Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 12:01 PM EDT

PDB ID	:	3FPB / pdb_00003fpb
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

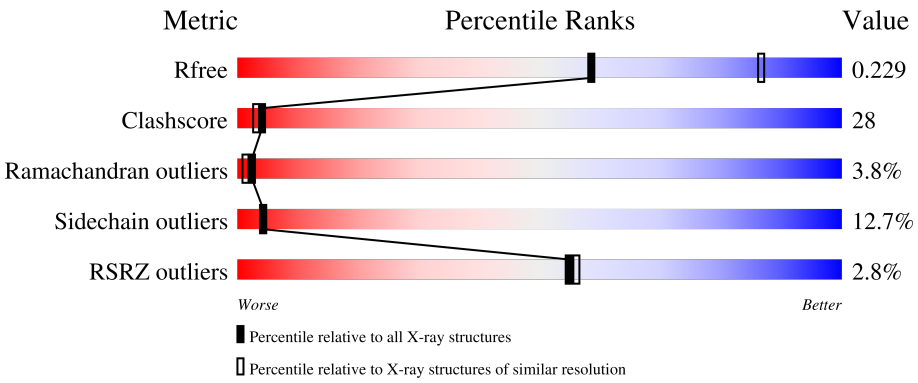
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	994	3%, 41%, 46%, 11%, •

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	-	-	-

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
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0

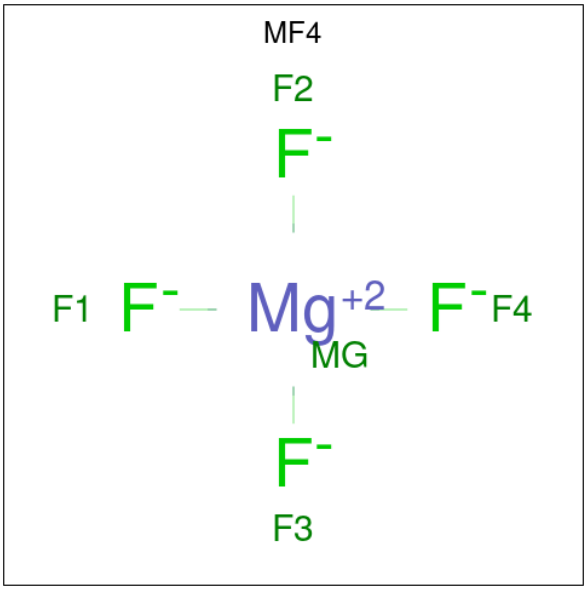
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F_4Mg).

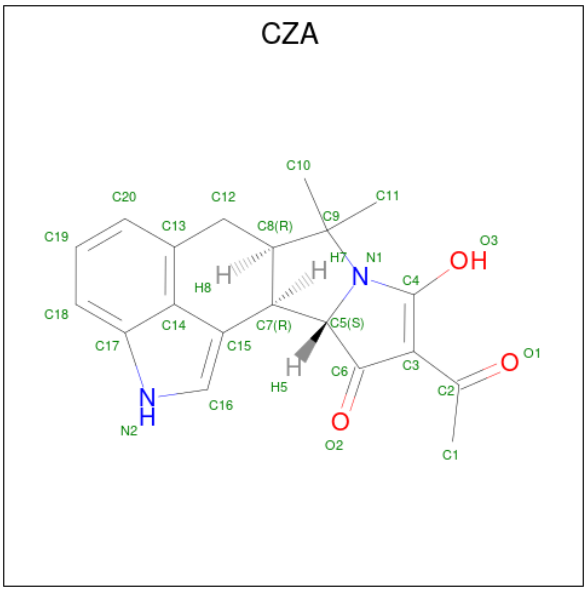


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	F	Mg		
3	A	1	5	4	1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

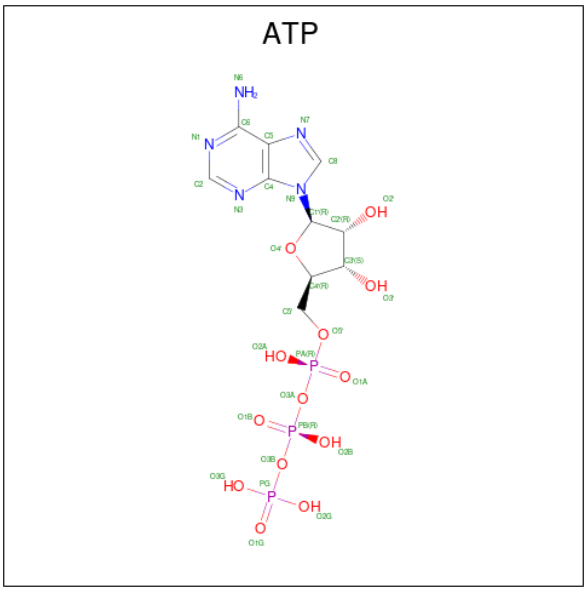
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0

- 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 (CCD ID: CZA) (formula: $C_{20}H_{20}N_2O_3$).



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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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.

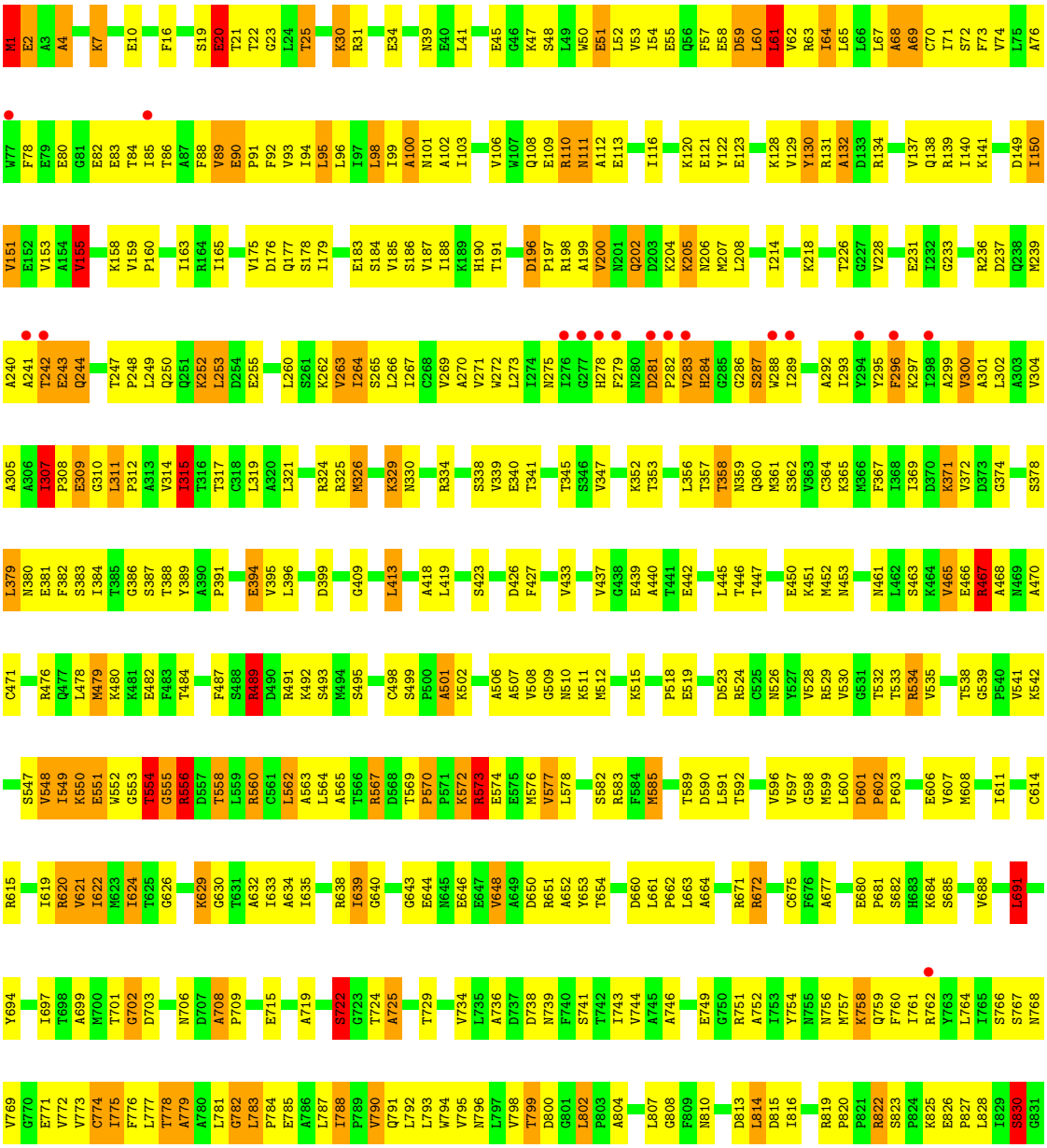
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	195	195	195	0	0

