



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:26 PM UTC

PDB ID : 3FPS / pdb_00003fps
Title : The Structure of Sarcoplasmic Reticulum Ca²⁺-ATPase Bound To Cyclopiazonic and ADP
Authors : Moncoq, K.; Morth, J.P.; Bublitz, M.; Laursen, M.; Nissen, P.; Young, H.S.
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

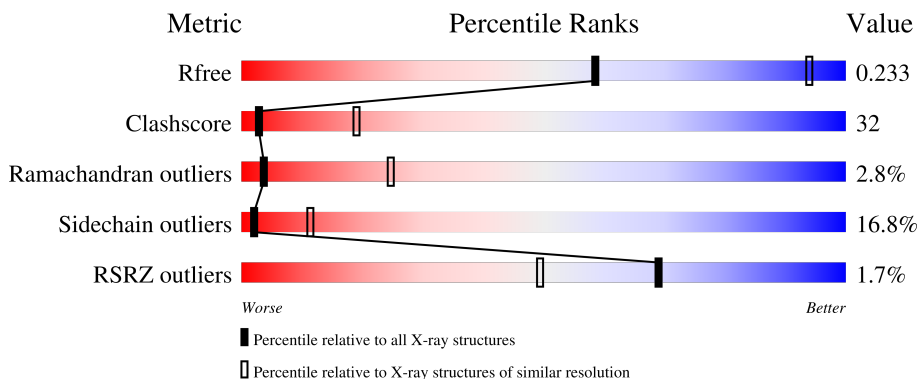
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	

2 Entry composition [i](#)

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

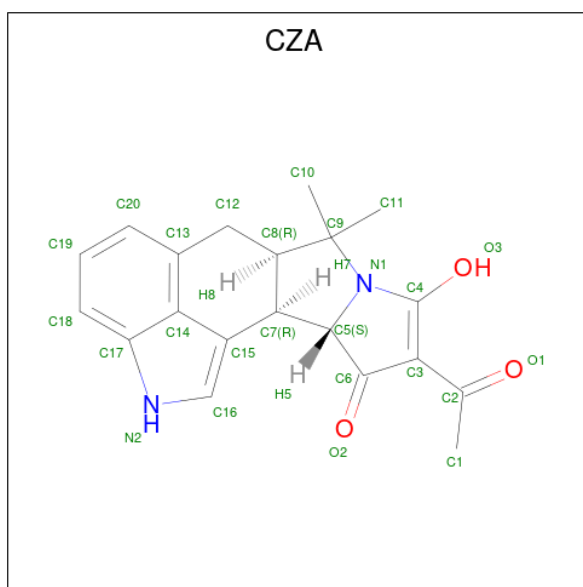
There is a discrepancy between the modelled and reference sequences:

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).

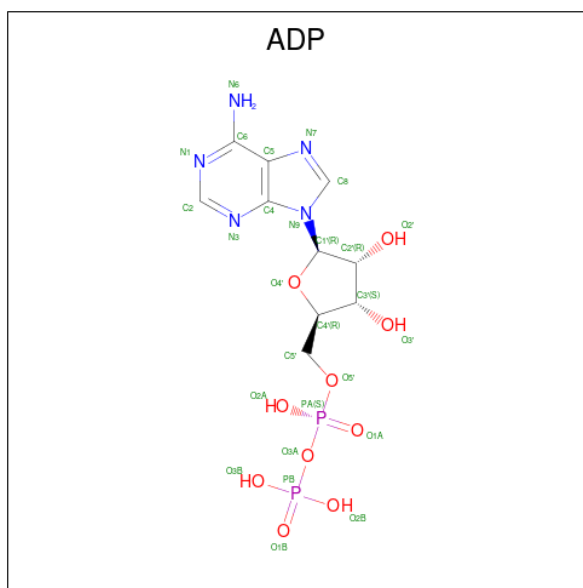
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- 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 (CCD ID: CZA) (formula: C₂₀H₂₀N₂O₃).



