



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:42 AM GMT

PDB ID : 3FPS
Title : The Structure of Sarcoplasmic Reticulum Ca²⁺-ATPase Bound To Cyclopiazonic and ADP
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Deposited on : 2009-01-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

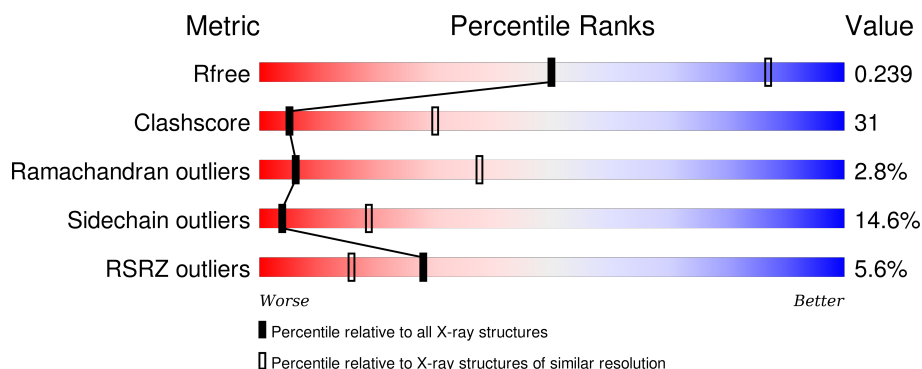
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>6%</div> <div>54%</div> <div>38%</div> <div>8%</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
4	ADP	A	1002	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7735 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			

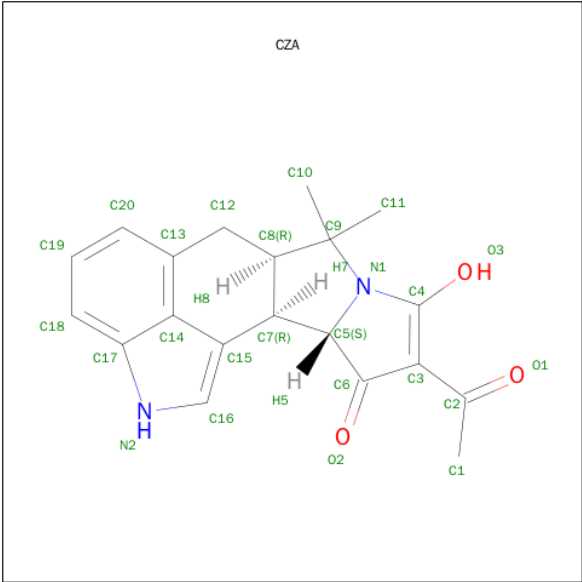
There is a discrepancy between the modelled and reference sequences:

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).

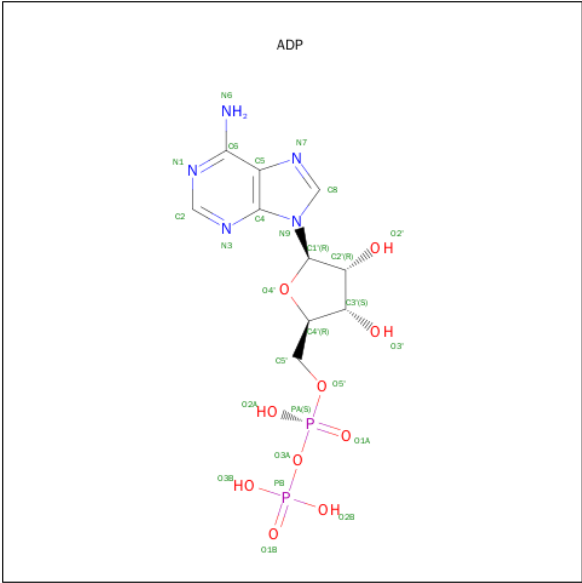
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: C₂₀H₂₀N₂O₃).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

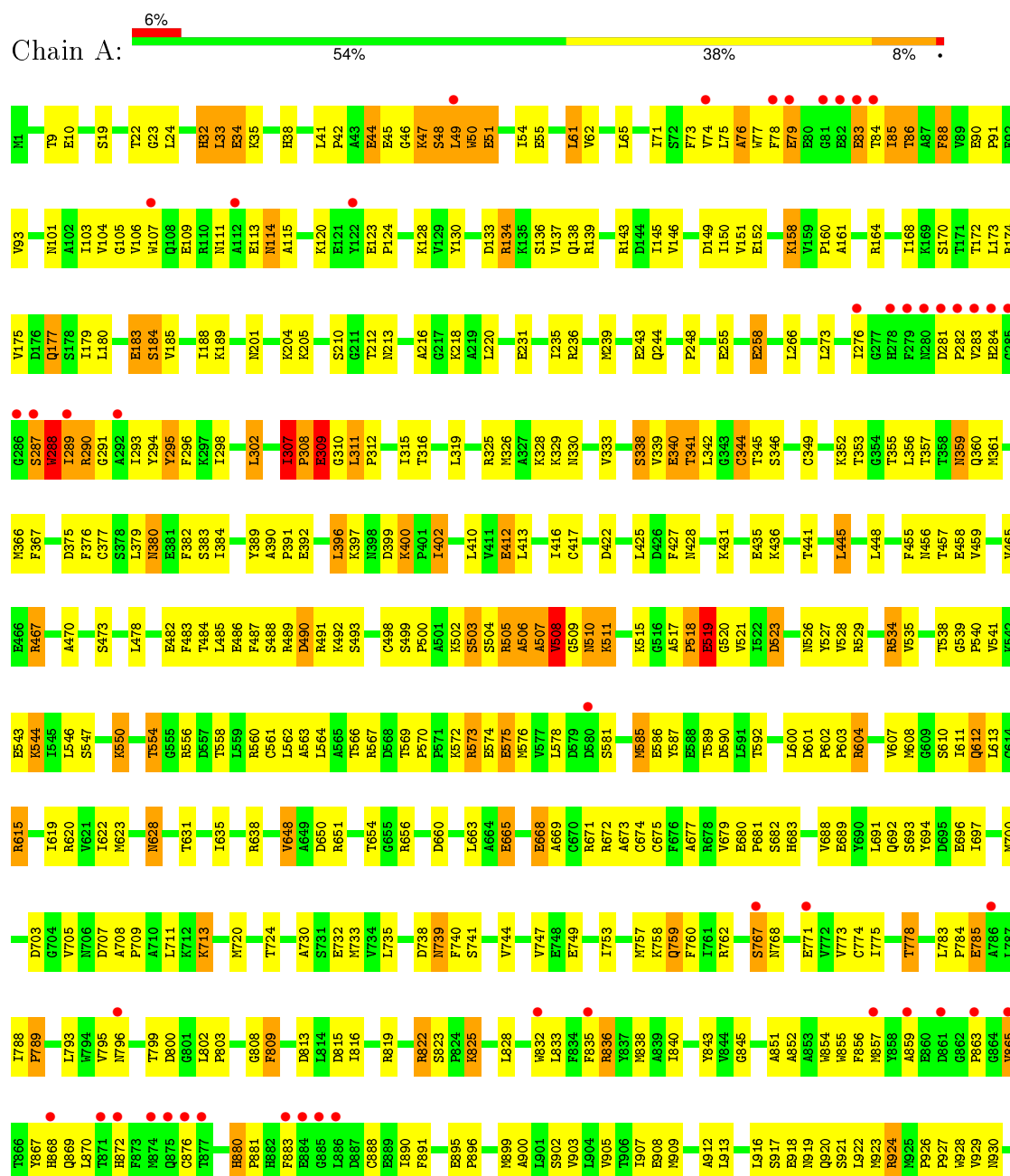
- Molecule 5 is water.