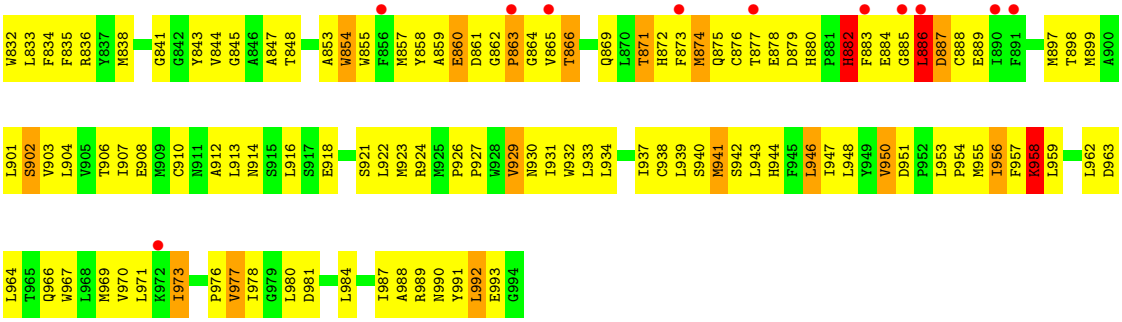
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain A:




W832 L833 F834 F835 R836 Y837 M838
G841 G842 Y843 V844 G845 A846 A847 T848
A853 W854 W855 F856 M857 Y858 A859 E860 D861 G862 P863 G864 V865 T866
Q869 L870 T871 H872 F873 M874 Q875 C876 T877 E878 D879 H880 P881 H882 F883 E884 G885 L886 D887 C888 E889 I890 F891
M897 T898 M899 A900
L901 S902 V903 L904 V905 T906 I907 E908 M909 C910 N911 A912 L913 N914 S915 L916 S917 E918
S921 L922 M923 R924 M925 P926 P927 W928 V929 N930 I931 W932 L933 L934
I937 C938 L939 S940 M941 S942 L943 H944 F945 L946 I947 L948 Y949 V950 D951 P952 L953 P954 M955 I956 F957 K958 L959
L962 D963
L964 T965 Q966 W967 L968 M969 V970 L971 K972 I973
P976 V977 I978 G979 L980 D981
L984
I987 A988 R989 N990 Y991 L992 E993 G994

4 Data and refinement statistics (i)

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 24.94 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.94-2.55) 99.7 (24.94-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.183 , 0.231 0.180 , 0.229	Depositor DCC
R_{free} test set	2775 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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^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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.65	114/7812 (1.5%)	1.58	127/10592 (1.2%)

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 (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ILE	CA-CB	14.41	1.73	1.54
1	A	132	ALA	CA-CB	-10.09	1.36	1.53
1	A	708	ALA	CA-CB	9.16	1.65	1.53
1	A	440	ALA	CA-CB	-8.17	1.40	1.53
1	A	597	VAL	CA-C	8.09	1.62	1.52
1	A	570	PRO	CA-C	8.06	1.59	1.52
1	A	352	LYS	CA-C	7.98	1.61	1.53
1	A	622	ILE	CA-C	7.60	1.62	1.52
1	A	822	ARG	C-O	-7.47	1.14	1.23
1	A	465	VAL	CA-CB	7.37	1.64	1.54
1	A	4	ALA	CA-CB	-7.22	1.41	1.53
1	A	499	SER	CA-C	-7.19	1.43	1.52
1	A	427	PHE	C-O	-7.18	1.15	1.24
1	A	664	ALA	CA-CB	7.03	1.64	1.53
1	A	183	GLU	CA-C	7.02	1.61	1.52
1	A	620	ARG	CA-C	6.99	1.61	1.52
1	A	200	VAL	CA-C	6.92	1.60	1.52
1	A	519	GLU	C-O	6.88	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	518	PRO	CA-CB	-6.86	1.44	1.53
1	A	463	SER	C-O	6.85	1.32	1.23
1	A	703	ASP	C-O	-6.79	1.16	1.24
1	A	554	THR	CA-CB	6.79	1.65	1.53
1	A	630	GLY	C-O	-6.72	1.15	1.23
1	A	358	THR	N-CA	6.70	1.54	1.46
1	A	159	VAL	CA-CB	-6.69	1.45	1.54
1	A	506	ALA	CA-CB	6.67	1.64	1.53
1	A	395	VAL	CA-CB	6.64	1.62	1.54
1	A	187	VAL	CA-CB	6.62	1.62	1.54
1	A	379	LEU	C-O	-6.62	1.15	1.23
1	A	565	ALA	CA-C	6.57	1.60	1.52
1	A	539	GLY	N-CA	6.56	1.50	1.44
1	A	524	ARG	CZ-NH1	6.51	1.41	1.32
1	A	468	ALA	N-CA	-6.49	1.38	1.46
1	A	484	THR	N-CA	-6.49	1.38	1.46
1	A	179	ILE	C-O	-6.47	1.15	1.24
1	A	418	ALA	C-O	-6.44	1.15	1.24
1	A	380	ASN	C-O	6.36	1.31	1.24
1	A	493	SER	CA-C	6.31	1.60	1.52
1	A	662	PRO	CA-C	-6.28	1.45	1.52
1	A	176	ASP	CA-C	6.22	1.60	1.52
1	A	445	LEU	C-O	6.22	1.31	1.24
1	A	199	ALA	CA-CB	-6.18	1.43	1.53
1	A	394	GLU	C-O	6.14	1.31	1.23
1	A	560	ARG	CA-C	6.11	1.61	1.52
1	A	736	ALA	CA-CB	-6.08	1.43	1.53
1	A	150	ILE	CA-CB	6.04	1.61	1.54
1	A	130	TYR	C-O	-6.01	1.16	1.24
1	A	364	CYS	CA-CB	5.96	1.62	1.53
1	A	715	GLU	C-O	-5.90	1.17	1.24
1	A	188	ILE	N-CA	-5.89	1.39	1.46
1	A	389	TYR	CB-CG	-5.89	1.38	1.51
1	A	685	SER	C-O	-5.88	1.16	1.24
1	A	538	THR	CA-C	-5.87	1.45	1.52
1	A	621	VAL	CA-CB	5.83	1.61	1.54
1	A	534	ARG	CA-C	5.76	1.59	1.52
1	A	589	THR	CA-CB	5.75	1.63	1.53
1	A	395	VAL	C-O	5.72	1.30	1.24
1	A	442	GLU	CA-C	-5.67	1.45	1.52
1	A	529	ARG	CA-C	5.67	1.60	1.52
1	A	391	PRO	CA-C	5.66	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	ASN	N-CA	-5.64	1.38	1.46
1	A	592	THR	N-CA	-5.60	1.39	1.46
1	A	381	GLU	C-O	-5.59	1.17	1.23
1	A	364	CYS	CB-SG	5.57	1.99	1.81
1	A	470	ALA	CA-CB	-5.56	1.44	1.53
1	A	640	GLY	C-O	-5.56	1.16	1.24
1	A	364	CYS	N-CA	5.55	1.53	1.46
1	A	590	ASP	CA-C	5.54	1.60	1.52
1	A	624	ILE	C-O	5.53	1.30	1.24
1	A	629	LYS	CA-C	5.52	1.59	1.52
1	A	163	ILE	C-O	5.51	1.29	1.24
1	A	724	THR	CB-CG2	5.50	1.70	1.52
1	A	532	THR	CA-C	-5.50	1.45	1.52
1	A	163	ILE	CA-CB	5.49	1.61	1.54
1	A	389	TYR	CD2-CE2	5.48	1.55	1.38
1	A	479	MET	CA-C	-5.47	1.46	1.52
1	A	703	ASP	N-CA	5.46	1.53	1.46
1	A	345	THR	CA-CB	5.45	1.62	1.53
1	A	633	ILE	N-CA	-5.44	1.40	1.46
1	A	439	GLU	CG-CD	5.44	1.65	1.52
1	A	734	VAL	CA-CB	5.43	1.61	1.54
1	A	691	LEU	CA-C	5.38	1.59	1.52
1	A	542	LYS	N-CA	5.37	1.52	1.46
1	A	601	ASP	C-O	-5.37	1.17	1.24
1	A	419	LEU	CA-C	5.34	1.59	1.52
1	A	563	ALA	CA-CB	-5.32	1.45	1.53
1	A	418	ALA	CA-CB	-5.32	1.45	1.53
1	A	708	ALA	C-O	-5.31	1.19	1.24
1	A	451	LYS	C-O	-5.31	1.18	1.24
1	A	736	ALA	C-O	-5.31	1.17	1.24
1	A	367	PHE	C-O	-5.30	1.17	1.23
1	A	447	THR	C-O	5.30	1.30	1.24
1	A	495	SER	CA-C	-5.30	1.46	1.52
1	A	433	VAL	CA-C	5.28	1.59	1.52
1	A	702	GLY	C-O	5.24	1.30	1.23
1	A	694	TYR	CG-CD1	5.23	1.50	1.39
1	A	326	MET	CA-C	5.22	1.59	1.52
1	A	743	ILE	CA-CB	-5.22	1.48	1.54
1	A	533	THR	CA-CB	5.19	1.61	1.53
1	A	177	GLN	CB-CG	-5.17	1.36	1.52
1	A	446	THR	CA-CB	5.16	1.61	1.53
1	A	23	GLY	C-O	5.15	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	SER	C-O	5.15	1.30	1.23
1	A	725	ALA	N-CA	-5.15	1.40	1.46
1	A	551	GLU	C-O	-5.14	1.18	1.24
1	A	233	GLY	CA-C	5.14	1.57	1.52
1	A	187	VAL	CB-CG1	5.12	1.69	1.52
1	A	697	ILE	C-O	5.12	1.29	1.24
1	A	369	ILE	CA-CB	-5.12	1.47	1.54
1	A	489	ARG	N-CA	5.11	1.52	1.46
1	A	648	VAL	CA-CB	5.08	1.61	1.54
1	A	214	ILE	CA-C	5.07	1.59	1.52
1	A	699	ALA	CA-C	5.03	1.59	1.52
1	A	361	MET	CA-CB	-5.02	1.45	1.53