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

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



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

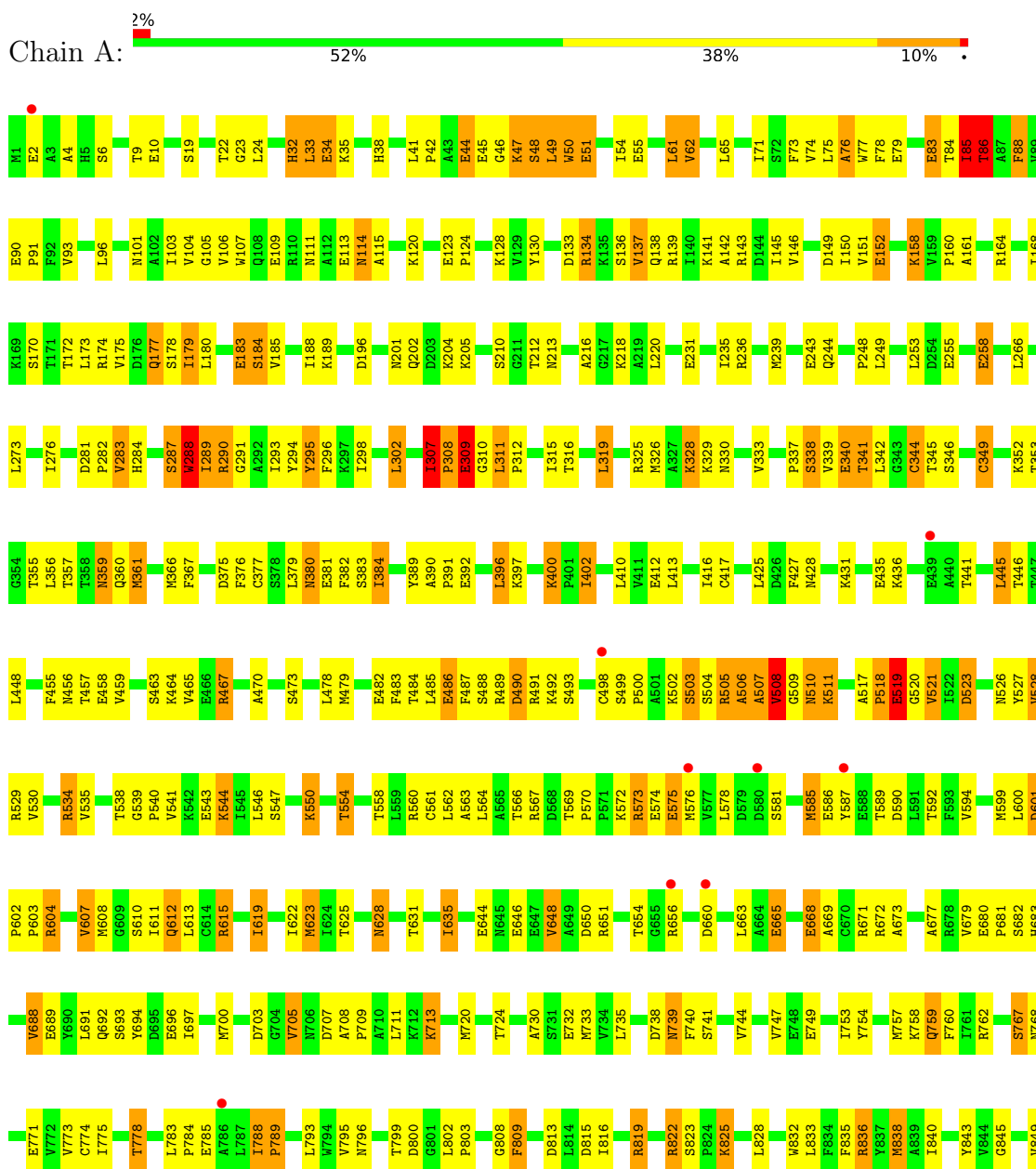
- Molecule 5 is water.