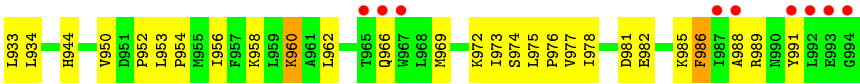
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.34Å 96.50Å 155.13Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	24.89 – 3.20 41.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.89-3.20) 99.1 (41.92-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.222 , 0.241 0.220 , 0.239	Depositor DCC
R_{free} test set	1532 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 75.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 30165 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7735	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	2/7812 (0.0%)	0.61	0/10592

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	675	CYS	CB-SG	-6.00	1.72	1.81
1	A	674	CYS	CB-SG	-5.68	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	GLU	Peptide
1	A	86	THR	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	476	1
2	A	2	0	0	0	0
3	A	25	0	20	6	0
4	A	27	0	12	0	0
5	A	10	0	0	0	0
All	All	7735	0	7796	476	1

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 31.

All (476) 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:287:SER:HB3	1:A:290:ARG:CB	1.31	1.56
1:A:287:SER:CB	1:A:290:ARG:HB2	1.40	1.49
1:A:287:SER:OG	1:A:290:ARG:HG3	1.22	1.33
1:A:307:ILE:HG22	1:A:309:GLU:CD	1.63	1.17
1:A:759:GLN:HA	1:A:759:GLN:HE21	1.09	1.16
1:A:924:ARG:HH21	1:A:924:ARG:HB2	1.08	1.16
1:A:307:ILE:CG2	1:A:309:GLU:HG3	1.76	1.15
1:A:287:SER:OG	1:A:290:ARG:CG	1.93	1.15
1:A:573:ARG:HG3	1:A:573:ARG:HH21	1.10	1.15
1:A:287:SER:CB	1:A:290:ARG:CB	2.11	1.13
1:A:759:GLN:HA	1:A:759:GLN:NE2	1.58	1.10
1:A:134:ARG:HH11	1:A:134:ARG:CG	1.63	1.09
1:A:507:ALA:O	1:A:508:VAL:HG23	1.53	1.08
1:A:290:ARG:HH11	1:A:290:ARG:HG2	0.98	1.06
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.37	1.06
1:A:290:ARG:HH11	1:A:290:ARG:CG	1.68	1.05
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.36	1.05
1:A:307:ILE:HG23	1:A:308:PRO:CD	1.85	1.04
1:A:134:ARG:HH11	1:A:134:ARG:HG2	0.93	1.04
1:A:615:ARG:HG2	1:A:615:ARG:HH11	1.20	1.04
1:A:307:ILE:CG2	1:A:309:GLU:H	1.71	1.04
1:A:307:ILE:HG22	1:A:308:PRO:N	1.71	1.02
1:A:307:ILE:HG21	1:A:309:GLU:CG	1.89	1.02
1:A:307:ILE:HG22	1:A:309:GLU:H	1.24	1.02
1:A:307:ILE:CG2	1:A:308:PRO:CD	2.38	1.01
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.40	1.01
1:A:307:ILE:CG2	1:A:309:GLU:CG	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HG21	1:A:309:GLU:HG3	1.03	1.01
1:A:924:ARG:NH2	1:A:924:ARG:HB2	1.76	1.00
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.41	1.00
1:A:575:GLU:HA	1:A:575:GLU:OE2	1.60	0.98
1:A:307:ILE:O	1:A:768:ASN:CG	2.03	0.97
1:A:615:ARG:HG2	1:A:615:ARG:NH1	1.77	0.97
1:A:518:PRO:O	1:A:520:GLY:N	1.97	0.96
1:A:307:ILE:HG23	1:A:308:PRO:HD2	1.47	0.96
1:A:128:LYS:HG2	1:A:139:ARG:HG2	1.49	0.94
1:A:311:LEU:HB3	1:A:312:PRO:CD	1.97	0.94
1:A:287:SER:CB	1:A:290:ARG:CG	2.44	0.93
1:A:47:LYS:C	1:A:47:LYS:HD3	1.88	0.93
1:A:287:SER:CB	1:A:290:ARG:HG3	1.98	0.93
1:A:573:ARG:HH21	1:A:573:ARG:CG	1.80	0.92
1:A:290:ARG:HG2	1:A:290:ARG:NH1	1.77	0.91
1:A:307:ILE:CG2	1:A:309:GLU:CD	2.38	0.91
1:A:114:ASN:N	1:A:114:ASN:HD22	1.67	0.91
1:A:307:ILE:CG2	1:A:308:PRO:N	2.33	0.91
1:A:308:PRO:HD2	1:A:309:GLU:H	1.37	0.90
1:A:201:ASN:HD21	1:A:231:GLU:HG2	1.36	0.89
1:A:291:GLY:O	1:A:294:TYR:HD2	1.54	0.89
1:A:130:TYR:CE2	1:A:137:VAL:HB	2.06	0.89
1:A:134:ARG:HG2	1:A:134:ARG:NH1	1.72	0.89
1:A:307:ILE:HG22	1:A:309:GLU:N	1.87	0.89
1:A:631:THR:O	1:A:635:ILE:HG12	1.71	0.89
1:A:836:ARG:HB2	1:A:836:ARG:HH21	1.37	0.88
1:A:502:LYS:HG3	1:A:503:SER:H	1.38	0.88
1:A:32:HIS:O	1:A:34:GLU:N	2.07	0.86
1:A:273:LEU:HD23	1:A:276:ILE:CD1	2.05	0.86
1:A:62:VAL:HG11	3:A:1001:CZA:H13	1.56	0.85
1:A:307:ILE:HG22	1:A:309:GLU:OE2	1.76	0.84
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.07	0.84
1:A:507:ALA:C	1:A:508:VAL:HG23	1.97	0.84
1:A:90:GLU:HG2	1:A:91:PRO:HD3	1.60	0.84
1:A:558:THR:HB	1:A:635:ILE:HD13	1.58	0.83
1:A:287:SER:HB3	1:A:290:ARG:HB3	1.57	0.83
1:A:287:SER:HG	1:A:290:ARG:HG3	1.02	0.81
1:A:291:GLY:O	1:A:294:TYR:CD2	2.34	0.80
1:A:307:ILE:O	1:A:768:ASN:ND2	2.14	0.80
1:A:308:PRO:HD2	1:A:309:GLU:N	1.96	0.80
1:A:510:ASN:HD22	1:A:510:ASN:H	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:GLN:HE21	1:A:759:GLN:CA	1.92	0.79
1:A:308:PRO:CD	1:A:309:GLU:H	1.90	0.79
1:A:507:ALA:C	1:A:508:VAL:CG2	2.50	0.79
1:A:307:ILE:CG2	1:A:309:GLU:OE2	2.31	0.78
1:A:307:ILE:HG22	1:A:309:GLU:CG	2.11	0.78
1:A:615:ARG:CG	1:A:615:ARG:HH11	1.90	0.78
1:A:491:ARG:HB2	1:A:585:MET:HG3	1.64	0.78
1:A:128:LYS:CG	1:A:139:ARG:HG2	2.13	0.78
1:A:307:ILE:CB	1:A:309:GLU:OE2	2.32	0.77
1:A:255:GLU:HA	1:A:258:GLU:HG2	1.66	0.77
1:A:510:ASN:H	1:A:510:ASN:ND2	1.82	0.77
1:A:307:ILE:O	1:A:768:ASN:OD1	2.02	0.77
1:A:114:ASN:HD22	1:A:114:ASN:H	1.30	0.76
1:A:380:ASN:HD21	1:A:397:LYS:HE3	1.48	0.76
1:A:114:ASN:N	1:A:114:ASN:ND2	2.33	0.76
1:A:201:ASN:ND2	1:A:231:GLU:HG2	2.01	0.76
1:A:795:VAL:HA	1:A:799:THR:HB	1.66	0.76
1:A:134:ARG:CG	1:A:134:ARG:NH1	2.33	0.75
1:A:510:ASN:N	1:A:510:ASN:ND2	2.34	0.75
1:A:507:ALA:C	1:A:509:GLY:H	1.90	0.74
1:A:574:GLU:HG2	1:A:574:GLU:O	1.86	0.74
1:A:47:LYS:O	1:A:48:SER:HB3	1.86	0.74
1:A:114:ASN:ND2	1:A:114:ASN:H	1.87	0.73
1:A:307:ILE:HB	1:A:309:GLU:OE2	1.88	0.72
1:A:308:PRO:C	1:A:309:GLU:OE1	2.28	0.72
1:A:47:LYS:HD3	1:A:48:SER:N	2.05	0.72
1:A:573:ARG:NH2	1:A:573:ARG:HG3	1.91	0.72
1:A:836:ARG:HH21	1:A:836:ARG:CB	2.02	0.71
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.72	0.71
1:A:978:ILE:O	1:A:982:GLU:HG2	1.90	0.71
1:A:309:GLU:N	1:A:309:GLU:CD	2.44	0.71
1:A:76:ALA:HB3	1:A:88:PHE:CZ	2.26	0.70
1:A:366:MET:HE1	1:A:448:LEU:HD21	1.73	0.69
1:A:183:GLU:O	1:A:185:VAL:N	2.26	0.69