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	THR	CA-C-N	-10.77	108.50	120.45
1	A	25	THR	C-N-CA	-10.77	108.50	120.45
1	A	556	ARG	N-CA-C	-10.54	97.00	111.87
1	A	467	ARG	NE-CZ-NH1	-9.12	112.38	121.50
1	A	122	TYR	N-CA-C	-8.89	101.97	113.17
1	A	576	MET	CA-C-N	-8.47	111.76	122.43
1	A	576	MET	C-N-CA	-8.47	111.76	122.43
1	A	341	THR	N-CA-C	8.18	120.92	111.11
1	A	467	ARG	NE-CZ-NH2	7.95	126.35	119.20
1	A	476	ARG	NE-CZ-NH1	-7.91	113.59	121.50
1	A	585	MET	N-CA-C	-7.41	103.28	111.36
1	A	315	ILE	N-CA-C	-7.19	103.84	110.82
1	A	501	ALA	CA-C-N	-7.13	112.12	124.82
1	A	501	ALA	C-N-CA	-7.13	112.12	124.82
1	A	461	ASN	N-CA-C	6.91	121.41	112.92
1	A	701	THR	CB-CA-C	-6.85	96.28	109.37
1	A	491	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	A	682	SER	CA-CB-OG	-6.78	97.55	111.10
1	A	535	VAL	CA-C-N	-6.78	112.98	119.76
1	A	535	VAL	C-N-CA	-6.78	112.98	119.76
1	A	534	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	A	539	GLY	CA-C-N	-6.73	111.43	119.84
1	A	539	GLY	C-N-CA	-6.73	111.43	119.84
1	A	578	LEU	N-CA-C	6.69	119.41	111.71
1	A	931	ILE	CB-CA-C	-6.59	103.41	112.24
1	A	492	LYS	N-CA-C	6.58	120.89	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	744	VAL	N-CA-C	-6.57	104.09	110.72
1	A	364	CYS	CB-CA-C	6.54	119.62	109.03
1	A	722	SER	CA-C-N	-6.50	115.41	122.55
1	A	722	SER	C-N-CA	-6.50	115.41	122.55
1	A	577	VAL	N-CA-C	6.49	117.85	107.73
1	A	569	THR	CA-C-N	-6.47	113.71	120.38
1	A	569	THR	C-N-CA	-6.47	113.71	120.38
1	A	200	VAL	N-CA-CB	-6.46	99.50	111.91
1	A	591	LEU	N-CA-C	6.44	119.58	110.50
1	A	577	VAL	CB-CA-C	6.37	119.35	111.25
1	A	601	ASP	CA-C-N	6.29	126.86	120.38
1	A	601	ASP	C-N-CA	6.29	126.86	120.38
1	A	476	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	A	20	GLU	N-CA-CB	-6.11	100.48	110.14
1	A	409	GLY	N-CA-C	6.07	120.23	112.83
1	A	129	VAL	N-CA-C	6.06	118.95	108.95
1	A	1	MET	N-CA-C	6.04	127.93	111.00
1	A	1	MET	N-CA-CB	6.02	120.74	110.50
1	A	615	ARG	N-CA-C	-6.02	104.80	111.36
1	A	724	THR	N-CA-C	5.98	118.42	110.53
1	A	476	ARG	CG-CD-NE	-5.95	98.91	112.00
1	A	603	PRO	CB-CA-C	-5.94	103.20	110.98
1	A	643	GLY	N-CA-C	-5.93	104.64	112.82
1	A	465	VAL	N-CA-CB	5.93	119.47	110.58
1	A	495	SER	N-CA-C	5.92	117.97	109.14
1	A	576	MET	N-CA-C	5.84	118.25	108.96
1	A	467	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	196	ASP	CA-C-N	5.80	125.42	119.56
1	A	196	ASP	C-N-CA	5.80	125.42	119.56
1	A	530	VAL	N-CA-CB	-5.76	105.18	112.15
1	A	231	GLU	N-CA-C	5.76	117.56	111.28
1	A	239	MET	CB-CG-SD	-5.75	95.46	112.70
1	A	140	ILE	N-CA-CB	-5.72	105.55	112.07
1	A	706	ASN	N-CA-C	-5.72	105.56	112.54
1	A	607	VAL	N-CA-C	5.71	115.91	110.42
1	A	523	ASP	CA-C-N	-5.71	113.52	122.65
1	A	523	ASP	C-N-CA	-5.71	113.52	122.65
1	A	820	PRO	CA-C-N	-5.68	114.75	120.31
1	A	820	PRO	C-N-CA	-5.68	114.75	120.31
1	A	585	MET	CA-C-N	-5.60	111.80	120.31
1	A	585	MET	C-N-CA	-5.60	111.80	120.31
1	A	534	ARG	NE-CZ-NH2	5.59	124.23	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	413	LEU	CA-CB-CG	5.58	135.84	116.30
1	A	7	LYS	N-CA-C	5.51	118.23	109.81
1	A	467	ARG	CG-CD-NE	-5.49	99.92	112.00
1	A	671	ARG	N-CA-C	-5.48	106.72	113.41
1	A	155	VAL	CB-CA-C	-5.47	102.32	111.29
1	A	426	ASP	CA-C-N	-5.42	114.54	122.19
1	A	426	ASP	C-N-CA	-5.42	114.54	122.19
1	A	386	GLY	N-CA-C	-5.40	100.38	113.18
1	A	826	GLU	CA-C-N	5.40	125.70	119.92
1	A	826	GLU	C-N-CA	5.40	125.70	119.92
1	A	25	THR	CB-CA-C	-5.39	99.53	109.51
1	A	629	LYS	CD-CE-NZ	-5.39	94.64	111.90
1	A	662	PRO	CB-CA-C	-5.39	104.17	111.12
1	A	697	ILE	CB-CG1-CD1	-5.38	102.49	113.80
1	A	175	VAL	N-CA-C	5.36	115.61	108.11
1	A	810	ASN	N-CA-C	5.36	116.16	109.57
1	A	529	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	697	ILE	N-CA-C	-5.34	100.63	108.54
1	A	59	ASP	N-CA-C	5.33	118.50	109.76
1	A	534	ARG	CG-CD-NE	-5.33	100.28	112.00
1	A	151	VAL	CB-CA-C	-5.32	102.18	110.69
1	A	708	ALA	CA-C-N	-5.31	113.72	119.24
1	A	708	ALA	C-N-CA	-5.31	113.72	119.24
1	A	367	PHE	N-CA-C	5.30	117.13	109.07
1	A	602	PRO	CA-C-N	5.30	125.20	119.85
1	A	602	PRO	C-N-CA	5.30	125.20	119.85
1	A	369	ILE	CB-CA-C	-5.27	103.86	111.34
1	A	347	VAL	CB-CA-C	-5.27	102.83	110.63
1	A	549	ILE	N-CA-CB	5.25	116.58	110.65
1	A	672	ARG	N-CA-C	-5.24	105.63	112.23
1	A	823	SER	CA-C-N	5.24	125.04	119.28
1	A	823	SER	C-N-CA	5.24	125.04	119.28
1	A	383	SER	N-CA-C	-5.23	101.41	109.52
1	A	47	LYS	N-CA-C	5.23	118.38	110.64
1	A	548	VAL	CA-C-N	-5.23	114.34	120.72
1	A	548	VAL	C-N-CA	-5.23	114.34	120.72
1	A	160	PRO	CA-C-O	-5.21	111.92	118.86
1	A	382	PHE	CA-C-N	-5.21	114.41	122.59
1	A	382	PHE	C-N-CA	-5.21	114.41	122.59
1	A	639	ILE	N-CA-C	5.19	120.13	109.34
1	A	471	CYS	N-CA-C	5.18	117.01	111.36
1	A	178	SER	N-CA-C	5.17	118.69	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	MET	N-CA-C	-5.17	107.02	113.38
1	A	207	MET	N-CA-C	5.16	118.00	109.85
1	A	378	SER	N-CA-C	5.16	118.47	110.17
1	A	553	GLY	N-CA-C	5.14	125.37	113.18
1	A	573	ARG	CG-CD-NE	-5.14	100.69	112.00
1	A	364	CYS	N-CA-C	-5.11	107.59	113.88
1	A	752	ALA	N-CA-C	-5.09	105.82	112.23
1	A	626	GLY	N-CA-C	5.07	120.03	114.40
1	A	358	THR	CA-C-N	-5.07	114.82	122.07
1	A	358	THR	C-N-CA	-5.07	114.82	122.07
1	A	307	ILE	CB-CA-C	-5.06	104.86	110.68
1	A	573	ARG	N-CA-CB	5.06	117.65	110.06
1	A	208	LEU	N-CA-C	-5.05	101.16	109.40
1	A	688	VAL	N-CA-C	5.04	115.66	110.36
1	A	830	SER	N-CA-C	5.01	116.54	108.32
1	A	200	VAL	CB-CA-C	5.00	118.40	111.49
1	A	183	GLU	O-C-N	-5.00	117.62	123.27