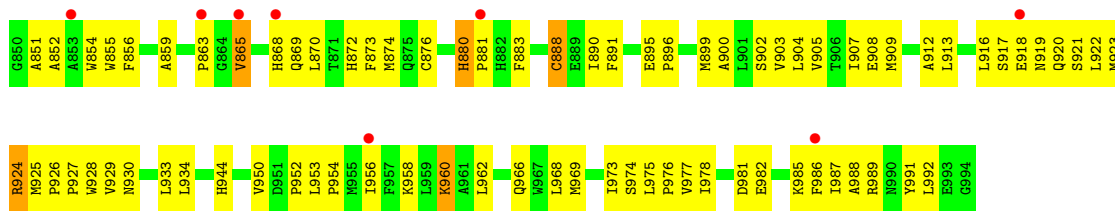
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0

3 Residue-property plots

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





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 24.89 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.89-3.20) 98.9 (24.89-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.222 , 0.241 0.218 , 0.233	Depositor DCC
R_{free} test set	1532 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7735	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtrriage'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, 0.333 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: MG, ADP, CZA

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	0.65	0/7812	0.94	14/10592 (0.1%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	CYS	N-CA-C	-10.14	101.47	114.04
1	A	196	ASP	CA-C-N	7.34	127.35	119.28
1	A	196	ASP	C-N-CA	7.34	127.35	119.28
1	A	2	GLU	N-CA-C	6.47	119.58	111.24
1	A	601	ASP	CA-C-N	6.13	126.70	120.38
1	A	601	ASP	C-N-CA	6.13	126.70	120.38
1	A	607	VAL	N-CA-C	6.03	117.49	110.62
1	A	381	GLU	N-CA-C	6.02	119.22	109.40
1	A	625	THR	N-CA-C	5.69	115.75	108.24
1	A	873	PHE	N-CA-C	5.46	117.32	108.26
1	A	594	VAL	CB-CA-C	-5.26	105.50	111.55
1	A	86	THR	N-CA-C	5.13	121.74	110.80
1	A	819	ARG	CA-C-N	5.06	125.59	120.38
1	A	819	ARG	C-N-CA	5.06	125.59	120.38

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 [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	504	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	504	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 32.