1:A:924:ARG:HH21	1:A:924:ARG:CB	1.98	0.69
1:A:32:HIS:O	1:A:35:LYS:N	2.26	0.69
1:A:975:LEU:N	1:A:976:PRO:HD2	2.07	0.69
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.08	0.69
1:A:62:VAL:CG1	3:A:1001:CZA:H13	2.23	0.68
1:A:308:PRO:O	1:A:310:GLY:N	2.26	0.68
1:A:307:ILE:C	1:A:309:GLU:OE2	2.32	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:LEU:HB3	1:A:784:PRO:CD	2.23	0.68
1:A:744:VAL:O	1:A:747:VAL:HG12	1.93	0.68
1:A:73:PHE:CE2	1:A:91:PRO:HB2	2.29	0.68
1:A:287:SER:O	1:A:291:GLY:N	2.26	0.68
1:A:310:GLY:O	1:A:311:LEU:C	2.31	0.68
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.76	0.68
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.77	0.67
1:A:235:ILE:HG23	1:A:709:PRO:HG3	1.76	0.67
1:A:823:SER:OG	1:A:825:LYS:HG3	1.95	0.67
1:A:669:ALA:O	1:A:673:ALA:HB2	1.95	0.66
1:A:248:PRO:HD2	1:A:340:GLU:OE2	1.95	0.66
1:A:507:ALA:O	1:A:508:VAL:CG2	2.38	0.66
1:A:325:ARG:HD2	1:A:749:GLU:OE2	1.96	0.66
1:A:307:ILE:CG2	1:A:309:GLU:N	2.49	0.65
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.79	0.65
1:A:145:ILE:C	1:A:146:VAL:HG13	2.16	0.65
1:A:950:VAL:O	1:A:954:PRO:HD2	1.95	0.65
1:A:288:TRP:O	1:A:291:GLY:N	2.29	0.65
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.78	0.65
1:A:507:ALA:O	1:A:509:GLY:N	2.29	0.65
1:A:518:PRO:O	1:A:519:GLU:C	2.36	0.64
1:A:828:LEU:H	1:A:828:LEU:HD12	1.62	0.64
1:A:688:VAL:HG23	1:A:700:MET:CE	2.27	0.64
1:A:130:TYR:HE2	1:A:137:VAL:HB	1.62	0.64
1:A:739:ASN:HD22	1:A:741:SER:H	1.42	0.64
1:A:916:LEU:HD21	1:A:930:ASN:HB2	1.79	0.64
1:A:561:CYS:C	1:A:562:LEU:HD12	2.19	0.64
1:A:62:VAL:HG22	3:A:1001:CZA:H7	1.79	0.63
1:A:161:ALA:HA	1:A:210:SER:HB2	1.79	0.63
1:A:307:ILE:CG2	1:A:308:PRO:HD2	2.16	0.63
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.80	0.63
1:A:175:VAL:HG12	1:A:212:THR:HG21	1.80	0.63
1:A:175:VAL:HG12	1:A:212:THR:CG2	2.28	0.63
1:A:307:ILE:N	1:A:307:ILE:HD13	2.14	0.63
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.29	0.63
1:A:600:LEU:HG	1:A:601:ASP:N	2.13	0.63
1:A:952:PRO:O	1:A:956:ILE:HG13	1.98	0.63
1:A:65:LEU:HD21	1:A:307:ILE:HG12	1.81	0.63
1:A:346:SER:OG	1:A:696:GLU:HG2	1.99	0.62
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.81	0.62
1:A:201:ASN:HD21	1:A:231:GLU:CG	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:CG	1:A:290:ARG:NH1	2.40	0.62
1:A:49:LEU:HD12	1:A:50:TRP:CE3	2.34	0.61
1:A:308:PRO:CD	1:A:309:GLU:N	2.48	0.61
1:A:128:LYS:HG2	1:A:139:ARG:CG	2.28	0.61
1:A:130:TYR:CE2	1:A:137:VAL:CB	2.80	0.61
1:A:49:LEU:HD12	1:A:50:TRP:HE3	1.66	0.61
1:A:688:VAL:HG11	1:A:713:LYS:HB3	1.83	0.61
1:A:762:ARG:NH1	1:A:833:LEU:HD21	2.16	0.61
1:A:539:GLY:O	1:A:543:GLU:HG2	2.01	0.61
1:A:550:LYS:O	1:A:554:THR:HG22	2.01	0.60
1:A:309:GLU:N	1:A:309:GLU:OE1	2.34	0.60
1:A:294:TYR:CG	1:A:295:TYR:N	2.70	0.60
1:A:10:GLU:N	1:A:10:GLU:OE1	2.26	0.60
1:A:985:LYS:O	1:A:989:ARG:HB2	2.02	0.60
1:A:880:HIS:N	1:A:881:PRO:HD2	2.17	0.60
1:A:895:GLU:N	1:A:896:PRO:HD2	2.17	0.59
1:A:918:GLU:HG2	1:A:919:ASN:HD22	1.67	0.59
1:A:307:ILE:HG23	1:A:308:PRO:HD3	1.79	0.59
1:A:366:MET:CE	1:A:448:LEU:HD11	2.32	0.59
1:A:856:PHE:HZ	1:A:891:PHE:HA	1.67	0.59
1:A:692:GLN:C	1:A:694:TYR:H	2.06	0.59
1:A:287:SER:HB3	1:A:290:ARG:HB2	0.63	0.59
1:A:307:ILE:HG23	1:A:309:GLU:H	1.66	0.59
1:A:345:THR:HA	1:A:697:ILE:HG22	1.85	0.59
1:A:101:ASN:HB3	3:A:1001:CZA:O3	2.04	0.58
1:A:344:CYS:SG	1:A:822:ARG:NH1	2.77	0.58
1:A:32:HIS:O	1:A:33:LEU:C	2.39	0.58
1:A:307:ILE:CD1	1:A:307:ILE:N	2.65	0.57
1:A:688:VAL:HG23	1:A:700:MET:HE3	1.85	0.57
1:A:489:ARG:NH1	1:A:489:ARG:HG3	2.18	0.57
1:A:507:ALA:C	1:A:509:GLY:N	2.57	0.57
1:A:180:LEU:HA	1:A:705:VAL:HG22	1.86	0.57
1:A:357:THR:HG22	1:A:603:PRO:HA	1.84	0.57
1:A:120:LYS:HG2	1:A:123:GLU:OE2	2.04	0.57
1:A:255:GLU:HA	1:A:258:GLU:CG	2.34	0.57
1:A:145:ILE:C	1:A:146:VAL:CG1	2.73	0.57
1:A:604:ARG:O	1:A:607:VAL:HG22	2.05	0.57
1:A:130:TYR:OH	1:A:152:GLU:OE2	2.09	0.57
1:A:161:ALA:CA	1:A:210:SER:HB2	2.35	0.57
1:A:326:MET:CE	1:A:333:VAL:HG21	2.35	0.57
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.04	0.57
1:A:145:ILE:O	1:A:146:VAL:CG1	2.53	0.57
1:A:902:SER:HA	1:A:944:HIS:HE1	1.68	0.57
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.87	0.56
1:A:518:PRO:C	1:A:519:GLU:OE1	2.44	0.56
1:A:502:LYS:HG3	1:A:503:SER:N	2.14	0.56
1:A:505:ARG:O	1:A:506:ALA:C	2.43	0.56
1:A:575:GLU:OE2	1:A:575:GLU:CA	2.42	0.56
1:A:974:SER:C	1:A:976:PRO:HD2	2.26	0.56
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.41	0.56
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.88	0.56
1:A:380:ASN:ND2	1:A:397:LYS:HE3	2.18	0.56
1:A:757:MET:HA	1:A:760:PHE:CE2	2.41	0.56
1:A:573:ARG:NH2	1:A:573:ARG:CG	2.51	0.55
1:A:76:ALA:HB1	1:A:77:TRP:CE3	2.42	0.55
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.72	0.55
1:A:483:PHE:CE2	1:A:578:LEU:HD21	2.41	0.55
1:A:288:TRP:O	1:A:289:ILE:C	2.45	0.55
1:A:986:PHE:HD1	1:A:989:ARG:CZ	2.20	0.55
1:A:130:TYR:HE2	1:A:137:VAL:CG2	2.20	0.55
1:A:338:SER:HA	1:A:341:THR:CG2	2.36	0.55
1:A:309:GLU:OE1	1:A:796:ASN:HB3	2.07	0.55
1:A:75:LEU:HD22	1:A:293:ILE:HG23	1.89	0.55
1:A:880:HIS:N	1:A:881:PRO:CD	2.70	0.55
1:A:329:LYS:O	1:A:330:ASN:HB2	2.07	0.54
1:A:309:GLU:HA	3:A:1001:CZA:H113	1.90	0.54
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.41	0.54
1:A:288:TRP:O	1:A:290:ARG:N	2.41	0.54
1:A:856:PHE:HE1	1:A:896:PRO:HG3	1.73	0.54
1:A:902:SER:HA	1:A:944:HIS:CE1	2.41	0.54
1:A:836:ARG:O	1:A:840:ILE:HG12	2.08	0.54
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.89	0.54
1:A:758:LYS:HG2	1:A:762:ARG:CZ	2.38	0.53
1:A:326:MET:HE1	1:A:333:VAL:HG21	1.89	0.53
1:A:212:THR:HG22	1:A:213:ASN:N	2.22	0.53
1:A:612:GLN:HA	1:A:615:ARG:HD2	1.89	0.53
1:A:32:HIS:C	1:A:34:GLU:N	2.61	0.53