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 (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	7671	0	7764	426	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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7930	0	7794	430	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 28.

All (430) 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:941:MET:HE3	1:A:941:MET:HA	1.46	0.97
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:O	1:A:600:LEU:HD23	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
1:A:754:TYR:CE1	1:A:758:LYS:HD2	2.22	0.73
6:A:1002:ATP:H5'1	6:A:1002:ATP:C8	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:941:MET:CE	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:88:PHE:HD2	1:A:92:PHE:HE1	1.41	0.69
1:A:120:LYS:HE2	1:A:123:GLU:OE2	1.93	0.69
1:A:886:LEU:HD12	1:A:887:ASP:N	2.09	0.68
1:A:72:SER:HB2	1:A:90:GLU:HG2	1.76	0.68
1:A:272:TRP:HD1	1:A:295:TYR:CE2	2.11	0.68
1:A:963:ASP:H	1:A:966:GLN:HG3	1.58	0.67
1:A:30:LYS:HD2	1:A:30:LYS:N	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:HD2	1:A:31:ARG:O	1.94	0.67
1:A:95:LEU:HD13	1:A:98:LEU:HD23	1.76	0.67
1:A:650:ASP:O	1:A:672:ARG:HD2	1.95	0.67
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.75	0.66
1:A:329:LYS:O	1:A:330:ASN:HB2	1.92	0.66
1:A:310:GLY:O	1:A:311:LEU:C	2.37	0.66
1:A:247:THR:H	1:A:250:GLN:NE2	1.93	0.66
1:A:958:LYS:HB3	1:A:958:LYS:HZ2	1.60	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:90:GLU:HB3	1:A:91:PRO:CD	2.27	0.64
1:A:879:ASP:HB3	1:A:882:HIS:CG	2.31	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:781:LEU:O	1:A:782:GLY:C	2.41	0.64
1:A:903:VAL:CG2	1:A:970:VAL:HG13	2.27	0.64
1:A:794:TRP:CZ2	1:A:947:ILE:HD11	2.32	0.64
1:A:914:ASN:HD22	1:A:922:LEU:HD11	1.62	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:834:PHE:CE1	1:A:838:MET:HE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:TRP:O	1:A:854:TRP:CE3	2.52	0.63
1:A:992:LEU:HD12	1:A:992:LEU:C	2.23	0.63
1:A:1:MET:HE3	1:A:4:ALA:HB2	1.79	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: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:61:LEU:C	1:A:64:ILE:HG22	2.25	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
1:A:85:ILE:O	1:A:85:ILE:HG13	1.99	0.61
6:A:1002:ATP:H8	6:A:1002:ATP:C5'	2.10	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:958:LYS:O	1:A:958:LYS:HG3	2.00	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: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:N	1:A:802:LEU:CD2	2.66	0.58
1:A:889:GLU:O	1:A:889:GLU:HG2	2.03	0.58
1:A:296:PHE:N	1:A:296:PHE:CD1	2.71	0.58
1:A:650:ASP:OD1	1:A:650:ASP:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:240:ALA:O	1:A:242:THR:N	2.36	0.58
1:A:487:PHE:CD1	1:A:487:PHE:C	2.82	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:777:LEU:C	1:A:779:ALA:H	2.11	0.57
1:A:977:VAL:CG1	1:A:978:ILE:N	2.67	0.57
1:A:293:ILE:HG22	1:A:293:ILE:O	2.05	0.57
1:A:279:PHE:O	1:A:279:PHE:CG	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
1:A:295:TYR:HB2	1:A:296:PHE:CD1	2.40	0.56
1:A:776:PHE:O	1:A:776:PHE:CD2	2.58	0.56
1:A:886:LEU:CD1	1:A:887:ASP:N	2.67	0.56
1:A:976:PRO:O	1:A:977:VAL:C	2.49	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:82:GLU:O	1:A:84:THR:N	2.38	0.56
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.88	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: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:198:ARG:NH1	1:A:660:ASP:OD1	2.37	0.54
1:A:296:PHE:HD1	1:A:296:PHE:H	1.55	0.54
1:A:304:VAL:HG13	1:A:793:LEU:HD21	1.88	0.54
1:A:360:GLN:HE21	1:A:388:THR:HG22	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:967:TRP:C	1:A:971:LEU:HD12	2.32	0.54
1:A:76:ALA:CB	1:A:91:PRO:HG2	2.38	0.54
1:A:72:SER:C	1:A:91:PRO:HG3	2.33	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:90:GLU:O	1:A:94:ILE:HG13	2.08	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:914:ASN:ND2	1:A:922:LEU:HD11	2.24	0.53
1:A:629:LYS:HE3	1:A:654:THR:HG23	1.91	0.53
1:A:887:ASP:CG	1:A:888:CYS:H	2.14	0.53
1:A:95:LEU:O	1:A:99:ILE:HG13	2.09	0.53
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:853:ALA:O	1:A:857:MET:HE2	2.09	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:74:VAL:O	1:A:78:PHE:HD1	1.92	0.52
1:A:113:GLU:OE1	1:A:113:GLU:N	2.41	0.52
1:A:20:GLU:HB3	7:A:1003:HOH:O	2.10	0.52
1:A:68:ALA:O	1:A:69:ALA:C	2.53	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:760:PHE:CD1	1:A:760:PHE:C	2.88	0.51
1:A:510:ASN:O	1:A:511:LYS:HD3	2.10	0.51
1:A:947:ILE:HG22	1:A:947:ILE:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:857:MET:C	1:A:859:ALA:H	2.19	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:263:VAL:O	1:A:264:ILE:C	2.54	0.50
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:832:TRP:CZ2	1:A:987:ILE:CG2	2.94	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: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:902:SER:HB3	1:A:970:VAL:HG11	1.94	0.49
1:A:295:TYR:C	1:A:297:LYS:H	2.20	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:85:ILE:O	1:A:86:THR:CG2	2.57	0.48
1:A:654:THR:HA	1:A:677:ALA:O	2.13	0.48
1:A:25:THR:HA	1:A:132:ALA:HB3	1.95	0.48
1:A:282:PRO:C	1:A:284:HIS:N	2.71	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:39:ASN:OD1	1:A:226:THR:HB	2.14	0.48
1:A:300:VAL:HG12	1:A:301:ALA:N	2.27	0.48
1:A:802:LEU:CD1	1:A:939:LEU:HD23	2.44	0.48
1:A:304:VAL:HG13	1:A:793:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ARG:HG3	7:A:1118:HOH:O	2.12	0.48
1:A:751:ARG:HB3	1:A:816:ILE:CG1	2.43	0.48
1:A:100:ALA:O	1:A:101:ASN:C	2.56	0.48
1:A:272:TRP:O	1:A:272:TRP:CD2	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:308:PRO:C	1:A:309:GLU:O	2.53	0.47