All (504) 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	1.22
1:A:759:GLN:HE21	1:A:759:GLN:HA	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:HH21	1:A:573:ARG:HG3	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:HG2	1:A:290:ARG:HH11	0.98	1.06
1:A:273:LEU:HD23	1:A:276:ILE:HD11	1.37	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ARG:CG	1:A:290:ARG:HH11	1.68	1.05
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.36	1.05
1:A:134:ARG:HH11	1:A:134:ARG:HG2	0.93	1.04
1:A:307:ILE:HG23	1:A:308:PRO:CD	1.85	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:HG22	1:A:309:GLU:H	1.24	1.02
1:A:307:ILE:HG21	1:A:309:GLU:CG	1.89	1.02
1:A:307:ILE:O	1:A:768:ASN:CG	2.03	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
1:A:307:ILE:HG21	1:A:309:GLU:HG3	1.03	1.01
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.41	1.00
1:A:924:ARG:HB2	1:A:924:ARG:NH2	1.76	1.00
1:A:575:GLU:HA	1:A:575:GLU:OE2	1.60	0.98
1:A:47:LYS:HD3	1:A:47:LYS:C	1.88	0.97
1:A:615:ARG:HG2	1:A:615:ARG:NH1	1.77	0.97
1:A:307:ILE:CG2	1:A:309:GLU:CD	2.38	0.96
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: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: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:507:ALA:C	1:A:508:VAL:HG23	1.97	0.89
1:A:631:THR:O	1:A:635:ILE:HG12	1.71	0.89
1:A:836:ARG:HH21	1:A:836:ARG:HB2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:507:ALA:C	1:A:508:VAL:CG2	2.50	0.84
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: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:H	1:A:510:ASN:HD22	1.28	0.79
1:A:759:GLN:HE21	1:A:759:GLN:CA	1.92	0.79
1:A:507:ALA:C	1:A:509:GLY:H	1.90	0.79
1:A:308:PRO:CD	1:A:309:GLU:H	1.90	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:HH11	1:A:615:ARG:CG	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:255:GLU:HA	1:A:258:GLU:HG2	1.66	0.77
1:A:307:ILE:CB	1:A:309:GLU:OE2	2.32	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:308:PRO:C	1:A:309:GLU:OE1	2.28	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:309:GLU:CD	1:A:309:GLU:N	2.44	0.75
1:A:134:ARG:CG	1:A:134:ARG:NH1	2.33	0.75
1:A:510:ASN:ND2	1:A:510:ASN:N	2.34	0.75
1:A:574:GLU:O	1:A:574:GLU:HG2	1.86	0.74
1:A:47:LYS:O	1:A:48:SER:HB3	1.86	0.73
1:A:114:ASN:H	1:A:114:ASN:ND2	1.87	0.73
1:A:307:ILE:C	1:A:309:GLU:OE2	2.32	0.73
1:A:307:ILE:HB	1:A:309:GLU:OE2	1.88	0.72
1:A:310:GLY:O	1:A:311:LEU:C	2.31	0.72
1:A:47:LYS:HD3	1:A:48:SER:N	2.05	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ARG:HG3	1:A:573:ARG:NH2	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:76:ALA:HB3	1:A:88:PHE:CZ	2.26	0.70
1:A:145:ILE:C	1:A:146:VAL:HG13	2.16	0.69
1:A:183:GLU:O	1:A:185:VAL:N	2.26	0.69
1:A:518:PRO:O	1:A:519:GLU:C	2.36	0.69
1:A:32:HIS:O	1:A:35:LYS:N	2.26	0.69
1:A:924:ARG:HH21	1:A:924:ARG:CB	1.98	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:561:CYS:C	1:A:562:LEU:HD12	2.19	0.68
1:A:744:VAL:O	1:A:747:VAL:HG12	1.93	0.68
1:A:783:LEU:HB3	1:A:784:PRO:CD	2.23	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: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:326:MET:HE3	1:A:333:VAL:HG21	1.77	0.67
1:A:248:PRO:HD2	1:A:340:GLU:OE2	1.95	0.66
1:A:669:ALA:O	1:A:673:ALA:HB2	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:925:MET:HA	1:A:925:MET:HE3	1.79	0.65
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.79	0.65
1:A:950:VAL:O	1:A:954:PRO:HD2	1.95	0.65
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.78	0.65
1:A:288:TRP:O	1:A:291:GLY:N	2.29	0.65