1:A:672:ARG:HH11	1:A:672:ARG:HB3	1.73	0.53
1:A:308:PRO:N	1:A:309:GLU:OE2	2.41	0.53
1:A:672:ARG:CZ	1:A:672:ARG:HB2	2.39	0.53
1:A:969:MET:HE3	1:A:972:LYS:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:CA	1:A:290:ARG:HB2	2.32	0.53
1:A:783:LEU:CB	1:A:784:PRO:CD	2.87	0.53
1:A:235:ILE:O	1:A:239:MET:HG3	2.09	0.53
1:A:22:THR:OG1	1:A:23:GLY:N	2.41	0.53
1:A:708:ALA:N	1:A:709:PRO:CD	2.71	0.53
1:A:692:GLN:C	1:A:694:TYR:N	2.60	0.53
1:A:654:THR:HG22	1:A:677:ALA:HB3	1.91	0.53
1:A:101:ASN:CB	3:A:1001:CZA:O3	2.56	0.53
1:A:76:ALA:CB	1:A:88:PHE:CZ	2.91	0.52
1:A:672:ARG:NH1	1:A:672:ARG:CB	2.72	0.52
1:A:809:PHE:N	1:A:809:PHE:CD2	2.77	0.52
1:A:505:ARG:O	1:A:506:ALA:O	2.28	0.52
1:A:905:VAL:O	1:A:909:MET:HG2	2.10	0.52
1:A:71:ILE:HA	1:A:74:VAL:HG12	1.91	0.52
1:A:366:MET:HE3	1:A:448:LEU:HD11	1.91	0.52
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.10	0.52
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.90	0.52
1:A:47:LYS:C	1:A:47:LYS:CD	2.70	0.52
1:A:71:ILE:O	1:A:75:LEU:HG	2.10	0.52
1:A:899:MET:O	1:A:903:VAL:HG23	2.09	0.52
1:A:133:ASP:O	1:A:134:ARG:NH1	2.42	0.52
1:A:836:ARG:NH2	1:A:836:ARG:CB	2.71	0.52
1:A:498:CYS:O	1:A:510:ASN:HB3	2.09	0.52
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.91	0.52
1:A:124:PRO:HB3	1:A:158:LYS:HD2	1.91	0.52
1:A:921:SER:HB2	1:A:989:ARG:HH22	1.75	0.51
1:A:735:LEU:HD13	1:A:739:ASN:O	2.09	0.51
1:A:809:PHE:HD2	1:A:809:PHE:N	2.09	0.51
1:A:51:GLU:O	1:A:55:GLU:HG3	2.10	0.51
1:A:319:LEU:HG	1:A:339:VAL:CG2	2.40	0.51
1:A:589:THR:HG22	1:A:590:ASP:N	2.25	0.51
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.93	0.51
1:A:145:ILE:O	1:A:146:VAL:HG12	2.11	0.51
1:A:502:LYS:CG	1:A:503:SER:H	2.17	0.51
1:A:73:PHE:CD2	1:A:91:PRO:HB2	2.45	0.51
1:A:795:VAL:HA	1:A:799:THR:CB	2.38	0.51
1:A:757:MET:HG2	1:A:760:PHE:HE2	1.75	0.51
1:A:488:SER:C	1:A:490:ASP:N	2.62	0.51
1:A:916:LEU:HD21	1:A:930:ASN:CB	2.40	0.51
1:A:519:GLU:CD	1:A:519:GLU:N	2.64	0.51
1:A:491:ARG:CB	1:A:585:MET:HG3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:MET:HG2	1:A:760:PHE:CE2	2.45	0.51
1:A:759:GLN:NE2	1:A:762:ARG:HH21	2.09	0.51
1:A:428:ASN:HB2	1:A:435:GLU:CG	2.41	0.51
1:A:488:SER:C	1:A:490:ASP:H	2.14	0.50
1:A:628:ASN:ND2	1:A:631:THR:HB	2.25	0.50
1:A:457:THR:O	1:A:459:VAL:HG13	2.11	0.50
1:A:397:LYS:HB3	1:A:402:ILE:HG21	1.94	0.50
1:A:539:GLY:N	1:A:540:PRO:HD2	2.25	0.50
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.27	0.50
1:A:33:LEU:HD23	1:A:33:LEU:O	2.12	0.50
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.42	0.50
1:A:308:PRO:N	1:A:309:GLU:CD	2.65	0.50
1:A:762:ARG:HH11	1:A:833:LEU:HD21	1.76	0.50
1:A:105:GLY:HA2	1:A:109:GLU:HG3	1.94	0.50
1:A:308:PRO:CA	1:A:309:GLU:OE1	2.60	0.50
1:A:130:TYR:HE2	1:A:137:VAL:CB	2.21	0.49
1:A:248:PRO:HB2	1:A:822:ARG:HH22	1.77	0.49
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.93	0.49
1:A:880:HIS:H	1:A:881:PRO:HD2	1.78	0.49
1:A:880:HIS:ND1	1:A:881:PRO:HD3	2.27	0.49
1:A:720:MET:HE1	1:A:738:ASP:O	2.12	0.49
1:A:150:ILE:CG2	1:A:220:LEU:HD11	2.43	0.49
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.93	0.49
1:A:502:LYS:O	1:A:504:SER:N	2.46	0.49
1:A:680:GLU:HG3	1:A:681:PRO:HD2	1.95	0.49
1:A:244:GLN:OE1	1:A:244:GLN:HA	2.12	0.49
1:A:390:ALA:C	1:A:392:GLU:H	2.15	0.49
1:A:33:LEU:HD21	1:A:38:HIS:NE2	2.28	0.49
1:A:281:ASP:HB3	1:A:282:PRO:HD2	1.95	0.48
1:A:375:ASP:O	1:A:376:PHE:C	2.51	0.48
1:A:294:TYR:O	1:A:296:PHE:N	2.47	0.48
1:A:822:ARG:O	1:A:822:ARG:HD3	2.14	0.48
1:A:315:ILE:HG22	1:A:316:THR:N	2.29	0.48
1:A:287:SER:OG	1:A:290:ARG:HB2	2.04	0.48
1:A:83:GLU:HB3	1:A:85:ILE:HG13	1.96	0.48
1:A:783:LEU:HB3	1:A:784:PRO:HD3	1.96	0.48
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.78	0.48
1:A:832:TRP:CD1	1:A:988:ALA:HB2	2.48	0.48
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.96	0.48
1:A:672:ARG:NH1	1:A:672:ARG:HB2	2.28	0.47
1:A:800:ASP:C	1:A:803:PRO:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:HB2	1:A:730:ALA:HA	1.96	0.47
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.94	0.47
1:A:856:PHE:CZ	1:A:891:PHE:HA	2.47	0.47
1:A:527:TYR:O	1:A:592:THR:HA	2.14	0.47
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.96	0.47
1:A:505:ARG:C	1:A:506:ALA:O	2.50	0.47
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.78	0.47
1:A:656:ARG:NE	1:A:660:ASP:OD2	2.41	0.47
1:A:345:THR:HB	1:A:747:VAL:CG2	2.45	0.47
1:A:357:THR:HB	1:A:602:PRO:O	2.15	0.47
1:A:868:HIS:O	1:A:869:GLN:C	2.53	0.47
1:A:679:VAL:HG22	1:A:683:HIS:ND1	2.30	0.47
1:A:412:GLU:OE2	1:A:529:ARG:HD2	2.15	0.47
1:A:926:PRO:O	1:A:929:VAL:HG23	2.15	0.47
1:A:800:ASP:OD1	1:A:908:GLU:HG3	2.15	0.47
1:A:294:TYR:C	1:A:296:PHE:H	2.19	0.47
1:A:688:VAL:HG12	1:A:689:GLU:N	2.29	0.47
1:A:506:ALA:O	1:A:507:ALA:HB2	2.15	0.47
1:A:47:LYS:O	1:A:48:SER:CB	2.58	0.47
1:A:183:GLU:O	1:A:184:SER:C	2.53	0.46
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.95	0.46
1:A:707:ASP:O	1:A:711:LEU:HG	2.15	0.46
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.97	0.46
1:A:562:LEU:N	1:A:562:LEU:HD12	2.31	0.46
1:A:417:CYS:SG	1:A:445:LEU:HG	2.56	0.46
1:A:307:ILE:HD13	1:A:307:ILE:H	1.80	0.46
1:A:499:SER:HA	1:A:510:ASN:HB3	1.97	0.46
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.98	0.46
1:A:558:THR:HB	1:A:635:ILE:CD1	2.38	0.46
1:A:333:VAL:HG22	1:A:733:MET:HG3	1.97	0.46
1:A:19:SER:HB3	1:A:22:THR:OG1	2.16	0.46
1:A:179:ILE:HG13	1:A:180:LEU:H	1.81	0.46
1:A:628:ASN:HD21	1:A:631:THR:CB	2.30	0.45
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.46	0.45
1:A:854:TRP:CZ2	1:A:969:MET:SD	3.09	0.45
1:A:319:LEU:HG	1:A:339:VAL:HG21	1.99	0.45
1:A:104:VAL:CG1	1:A:104:VAL:O	2.64	0.45
1:A:76:ALA:HB3	1:A:88:PHE:HZ	1.78	0.45