1:A:326:MET:HE2	1:A:746:ALA:HB2	1.94	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:777:LEU:C	1:A:779:ALA:N	2.72	0.47
1:A:782:GLY:C	1:A:873:PHE:HE2	2.22	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:HD12	1:A:253:LEU:HA	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
1:A:885:GLY:O	1:A:886:LEU:HB3	2.15	0.47
1:A:897:MET:SD	1:A:958:LYS:HD2	2.55	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:562:LEU:HD22	1:A:599:MET:HE3	1.97	0.47
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.44	0.47
1:A:73:PHE:CA	1:A:91:PRO:HG3	2.44	0.47
1:A:113:GLU:OE2	1:A:334:ARG:NH1	2.47	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:112:ALA:O	1:A:113:GLU:C	2.58	0.46
1:A:287:SER:C	1:A:289:ILE:H	2.23	0.46
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.50	0.46
1:A:325:ARG:NH1	1:A:749:GLU:CD	2.73	0.46
1:A:550:LYS:O	1:A:551:GLU:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:913:LEU:O	1:A:914:ASN:C	2.57	0.46
1:A:939:LEU:O	1:A:939:LEU:HD12	2.15	0.46
1:A:946:LEU:HD12	1:A:946:LEU:HA	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:2:GLU:OE1	1:A:2:GLU:HA	2.15	0.46
1:A:196:ASP:HA	1:A:197:PRO:HD3	1.65	0.46
1:A:725:ALA:O	1:A:729:THR:HG23	2.16	0.46
1:A:99:ILE:O	1:A:100:ALA:C	2.57	0.46
1:A:622:ILE:HD13	1:A:622:ILE:HG21	1.75	0.46
1:A:768:ASN:O	1:A:772:VAL:HG23	2.16	0.46
1:A:901:LEU:O	1:A:901:LEU:HD12	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:52:LEU:O	1:A:53:VAL:C	2.60	0.45
1:A:70:CYS:O	1:A:74:VAL:N	2.47	0.45
1:A:269:VAL:CG1	1:A:270:ALA:N	2.80	0.45
1:A:61:LEU:HA	1:A:64:ILE:HG22	1.98	0.45
1:A:90:GLU:O	1:A:91:PRO:C	2.59	0.45
1:A:99:ILE:O	1:A:103:ILE:HG13	2.17	0.45
1:A:131:ARG:HH21	1:A:149:ASP:CG	2.25	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
1:A:879:ASP:HB3	1:A:882:HIS:HB2	1.98	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:785:GLU:HB2	1:A:897:MET:HE2	1.99	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:843:TYR:CD2	1:A:843:TYR:C	2.95	0.45
1:A:855:TRP:O	1:A:855:TRP:CE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:778:THR:OG1	1:A:784:PRO:O	2.35	0.44
1:A:606:GLU:H	1:A:606:GLU:CD	2.26	0.44
1:A:757:MET:HE2	1:A:757:MET:HB3	1.78	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:88:PHE:O	1:A:92:PHE:HD1	2.01	0.44
1:A:798:VAL:O	1:A:802:LEU:HD23	2.18	0.44
1:A:836:ARG:HH21	1:A:981:ASP:CG	2.26	0.44
1:A:236:ARG:HD3	1:A:236:ARG:C	2.43	0.44
1:A:984:LEU:C	1:A:987:ILE:HG22	2.42	0.44
1:A:272:TRP:O	1:A:272:TRP:CG	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:479:MET:HE3	1:A:498:CYS:HB3	2.00	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:96:LEU:HD12	1:A:96:LEU:O	2.19	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:252:LYS:HD3	1:A:252:LYS:HA	1.60	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: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:859:ALA:C	1:A:861:ASP:N	2.76	0.43
1:A:65:LEU:C	1:A:67:LEU:N	2.75	0.43
1:A:73:PHE:HA	1:A:91:PRO:CG	2.48	0.43
1:A:242:THR:O	1:A:243:GLU:C	2.60	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:184:SER:O	1:A:185:VAL:C	2.62	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: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:452:MET:O	1:A:453:ASN:C	2.62	0.43
1:A:653:TYR:OH	1:A:672:ARG:NH2	2.51	0.43
1:A:847:ALA:HB1	1:A:973:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:854:TRP:CE3	1:A:854:TRP:C	2.97	0.42
1:A:55:GLU:O	1:A:58:GLU:HB2	2.18	0.42
1:A:190:HIS:ND1	1:A:190:HIS:C	2.77	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:204:LYS:NZ	7:A:1086:HOH:O	2.53	0.42
1:A:762:ARG:HE	1:A:762:ARG:HB3	1.47	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:921:SER:C	1:A:923:MET:N	2.75	0.42
1:A:50:TRP:HE1	1:A:54:ILE:HD11	1.80	0.42
1:A:89:VAL:HG12	1:A:93:VAL:HG23	2.00	0.42
1:A:134:ARG:NE	1:A:138:GLN:HG2	2.34	0.42
1:A:680:GLU:HB3	1:A:681:PRO:CD	2.49	0.42
1:A:757:MET:C	1:A:761:ILE:HD12	2.44	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:574:GLU:H	1:A:574:GLU:CD	2.28	0.42
1:A:60:LEU:O	1:A:63:ARG:N	2.53	0.42
1:A:101:ASN:OD1	1:A:312:PRO:HB2	2.20	0.42
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.70	0.42
1:A:883:PHE:C	1:A:884:GLU:HG2	2.45	0.42
1:A:80:GLU:O	1:A:82:GLU:N	2.46	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:769:VAL:CG1	1:A:841:GLY:HA3	2.50	0.42
1:A:963:ASP:N	1:A:966:GLN:HG3	2.29	0.42
1:A:86:THR:O	1:A:89:VAL:HG23	2.20	0.41
1:A:708:ALA:O	1:A:709:PRO:C	2.62	0.41
1:A:854:TRP:O	1:A:854:TRP:CG	2.73	0.41
1:A:71:ILE:HA	1:A:74:VAL:CG2	2.50	0.41
1:A:153:VAL:O	1:A:153:VAL:HG23	2.20	0.41
1:A:984:LEU:HA	1:A:987:ILE:CG2	2.50	0.41
1:A:396:LEU:HD13	1:A:399:ASP:HA	2.01	0.41
1:A:309:GLU:CD	1:A:309:GLU:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH21	1:A:198:ARG:HD3	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: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:101:ASN:CB	5:A:1001:CZA:O3	2.69	0.41
1:A:992:LEU:HD12	1:A:992:LEU:O	2.21	0.41
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.92	0.41
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.87	0.41
1:A:560:ARG:O	1:A:598:GLY:HA2	2.20	0.41
1:A:652:ALA:HA	1:A:675:CYS:O	2.20	0.41
1:A:924:ARG:NH2	1:A:989:ARG:NH2	2.69	0.41
1:A:269:VAL:HG13	1:A:270:ALA:N	2.35	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:243:GLU:O	1:A:244:GLN:C	2.64	0.40
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:HA	1:A:793:LEU:HD23	1.68	0.40
1:A:794:TRP:CZ3	1:A:947:ILE:CD1	3.03	0.40
1:A:814:LEU:N	1:A:814:LEU:CD1	2.84	0.40
1:A:843:TYR:OH	1:A:976:PRO:HB2	2.21	0.40
1:A:947:ILE:HG23	1:A:957:PHE:CD1	2.56	0.40
1:A:950:VAL:O	1:A:951:ASP:C	2.63	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 (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	992/994 (100%)	865 (87%)	89 (9%)	38 (4%)	2 1

