.87	0.41
1:A:652:ALA:HA	1:A:675:CYS:O	2.20	0.41
1:A:269:VAL:HG13	1:A:270:ALA:N	2.35	0.41
1:A:52:LEU:O	1:A:53:VAL:C	2.60	0.41
1:A:572:LYS:HB3	1:A:574:GLU:OE1	2.20	0.41
1:A:953:LEU:O	1:A:956:ILE:HG12	2.21	0.41
1:A:269:VAL:HA	1:A:272:TRP:HB3	2.02	0.40
1:A:585:MET:HE3	7:A:1169:HOH:O	2.20	0.40
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.68	0.40
1:A:90:GLU:O	1:A:91:PRO:C	2.59	0.40
1:A:794:TRP:CZ3	1:A:947:ILE:CD1	3.03	0.40
1:A:814:LEU:CD1	1:A:814:LEU:N	2.84	0.40
1:A:843:TYR:OH	1:A:976:PRO:HB2	2.21	0.40
1:A:921:SER:C	1:A:923:MET:N	2.75	0.40
1:A:947:ILE:HG23	1:A:957:PHE:CD1	2.56	0.40
1:A:267:ILE:HG22	1:A:302:LEU:CD1	2.51	0.40
1:A:379:LEU:HD12	1:A:548:VAL:HG21	2.02	0.40
1:A:963:ASP:HB2	1:A:966:GLN:CG	2.52	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%)	<div>4</div> <div>4</div>

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

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Mol	Chain	Res	Type
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 [i](#)

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%)	<b>7</b> <b>12</b>

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	202	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	284	HIS
1	A	359	ASN
1	A	360	GLN
1	A	756	ASN
1	A	875	GLN
1	A	914	ASN
1	A	944	HIS
1	A	990	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	27,29,29	2.01	8 (29%)	24,48,48	2.05	5 (20%)
6	ATP	A	1002	-	27,33,33	2.60	12 (44%)	25,52,52	3.41	9 (36%)
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	0/5/5/5
6	ATP	A	1002	-	1/1/7/7	0/18/38/38	0/3/3/3
3	MF4	A	996	1	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	CZA	C4-N1	-5.80	1.33	1.39
5	A	1001	CZA	C3-C4	-2.74	1.35	1.40
5	A	1001	CZA	C13-C14	-2.28	1.39	1.43
6	A	1002	ATP	C5-C4	-2.18	1.35	1.40
5	A	1001	CZA	O3-C4	2.01	1.36	1.31
6	A	1002	ATP	PG-O2G	2.24	1.64	1.54
6	A	1002	ATP	C5'-C4'	2.26	1.58	1.51
6	A	1002	ATP	C6-N6	2.43	1.44	1.34
5	A	1001	CZA	C20-C13	2.54	1.42	1.37
5	A	1001	CZA	C19-C18	3.00	1.43	1.36
6	A	1002	ATP	PA-O5'	3.11	1.72	1.59
5	A	1001	CZA	C1-C2	3.20	1.56	1.50
6	A	1002	ATP	O4'-C1'	3.37	1.45	1.41
5	A	1001	CZA	C12-C8	3.42	1.58	1.53
6	A	1002	ATP	PB-O1B	4.04	1.66	1.50
6	A	1002	ATP	PA-O1A	4.14	1.66	1.50
6	A	1002	ATP	C8-N7	4.63	1.43	1.34
6	A	1002	ATP	PG-O3B	4.70	1.67	1.60
6	A	1002	ATP	PG-O1G	4.71	1.66	1.50
6	A	1002	ATP	C2-N3	5.03	1.40	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	ATP	N3-C2-N1	-12.34	118.11	128.86
6	A	1002	ATP	C4'-O4'-C1'	-6.46	102.90	109.77
5	A	1001	CZA	C12-C13-C14	-6.01	114.36	119.44
5	A	1001	CZA	O2-C6-C5	-2.77	122.07	124.69
6	A	1002	ATP	O4'-C4'-C3'	-2.06	101.08	105.17
6	A	1002	ATP	O3'-C3'-C2'	2.32	119.27	111.83
5	A	1001	CZA	O2-C6-C3	2.46	134.47	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	CZA	C18-C17-N2	2.93	138.92	130.80
6	A	1002	ATP	O4'-C4'-C5'	3.52	121.29	109.40
6	A	1002	ATP	O2'-C2'-C3'	3.60	123.36	111.83
5	A	1001	CZA	C13-C14-C15	3.79	126.96	123.49
6	A	1002	ATP	O2'-C2'-C1'	3.81	123.52	111.61
6	A	1002	ATP	O3'-C3'-C4'	3.97	122.69	111.09
6	A	1002	ATP	O5'-C5'-C4'	3.98	123.11	109.00