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.99	0.45
1:A:775:ILE:HA	1:A:778:THR:HG22	1.97	0.45
1:A:924:ARG:O	1:A:926:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:LEU:HD23	1:A:975:LEU:C	2.36	0.45
1:A:907:ILE:HG23	1:A:977:VAL:HG11	1.99	0.45
1:A:610:SER:OG	1:A:741:SER:HB2	2.17	0.45
1:A:174:ARG:NH1	1:A:188:ILE:HD11	2.32	0.45
1:A:50:TRP:O	1:A:54:ILE:HG12	2.17	0.45
1:A:813:ASP:HB3	1:A:815:ASP:OD1	2.17	0.45
1:A:517:ALA:O	1:A:518:PRO:O	2.35	0.45
1:A:635:ILE:HG12	1:A:635:ILE:H	1.62	0.45
1:A:802:LEU:N	1:A:803:PRO:CD	2.80	0.45
1:A:248:PRO:CB	1:A:822:ARG:HH12	2.29	0.45
1:A:428:ASN:HB2	1:A:435:GLU:HG2	1.97	0.45
1:A:133:ASP:O	1:A:134:ARG:HG2	2.17	0.45
1:A:124:PRO:HB3	1:A:158:LYS:CD	2.46	0.45
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.99	0.45
1:A:273:LEU:HA	1:A:276:ILE:CD1	2.47	0.44
1:A:78:PHE:CG	1:A:79:GLU:N	2.84	0.44
1:A:168:ILE:CG2	1:A:173:LEU:HB2	2.47	0.44
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.47	0.44
1:A:307:ILE:HA	1:A:308:PRO:HD3	1.76	0.44
1:A:519:GLU:O	1:A:523:ASP:HB2	2.17	0.44
1:A:42:PRO:O	1:A:120:LYS:NZ	2.51	0.44
1:A:672:ARG:CB	1:A:672:ARG:HH11	2.29	0.44
1:A:84:THR:HG23	1:A:84:THR:O	2.17	0.44
1:A:396:LEU:HB2	1:A:400:LYS:H	1.81	0.44
1:A:648:VAL:HA	1:A:651:ARG:HG3	1.98	0.44
1:A:44:GLU:OE2	1:A:46:GLY:HA2	2.18	0.44
1:A:778:THR:OG1	1:A:785:GLU:HA	2.18	0.44
1:A:359:ASN:HA	1:A:359:ASN:HD22	1.48	0.44
1:A:912:ALA:HB1	1:A:933:LEU:HD11	1.99	0.44
1:A:917:SER:OG	1:A:920:GLN:HB2	2.17	0.44
1:A:921:SER:HB3	1:A:924:ARG:HH22	1.83	0.44
1:A:960:LYS:HD3	1:A:960:LYS:HA	1.78	0.44
1:A:985:LYS:HB3	1:A:989:ARG:HH21	1.81	0.44
1:A:345:THR:HB	1:A:747:VAL:HG21	2.00	0.44
1:A:311:LEU:CB	1:A:312:PRO:CD	2.76	0.43
1:A:397:LYS:H	1:A:402:ILE:HG23	1.82	0.43
1:A:361:MET:HA	1:A:600:LEU:O	2.18	0.43
1:A:962:LEU:HB3	1:A:966:GLN:HB2	2.00	0.43
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.89	0.43
1:A:534:ARG:HG2	1:A:535:VAL:N	2.28	0.43
1:A:921:SER:HB3	1:A:924:ARG:NH2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:HA	1:A:470:ALA:HB2	1.99	0.43
1:A:41:LEU:HD23	1:A:236:ARG:HG3	2.00	0.43
1:A:201:ASN:HA	1:A:204:LYS:HD2	2.01	0.43
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.80	0.43
1:A:75:LEU:HD21	1:A:296:PHE:HB2	2.00	0.43
1:A:783:LEU:HD22	1:A:870:LEU:HB2	2.01	0.43
1:A:519:GLU:O	1:A:523:ASP:N	2.35	0.43
1:A:38:HIS:CE1	1:A:143:ARG:HH12	2.37	0.43
1:A:73:PHE:HE2	1:A:91:PRO:HB2	1.79	0.43
1:A:953:LEU:HB2	1:A:954:PRO:HD3	2.01	0.43
1:A:563:ALA:O	1:A:564:LEU:HD23	2.18	0.43
1:A:93:VAL:HG12	1:A:793:LEU:HD13	2.01	0.43
1:A:601:ASP:HA	1:A:602:PRO:HD2	1.86	0.42
1:A:177:GLN:H	1:A:177:GLN:HG2	1.70	0.42
1:A:825:LYS:HE2	1:A:825:LYS:HB2	1.80	0.42
1:A:356:LEU:HA	1:A:607:VAL:HG11	2.01	0.42
1:A:179:ILE:HG13	1:A:180:LEU:HG	2.01	0.42
1:A:546:LEU:HA	1:A:546:LEU:HD23	1.89	0.42
1:A:349:CYS:HA	1:A:622:ILE:O	2.19	0.42
1:A:628:ASN:N	1:A:628:ASN:HD22	2.18	0.42
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.33	0.42
1:A:924:ARG:NH2	1:A:989:ARG:HH12	2.18	0.42
1:A:352:LYS:HD2	1:A:635:ILE:HG21	2.02	0.42
1:A:24:LEU:HG	1:A:149:ASP:HA	2.02	0.42
1:A:174:ARG:HH12	1:A:188:ILE:HD11	1.85	0.42
1:A:880:HIS:H	1:A:881:PRO:CD	2.32	0.42
1:A:179:ILE:HG13	1:A:180:LEU:N	2.35	0.42
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.85	0.42
1:A:124:PRO:HG3	1:A:160:PRO:HA	2.01	0.42
1:A:631:THR:HG22	1:A:635:ILE:HD11	2.02	0.42
1:A:975:LEU:N	1:A:976:PRO:CD	2.81	0.42
1:A:105:GLY:C	1:A:109:GLU:HB2	2.40	0.42
1:A:808:GLY:C	1:A:809:PHE:HD2	2.23	0.42
1:A:775:ILE:O	1:A:775:ILE:HG22	2.18	0.42
1:A:851:ALA:HB2	1:A:973:ILE:HG21	2.01	0.42
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.52	0.42
1:A:607:VAL:O	1:A:611:ILE:HG12	2.20	0.42
1:A:908:GLU:OE2	1:A:908:GLU:HA	2.20	0.42
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.77	0.42
1:A:383:SER:C	1:A:384:ILE:HD13	2.40	0.42
1:A:130:TYR:HE2	1:A:137:VAL:HG23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:HA	1:A:570:PRO:HG3	2.02	0.41
1:A:720:MET:HE3	1:A:738:ASP:CB	2.49	0.41
1:A:168:ILE:HG23	1:A:173:LEU:HB2	2.03	0.41
1:A:84:THR:O	1:A:86:THR:N	2.53	0.41
1:A:650:ASP:N	1:A:650:ASP:OD2	2.52	0.41
1:A:455:PHE:O	1:A:456:ASN:HB2	2.20	0.41
1:A:389:TYR:HB3	1:A:425:LEU:CD2	2.48	0.41
1:A:518:PRO:O	1:A:521:VAL:N	2.52	0.41
1:A:688:VAL:HG23	1:A:700:MET:HE2	1.98	0.41
1:A:377:CYS:HB3	1:A:544:LYS:HG3	2.03	0.41
1:A:133:ASP:O	1:A:134:ARG:CG	2.68	0.41
1:A:23:GLY:HA3	1:A:130:TYR:O	2.21	0.41
1:A:499:SER:HA	1:A:500:PRO:HD3	1.91	0.41
1:A:903:VAL:O	1:A:907:ILE:HG13	2.21	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.82	0.41
1:A:137:VAL:HG22	1:A:137:VAL:O	2.21	0.41
1:A:488:SER:O	1:A:490:ASP:N	2.53	0.41
1:A:288:TRP:C	1:A:290:ARG:N	2.74	0.41
1:A:612:GLN:OE1	1:A:615:ARG:HD3	2.21	0.41
1:A:338:SER:O	1:A:342:LEU:HB2	2.21	0.41
1:A:342:LEU:HD11	1:A:733:MET:HE1	2.03	0.41
1:A:188:ILE:HD13	1:A:486:GLU:HG2	2.02	0.41
1:A:109:GLU:O	1:A:111:ASN:ND2	2.54	0.41
1:A:175:VAL:HG23	1:A:189:LYS:HG2	2.03	0.40
1:A:665:GLU:HA	1:A:668:GLU:HB2	2.03	0.40
1:A:298:ILE:O	1:A:302:LEU:HB2	2.21	0.40
1:A:612:GLN:O	1:A:615:ARG:HB2	2.22	0.40
1:A:739:ASN:HD22	1:A:740:PHE:N	2.20	0.40
1:A:852:ALA:HB2	1:A:900:ALA:HB2	2.03	0.40
1:A:767:SER:O	1:A:771:GLU:HG3	2.21	0.40
1:A:487:PHE:HA	1:A:493:SER:O	2.22	0.40
1:A:170:SER:OG	1:A:218:LYS:N	2.46	0.40
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.56	0.40
1:A:498:CYS:O	1:A:510:ASN:CB	2.69	0.40
1:A:382:PHE:CE1	1:A:410:LEU:HD11	2.56	0.40
1:A:515:LYS:O	1:A:515:LYS:HG2	2.20	0.40
1:A:888:CYS:C	1:A:890:ILE:H	2.25	0.40
1:A:287:SER:C	1:A:290:ARG:HB2	2.42	0.40
1:A:832:TRP:CZ3	1:A:835:PHE:HD1	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:NH1	1:A:650:ASP:OD1[1_655]	1.97	0.23