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 (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%)	733 (87%)	107 (13%)	4 4

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	7	LYS
1	A	10	GLU
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	89	VAL
1	A	95	LEU
1	A	98	LEU
1	A	108	GLN
1	A	116	ILE
1	A	121	GLU
1	A	141	LYS
1	A	150	ILE
1	A	151	VAL
1	A	155	VAL
1	A	158	LYS
1	A	200	VAL
1	A	202	GLN
1	A	205	LYS
1	A	218	LYS
1	A	228	VAL
1	A	242	THR

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	252	LYS
1	A	253	LEU
1	A	255	GLU
1	A	271	VAL
1	A	278	HIS
1	A	296	PHE
1	A	300	VAL
1	A	307	ILE
1	A	309	GLU
1	A	311	LEU
1	A	314	VAL
1	A	315	ILE
1	A	319	LEU
1	A	324	ARG
1	A	329	LYS
1	A	338	SER
1	A	339	VAL
1	A	356	LEU
1	A	371	LYS
1	A	394	GLU
1	A	413	LEU
1	A	465	VAL
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	554	THR
1	A	556	ARG
1	A	562	LEU
1	A	567	ARG
1	A	572	LYS
1	A	573	ARG
1	A	577	VAL
1	A	582	SER
1	A	620	ARG
1	A	648	VAL
1	A	663	LEU
1	A	691	LEU

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Mol	Chain	Res	Type
1	A	722	SER
1	A	758	LYS
1	A	759	GLN
1	A	766	SER
1	A	774	CYS
1	A	775	ILE
1	A	783	LEU
1	A	788	ILE
1	A	790	VAL
1	A	799	THR
1	A	802	LEU
1	A	814	LEU
1	A	825	LYS
1	A	828	LEU
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	886	LEU
1	A	902	SER
1	A	906	THR
1	A	932	TRP
1	A	941	MET
1	A	946	LEU
1	A	950	VAL
1	A	955	MET
1	A	956	ILE
1	A	958	LYS
1	A	964	LEU
1	A	973	ILE
1	A	977	VAL
1	A	992	LEU

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

Mol	Chain	Res	Type
1	A	38	HIS
1	A	108	GLN
1	A	111	ASN

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Mol	Chain	Res	Type
1	A	202	GLN
1	A	250	GLN
1	A	284	HIS
1	A	360	GLN
1	A	756	ASN
1	A	768	ASN
1	A	868	HIS
1	A	875	GLN
1	A	914	ASN
1	A	944	HIS
1	A	966	GLN