1:A:507:ALA:O	1:A:509:GLY:N	2.29	0.65
1:A:688:VAL:HG23	1:A:700:MET:CE	2.27	0.64
1:A:828:LEU:H	1:A:828:LEU:HD12	1.62	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:692:GLN:C	1:A:694:TYR:H	2.06	0.64
1:A:916:LEU:HD21	1:A:930:ASN:HB2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:VAL:HG12	1:A:212:THR:CG2	2.28	0.63
1:A:175:VAL:HG12	1:A:212:THR:HG21	1.80	0.63
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.80	0.63
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.29	0.63
1:A:307:ILE:HD13	1:A:307:ILE:N	2.14	0.63
1:A:600:LEU:HG	1:A:601:ASP:N	2.13	0.63
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.80	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:32:HIS:O	1:A:33:LEU:C	2.39	0.62
1:A:201:ASN:HD21	1:A:231:GLU:CG	2.10	0.62
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:145:ILE:C	1:A:146:VAL:CG1	2.73	0.61
1:A:308:PRO:CD	1:A:309:GLU:N	2.48	0.61
1:A:49:LEU:HD12	1:A:50:TRP:HE3	1.66	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:518:PRO:C	1:A:519:GLU:OE1	2.44	0.61
1:A:688:VAL:HG11	1:A:713:LYS:HB3	1.83	0.61
1:A:505:ARG:O	1:A:506:ALA:C	2.43	0.61
1:A:539:GLY:O	1:A:543:GLU:HG2	2.01	0.61
1:A:762:ARG:NH1	1:A:833:LEU:HD21	2.16	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:974:SER:C	1:A:976:PRO:HD2	2.26	0.60
1:A:294:TYR:CG	1:A:295:TYR:N	2.70	0.60
1:A:10:GLU:OE1	1:A:10:GLU:N	2.26	0.60
1:A:985:LYS:O	1:A:989:ARG:HB2	2.02	0.60
1:A:288:TRP:O	1:A:289:ILE:C	2.45	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:366:MET:HE3	1:A:384:ILE:HD11	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	1:A:34:GLU:N	2.61	0.58
1:A:307:ILE:N	1:A:307:ILE:CD1	2.65	0.57
1:A:489:ARG:NH1	1:A:489:ARG:HG3	2.18	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:604:ARG:O	1:A:607:VAL:HG22	2.05	0.57
1:A:507:ALA:C	1:A:509:GLY:N	2.57	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
1:A:145:ILE:O	1:A:146:VAL:CG1	2.53	0.57
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.04	0.57
1:A:902:SER:HA	1:A:944:HIS:HE1	1.68	0.57
1:A:47:LYS:C	1:A:47:LYS:CD	2.70	0.56
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.87	0.56
1:A:502:LYS:HG3	1:A:503:SER:N	2.14	0.56
1:A:575:GLU:OE2	1:A:575:GLU:CA	2.42	0.56
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.87	0.56
1:A:488:SER:C	1:A:490:ASP:H	2.14	0.56
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.41	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:76:ALA:HB1	1:A:77:TRP:CE3	2.42	0.55
1:A:519:GLU:CD	1:A:519:GLU:N	2.64	0.55
1:A:573:ARG:CG	1:A:573:ARG:NH2	2.51	0.55
1:A:483:PHE:CE2	1:A:578:LEU:HD21	2.41	0.55
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.72	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:986:PHE:HD1	1:A:989:ARG:CZ	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:SER:C	1:A:490:ASP:N	2.62	0.55
1:A:308:PRO:N	1:A:309:GLU:CD	2.65	0.54
1:A:390:ALA:C	1:A:392:GLU:H	2.15	0.54
1:A:692:GLN:C	1:A:694:TYR:N	2.60	0.54
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:799:THR:HG21	1:A:905:VAL:HG22	1.89	0.54
1:A:836:ARG:O	1:A:840:ILE:HG12	2.08	0.54
1:A:212:THR:HG22	1:A:213:ASN:N	2.22	0.53
1:A:758:LYS:HG2	1:A:762:ARG:CZ	2.38	0.53
1:A:612:GLN:HA	1:A:615:ARG:HD2	1.89	0.53
1:A:375:ASP:O	1:A:376:PHE:C	2.51	0.53
1:A:672:ARG:HH11	1:A:672:ARG:HB3	1.73	0.53
1:A:800:ASP:C	1:A:803:PRO:HD2	2.33	0.53
1:A:308:PRO:N	1:A:309:GLU:OE2	2.41	0.53
1:A:672:ARG:HB2	1:A:672:ARG:CZ	2.39	0.53
1:A:235:ILE:O	1:A:239:MET:HG3	2.09	0.53
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:22:THR:OG1	1:A:23:GLY:N	2.41	0.53