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%)	864 (87%)	100 (10%)	28 (3%)	6	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	85	ILE
1	A	184	SER
1	A	288	TRP
1	A	308	PRO
1	A	309	GLU
1	A	311	LEU
1	A	503	SER
1	A	508	VAL
1	A	518	PRO
1	A	519	GLU
1	A	883	PHE
1	A	48	SER
1	A	76	ALA
1	A	289	ILE
1	A	506	ALA
1	A	648	VAL
1	A	295	TYR
1	A	338	SER
1	A	482	GLU
1	A	507	ALA
1	A	789	PRO
1	A	32	HIS

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Mol	Chain	Res	Type
1	A	693	SER
1	A	863	PRO
1	A	106	VAL
1	A	307	ILE
1	A	391	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/840 (100%)	717 (85%)	123 (15%)	4 19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	34	GLU
1	A	44	GLU
1	A	45	GLU
1	A	47	LYS
1	A	49	LEU
1	A	50	TRP
1	A	51	GLU
1	A	61	LEU
1	A	79	GLU
1	A	88	PHE
1	A	103	ILE
1	A	107	TRP
1	A	113	GLU
1	A	114	ASN
1	A	134	ARG
1	A	136	SER
1	A	138	GLN
1	A	151	VAL
1	A	158	LYS
1	A	164	ARG