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 oligosaccharides 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	$\#\|Z\| > 2$
3	MF4	A	996	1	0,4,4	-	-	-		
6	ATP	A	1002	-	32,33,33	3.53	14 (43%)	48,52,52	2.50	17 (35%)
5	CZA	A	1001	2	28,29,29	1.97	6 (21%)	29,48,48	1.92	7 (24%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	ATP	PB-O3B	8.92	1.69	1.59
6	A	1002	ATP	PA-O3A	8.23	1.68	1.59
6	A	1002	ATP	PB-O3A	6.84	1.66	1.59
6	A	1002	ATP	C8-N7	6.07	1.43	1.31
5	A	1001	CZA	C4-N1	-5.95	1.33	1.39
6	A	1002	ATP	PG-O1G	5.24	1.66	1.50
6	A	1002	ATP	PA-O1A	4.51	1.66	1.50
6	A	1002	ATP	PB-O1B	4.40	1.66	1.50
6	A	1002	ATP	C4-N9	3.85	1.45	1.37
6	A	1002	ATP	C6-N6	3.84	1.44	1.34
6	A	1002	ATP	C2-N3	3.72	1.40	1.33
5	A	1001	CZA	C12-C8	3.46	1.58	1.53
5	A	1001	CZA	C1-C2	3.35	1.56	1.50
6	A	1002	ATP	PA-O5'	3.33	1.72	1.59
5	A	1001	CZA	C19-C18	2.81	1.43	1.38
5	A	1001	CZA	C3-C4	-2.69	1.35	1.40
6	A	1002	ATP	PG-O2G	2.48	1.64	1.54
6	A	1002	ATP	C5'-C4'	2.38	1.58	1.51
6	A	1002	ATP	PG-O3G	-2.05	1.47	1.54
5	A	1001	CZA	O2-C6	2.00	1.25	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	ATP	N3-C2-N1	-6.92	118.11	128.58
6	A	1002	ATP	C5-C4-N3	-6.59	117.64	126.72
6	A	1002	ATP	C2-N3-C4	5.39	125.00	111.83
5	A	1001	CZA	C18-C17-N2	5.11	138.92	130.74
6	A	1002	ATP	O5'-C5'-C4'	4.15	123.11	108.99
5	A	1001	CZA	C17-C14-C15	4.12	112.27	107.59
6	A	1002	ATP	O3'-C3'-C4'	4.04	122.69	111.08
6	A	1002	ATP	C5-C4-N9	3.99	110.16	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	ATP	O2'-C2'-C1'	3.90	123.52	110.10
6	A	1002	ATP	O2G-PG-O3B	3.74	117.16	104.64
6	A	1002	ATP	O4'-C4'-C5'	3.73	121.29	109.33
6	A	1002	ATP	O2'-C2'-C3'	3.60	123.36	111.82
5	A	1001	CZA	C14-C17-N2	-3.13	102.09	106.88
6	A	1002	ATP	O4'-C1'-N9	3.02	113.89	108.09
6	A	1002	ATP	C4'-O4'-C1'	-2.98	102.90	109.47
6	A	1002	ATP	N3-C4-N9	2.95	132.19	127.17
5	A	1001	CZA	C17-N2-C16	2.77	111.54	109.08
5	A	1001	CZA	C9-N1-C5	2.64	115.66	112.27
5	A	1001	CZA	O2-C6-C3	2.59	134.47	128.42
6	A	1002	ATP	O3'-C3'-C2'	2.33	119.27	111.82
6	A	1002	ATP	C4-C5-N7	-2.17	108.10	110.58
5	A	1001	CZA	C12-C13-C14	-2.12	114.36	117.87
6	A	1002	ATP	O4'-C4'-C3'	-2.05	101.08	105.15
6	A	1002	ATP	C5-C6-N1	2.02	122.65	117.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1002	ATP	C3'

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	ATP	PB-O3B-PG-O2G
6	A	1002	ATP	C5'-O5'-PA-O1A
6	A	1002	ATP	C5'-O5'-PA-O2A
6	A	1002	ATP	C5'-O5'-PA-O3A
6	A	1002	ATP	C4'-C5'-O5'-PA
5	A	1001	CZA	O1-C2-C3-C6
6	A	1002	ATP	O4'-C4'-C5'-O5'
5	A	1001	CZA	O1-C2-C3-C4
6	A	1002	ATP	PB-O3B-PG-O1G

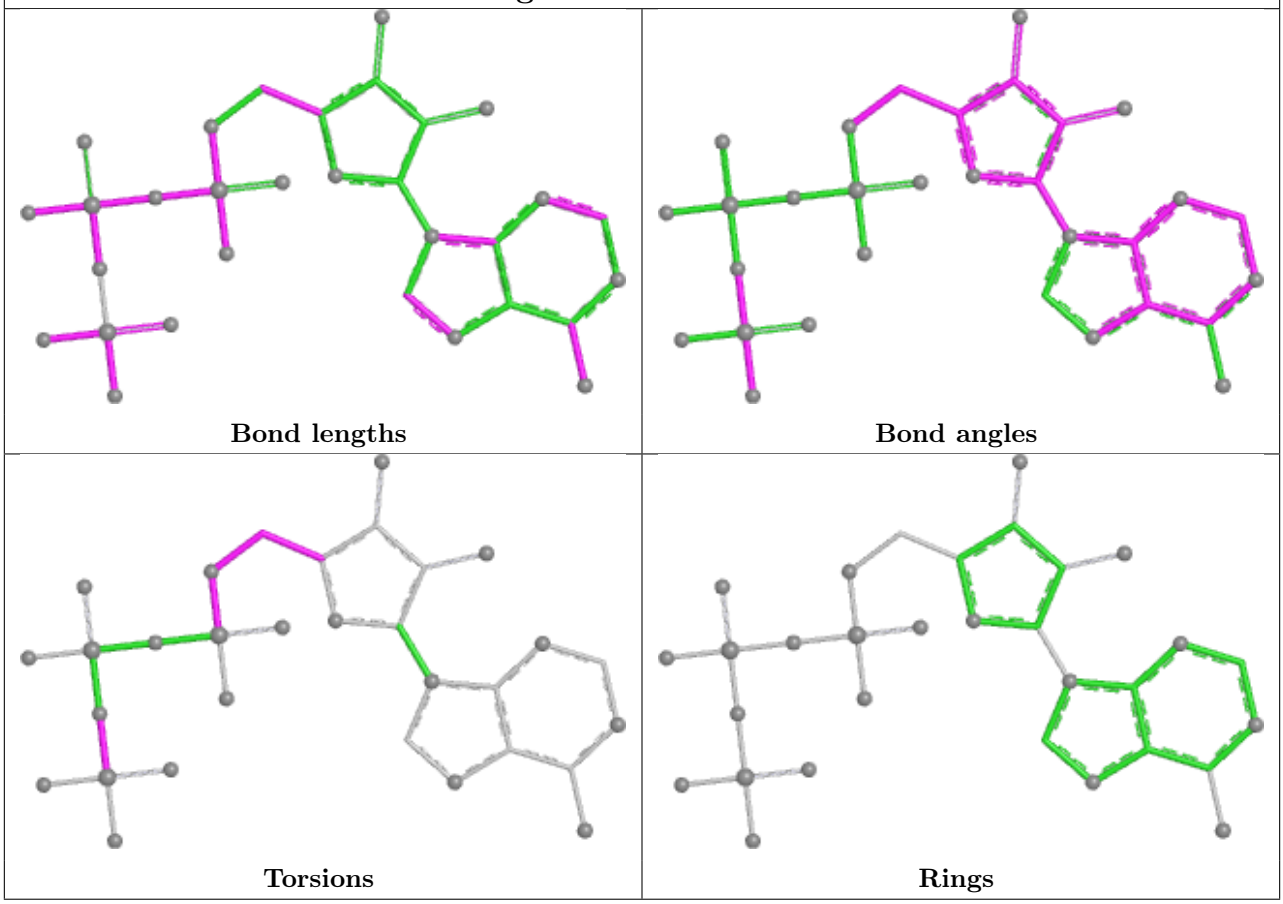
There are no ring outliers.