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.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	CZA	5	0
6	A	1002	ATP	6	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	994/994 (100%)	0.70	128 (12%) 4 4	34, 72, 209, 337	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	12.0
1	A	282	PRO	10.9
1	A	867	TYR	10.9
1	A	280	ASN	10.8
1	A	279	PHE	9.9
1	A	77	TRP	9.6
1	A	891	PHE	9.1
1	A	278	HIS	8.7
1	A	287	SER	8.7
1	A	298	ILE	8.6
1	A	290	ARG	8.4
1	A	856	PHE	8.3
1	A	890	ILE	8.3
1	A	286	GLY	8.0
1	A	288	TRP	7.8
1	A	991	TYR	7.3
1	A	85	ILE	7.3
1	A	283	VAL	7.1
1	A	870	LEU	6.9
1	A	284	HIS	6.8
1	A	289	ILE	6.7
1	A	881	PRO	6.5
1	A	295	TYR	6.3
1	A	277	GLY	6.2
1	A	274	ILE	6.1
1	A	285	GLY	6.1
1	A	291	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	84	THR	5.8
1	A	86	THR	5.7
1	A	294	TYR	5.5
1	A	855	TRP	5.5
1	A	780	ALA	5.5
1	A	967	TRP	5.4
1	A	873	PHE	5.3
1	A	874	MET	5.3
1	A	964	LEU	5.3
1	A	784	PRO	5.2
1	A	858	TYR	5.1
1	A	787	LEU	5.1
1	A	888	CYS	5.0
1	A	929	VAL	5.0
1	A	928	TRP	4.9
1	A	957	PHE	4.9
1	A	953	LEU	4.8
1	A	877	THR	4.8
1	A	275	ASN	4.7
1	A	78	PHE	4.7
1	A	276	ILE	4.7
1	A	302	LEU	4.7
1	A	889	GLU	4.6
1	A	853	ALA	4.6
1	A	949	TYR	4.5
1	A	271	VAL	4.5
1	A	81	GLY	4.4
1	A	886	LEU	4.3
1	A	925	MET	4.3
1	A	965	THR	4.2
1	A	876	CYS	4.0
1	A	267	ILE	4.0
1	A	75	LEU	3.9
1	A	951	ASP	3.9
1	A	244	GLN	3.9
1	A	293	ILE	3.8
1	A	863	PRO	3.6
1	A	868	HIS	3.6
1	A	775	ILE	3.6
1	A	272	TRP	3.5
1	A	866	THR	3.5
1	A	83	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	970	VAL	3.5
1	A	950	VAL	3.4
1	A	959	LEU	3.4
1	A	849	VAL	3.4
1	A	986	PHE	3.4
1	A	270	ALA	3.4
1	A	875	GLN	3.4
1	A	865	VAL	3.3
1	A	57	PHE	3.3
1	A	993	GLU	3.3
1	A	273	LEU	3.3
1	A	857	MET	3.3
1	A	786	ALA	3.2
1	A	948	LEU	3.2
1	A	76	ALA	3.2
1	A	79	GLU	3.2
1	A	864	GLY	3.2
1	A	887	ASP	3.2
1	A	994	GLY	3.2
1	A	883	PHE	3.1
1	A	962	LEU	3.0
1	A	923	MET	3.0
1	A	82	GLU	2.9
1	A	926	PRO	2.9
1	A	292	ALA	2.9
1	A	269	VAL	2.8
1	A	924	ARG	2.8
1	A	859	ALA	2.8
1	A	60	LEU	2.8
1	A	260	LEU	2.8
1	A	882	HIS	2.8
1	A	880	HIS	2.8
1	A	968	LEU	2.7
1	A	296	PHE	2.7
1	A	781	LEU	2.7
1	A	51	GLU	2.7
1	A	871	THR	2.7
1	A	80	GLU	2.6
1	A	972	LYS	2.5
1	A	266	LEU	2.5
1	A	931	ILE	2.4
1	A	814	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	241	ALA	2.4
1	A	809	PHE	2.4
1	A	778	THR	2.3
1	A	812	PRO	2.3
1	A	264	ILE	2.3
1	A	88	PHE	2.3
1	A	779	ALA	2.3
1	A	61	LEU	2.3
1	A	916	LEU	2.2
1	A	792	LEU	2.2
1	A	305	ALA	2.2
1	A	259	GLN	2.2
1	A	261	SER	2.2
1	A	45	GLU	2.1
1	A	969	MET	2.0
1	A	920	GLN	2.0
1	A	810	ASN	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
6	ATP	A	1002	31/31	0.78	0.29	4.67	42,87,197,402	31
3	MF4	A	996	5/5	0.99	0.22	1.35	34,38,47,58	0
2	MG	A	995	1/1	0.97	0.21	1.09	37,37,37,37	0
4	K	A	997	1/1	0.94	0.16	-0.55	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CZA	A	1001	25/25	0.96	0.13	-0.56	83,103,107,115	0
2	MG	A	1000	1/1	0.92	0.07	-	107,107,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.