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Mol	Chain	Res	Type
1	A	172	THR
1	A	177	GLN
1	A	183	GLU
1	A	205	LYS
1	A	243	GLU
1	A	258	GLU
1	A	266	LEU
1	A	287	SER
1	A	288	TRP
1	A	290	ARG
1	A	302	LEU
1	A	307	ILE
1	A	309	GLU
1	A	340	GLU
1	A	341	THR
1	A	344	CYS
1	A	353	THR
1	A	359	ASN
1	A	360	GLN
1	A	380	ASN
1	A	396	LEU
1	A	399	ASP
1	A	400	LYS
1	A	402	ILE
1	A	412	GLU
1	A	422	ASP
1	A	431	LYS
1	A	436	LYS
1	A	441	THR
1	A	445	LEU
1	A	458	GLU
1	A	467	ARG
1	A	473	SER
1	A	478	LEU
1	A	484	THR
1	A	490	ASP
1	A	492	LYS
1	A	505	ARG
1	A	508	VAL
1	A	510	ASN
1	A	511	LYS
1	A	519	GLU

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Mol	Chain	Res	Type
1	A	523	ASP
1	A	534	ARG
1	A	538	THR
1	A	544	LYS
1	A	547	SER
1	A	550	LYS
1	A	554	THR
1	A	556	ARG
1	A	560	ARG
1	A	569	THR
1	A	572	LYS
1	A	573	ARG
1	A	575	GLU
1	A	581	SER
1	A	585	MET
1	A	586	GLU
1	A	604	ARG
1	A	608	MET
1	A	612	GLN
1	A	613	LEU
1	A	615	ARG
1	A	619	ILE
1	A	620	ARG
1	A	623	MET
1	A	628	ASN
1	A	638	ARG
1	A	663	LEU
1	A	665	GLU
1	A	668	GLU
1	A	682	SER
1	A	691	LEU
1	A	703	ASP
1	A	713	LYS
1	A	724	THR
1	A	732	GLU
1	A	739	ASN
1	A	759	GLN
1	A	767	SER
1	A	774	CYS
1	A	778	THR
1	A	785	GLU
1	A	809	PHE