2 monomers are involved in 11 short contacts:

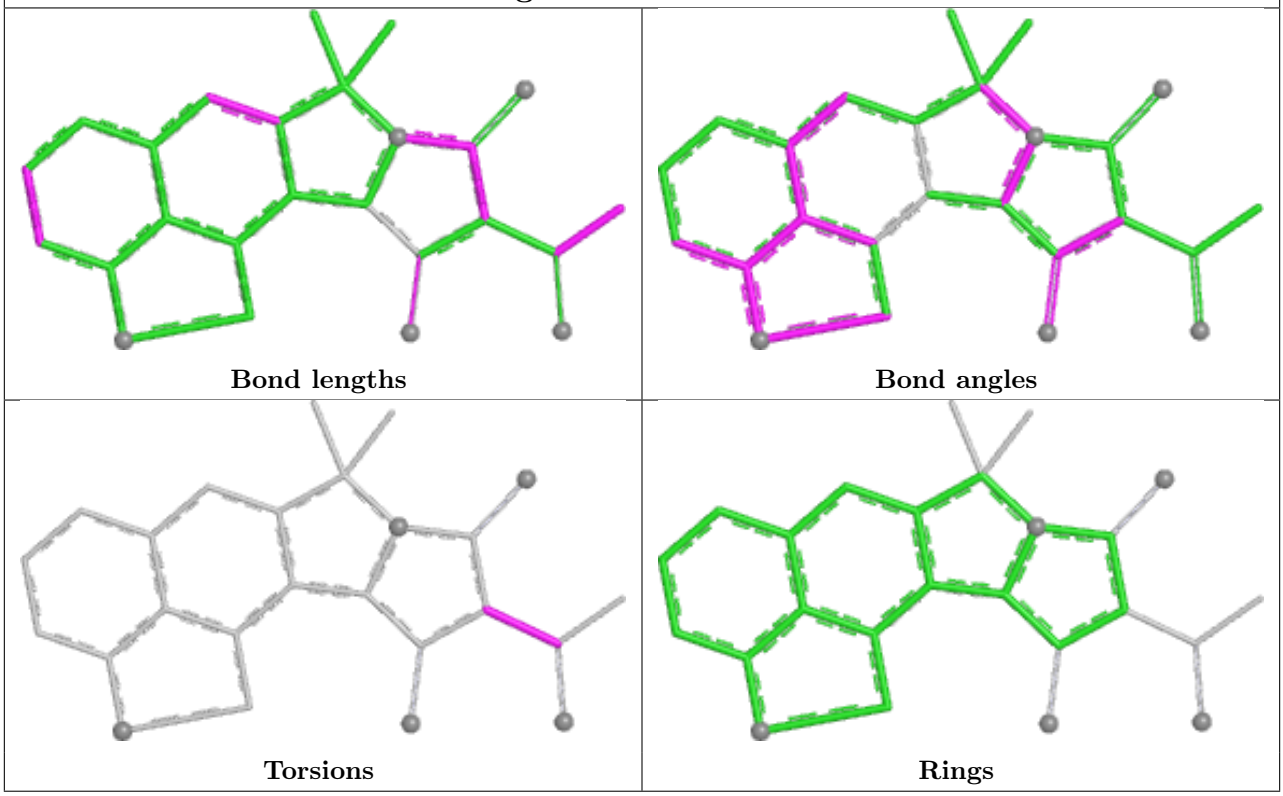
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1002	ATP	6	0
5	A	1001	CZA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 1002



Ligand CZA A 1001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.10	28 (2%) 55 56	34, 72, 209, 337	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	PHE	5.5
1	A	278	HIS	4.9
1	A	281	ASP	4.1
1	A	283	VAL	3.6
1	A	289	ILE	3.6
1	A	883	PHE	3.5
1	A	294	TYR	3.4
1	A	885	GLY	2.8
1	A	288	TRP	2.8
1	A	77	TRP	2.7
1	A	886	LEU	2.7
1	A	873	PHE	2.6
1	A	891	PHE	2.6
1	A	762	ARG	2.6
1	A	863	PRO	2.5
1	A	85	ILE	2.5
1	A	856	PHE	2.5
1	A	276	ILE	2.4
1	A	890	ILE	2.4
1	A	865	VAL	2.4
1	A	282	PRO	2.3
1	A	972	LYS	2.3
1	A	298	ILE	2.2
1	A	241	ALA	2.1
1	A	296	PHE	2.0
1	A	277	GLY	2.0
1	A	242	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	877	THR	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 oligosaccharides in this entry.

6.4 Ligands (i)

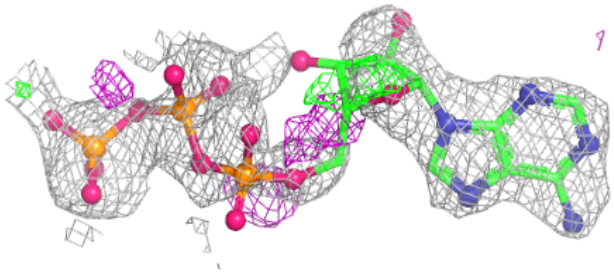
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

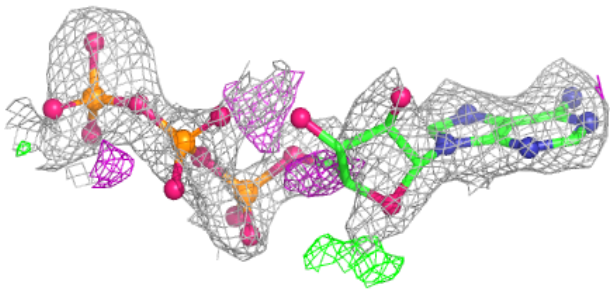
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ATP	A	1002	31/31	0.82	0.14	42,87,197,402	31
5	CZA	A	1001	25/25	0.96	0.07	83,103,107,115	0
4	K	A	997	1/1	0.96	0.09	107,107,107,107	0
3	MF4	A	996	5/5	0.98	0.07	34,38,47,58	0
2	MG	A	1000	1/1	0.99	0.02	107,107,107,107	0
2	MG	A	995	1/1	1.00	0.02	37,37,37,37	0

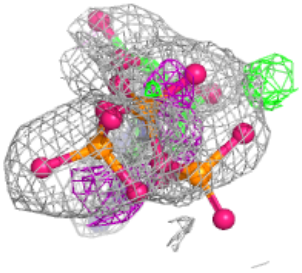
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

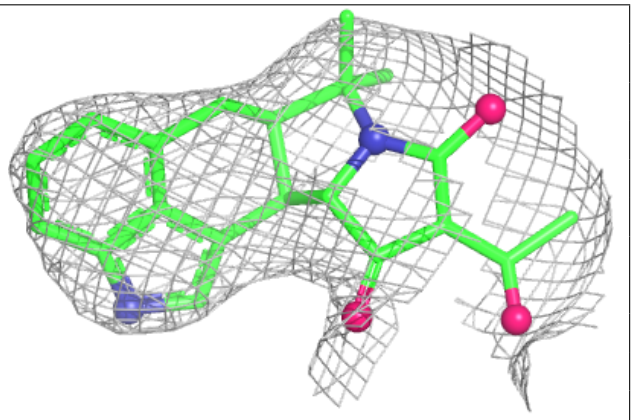


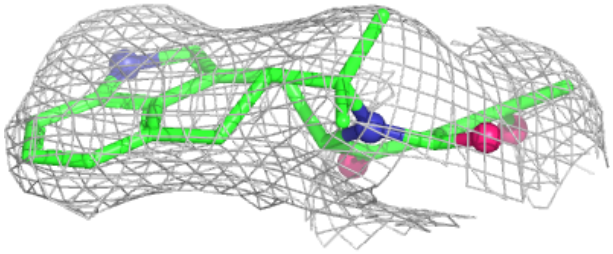


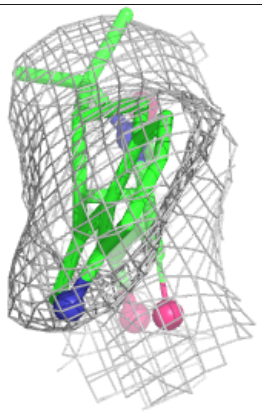


Electron density around CZA A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.