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Mol	Chain	Res	Type
1	A	816	ILE
1	A	819	ARG
1	A	822	ARG
1	A	825	LYS
1	A	836	ARG
1	A	838	MET
1	A	857	MET
1	A	865	VAL
1	A	867	TYR
1	A	876	CYS
1	A	880	HIS
1	A	923	MET
1	A	924	ARG
1	A	958	LYS
1	A	960	LYS
1	A	981	ASP
1	A	986	PHE
1	A	991	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	114	ASN
1	A	201	ASN
1	A	202	GLN
1	A	275	ASN
1	A	359	ASN
1	A	380	ASN
1	A	398	ASN
1	A	510	ASN
1	A	526	ASN
1	A	628	ASN
1	A	739	ASN
1	A	755	ASN
1	A	759	GLN
1	A	914	ASN
1	A	919	ASN
1	A	944	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	CZA	A	1001	2	25,29,29	1.61	7 (28%)	22,48,48	1.39	2 (9%)
4	ADP	A	1002	2	22,29,29	1.19	2 (9%)	27,45,45	1.62	4 (14%)

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
3	CZA	A	1001	2	-	0/4/52/52	0/5/5/5
4	ADP	A	1002	2	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	CZA	C4-N1	-2.90	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	CZA	C3-C4	-2.20	1.36	1.40
3	A	1001	CZA	C13-C14	-2.15	1.39	1.44
3	A	1001	CZA	C19-C18	2.17	1.41	1.36
3	A	1001	CZA	C20-C13	2.18	1.41	1.37
4	A	1002	ADP	PB-O1B	2.19	1.58	1.51
3	A	1001	CZA	O3-C4	2.42	1.37	1.31
4	A	1002	ADP	C2-N3	2.80	1.37	1.32
3	A	1001	CZA	C12-C8	3.67	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	O3A-PA-O5'	-4.01	92.30	102.94
4	A	1002	ADP	O2'-C2'-C3'	-2.45	103.87	111.83
4	A	1002	ADP	C2-N1-C6	-2.18	114.88	118.77
3	A	1001	CZA	C18-C17-N2	2.17	136.89	130.75
4	A	1002	ADP	O3B-PB-O3A	2.50	116.44	105.09
3	A	1001	CZA	C13-C14-C15	3.92	127.22	123.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	CZA	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, 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%)	0.06	56 (5%)	28 16	56, 115, 268, 410	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	HIS	8.3
1	A	276	ILE	8.0
1	A	994	GLY	7.3
1	A	863	PRO	6.6
1	A	875	GLN	6.5
1	A	279	PHE	6.4
1	A	283	VAL	6.2
1	A	886	LEU	6.2
1	A	786	ALA	5.0
1	A	883	PHE	4.6
1	A	987	ILE	4.5
1	A	872	HIS	3.7
1	A	81	GLY	3.6
1	A	107	TRP	3.6
1	A	832	TRP	3.6
1	A	991	TYR	3.6
1	A	292	ALA	3.3
1	A	877	THR	3.3
1	A	82	GLU	3.2
1	A	84	THR	3.1
1	A	884	GLU	3.1
1	A	122	TYR	3.1
1	A	286	GLY	3.0
1	A	74	VAL	3.0
1	A	966	GLN	3.0
1	A	988	ALA	2.9
1	A	876	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	993	GLU	2.9
1	A	796	ASN	2.9
1	A	79	GLU	2.9
1	A	885	GLY	2.8
1	A	868	HIS	2.8
1	A	857	MET	2.8
1	A	289	ILE	2.8
1	A	78	PHE	2.7
1	A	859	ALA	2.6
1	A	280	ASN	2.5
1	A	767	SER	2.5
1	A	83	GLU	2.5
1	A	771	GLU	2.4
1	A	580	ASP	2.4
1	A	871	THR	2.3
1	A	874	MET	2.3
1	A	287	SER	2.3
1	A	865	VAL	2.3
1	A	285	GLY	2.3
1	A	112	ALA	2.2
1	A	278	HIS	2.2
1	A	835	PHE	2.2
1	A	282	PRO	2.1
1	A	965	THR	2.1
1	A	967	TRP	2.1
1	A	992	LEU	2.0
1	A	861	ASP	2.0
1	A	281	ASP	2.0
1	A	49	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	ADP	A	1002	27/27	0.83	0.35	4.75	110,110,110,110	0
3	CZA	A	1001	25/25	0.91	0.23	0.32	154,154,154,154	0
2	MG	A	995	1/1	0.95	0.59	-	61,61,61,61	0
2	MG	A	996	1/1	0.97	0.42	-	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.