1:A:654:THR:HG22	1:A:677:ALA:HB3	1.91	0.53
1:A:708:ALA:N	1:A:709:PRO:CD	2.71	0.53
1:A:101:ASN:CB	3:A:1001:CZA:O3	2.56	0.53
1:A:479:MET:HE3	1:A:498:CYS:HB3	1.90	0.53
1:A:688:VAL:HG23	1:A:700:MET:HE2	1.91	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: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:71:ILE:O	1:A:75:LEU:HG	2.10	0.52
1:A:505:ARG:C	1:A:506:ALA:O	2.50	0.52
1:A:868:HIS:O	1:A:869:GLN:C	2.53	0.52
1:A:899:MET:O	1:A:903:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:O	1:A:134:ARG:NH1	2.42	0.52
1:A:836:ARG:CB	1:A:836:ARG:NH2	2.71	0.52
1:A:124:PRO:HB3	1:A:158:LYS:HD2	1.91	0.52
1:A:326:MET:HG2	1:A:749:GLU:HG2	1.91	0.52
1:A:498:CYS:O	1:A:510:ASN:HB3	2.09	0.52
1:A:294:TYR:C	1:A:296:PHE:H	2.19	0.51
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:N	1:A:809:PHE:HD2	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:183:GLU:O	1:A:184:SER:C	2.53	0.51
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.93	0.51
1:A:589:THR:HG22	1:A:590:ASP:N	2.25	0.51
1:A:145:ILE:O	1:A:146:VAL:HG12	2.11	0.51
1:A:73:PHE:CD2	1:A:91:PRO:HB2	2.45	0.51
1:A:502:LYS:CG	1:A:503:SER:H	2.17	0.51
1:A:757:MET:HG2	1:A:760:PHE:HE2	1.75	0.51
1:A:795:VAL:HA	1:A:799:THR:CB	2.38	0.51
1:A:975:LEU:C	1:A:975:LEU:HD23	2.36	0.51
1:A:916:LEU:HD21	1:A:930:ASN:CB	2.40	0.51
1:A:491:ARG:CB	1:A:585:MET:HG3	2.36	0.51
1:A:757:MET:HG2	1:A:760:PHE:CE2	2.45	0.51
1:A:428:ASN:HB2	1:A:435:GLU:CG	2.41	0.51
1:A:759:GLN:NE2	1:A:762:ARG:HH21	2.09	0.51
1:A:457:THR:O	1:A:459:VAL:HG13	2.11	0.50
1:A:628:ASN:ND2	1:A:631:THR:HB	2.25	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:688:VAL:HG23	1:A:700:MET:HE3	1.92	0.50
1:A:33:LEU:O	1:A:33:LEU:HD23	2.12	0.50
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.42	0.50
1:A:105:GLY:HA2	1:A:109:GLU:HG3	1.94	0.50
1:A:762:ARG:HH11	1:A:833:LEU:HD21	1.76	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:GLN:OE1	1:A:244:GLN:HA	2.12	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:835:PHE:CD2	1:A:838:MET:HE3	2.47	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: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:720:MET:HE1	1:A:738:ASP:O	2.13	0.48
1:A:83:GLU:HB3	1:A:85:ILE:HG13	1.96	0.48
1:A:287:SER:OG	1:A:290:ARG:HB2	2.04	0.48
1:A:604:ARG:HG3	1:A:604:ARG:HH11	1.78	0.48
1:A:783:LEU:HB3	1:A:784:PRO:HD3	1.96	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:115:ALA:HB2	1:A:730:ALA:HA	1.96	0.47
1:A:672:ARG:HB2	1:A:672:ARG:NH1	2.28	0.47
1:A:969:MET:HA	1:A:969:MET:HE3	1.96	0.47
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.94	0.47
1:A:527:TYR:O	1:A:592:THR:HA	2.14	0.47
1:A:856:PHE:CZ	1:A:891:PHE:HA	2.47	0.47
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.96	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:412:GLU:OE2	1:A:529:ARG:HD2	2.15	0.47
1:A:679:VAL:HG22	1:A:683:HIS:ND1	2.30	0.47
1:A:800:ASP:OD1	1:A:908:GLU:HG3	2.15	0.47
1:A:926:PRO:O	1:A:929:VAL:HG23	2.15	0.47
1:A:105:GLY:C	1:A:109:GLU:HB2	2.40	0.47
1:A:47:LYS:O	1:A:48:SER:CB	2.58	0.47
1:A:506:ALA:O	1:A:507:ALA:HB2	2.15	0.47
1:A:623:MET:HE1	1:A:635:ILE:HB	1.97	0.47
1:A:383:SER:C	1:A:384:ILE:HD13	2.40	0.46
1:A:707:ASP:O	1:A:711:LEU:HG	2.15	0.46
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.95	0.46
1:A:688:VAL:HG12	1:A:689:GLU:N	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.97	0.46
1:A:417:CYS:SG	1:A:445:LEU:HG	2.56	0.46
1:A:808:GLY:C	1:A:809:PHE:HD2	2.23	0.46
1:A:562:LEU:HD12	1:A:562:LEU:N	2.31	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:585:MET:HB3	1:A:585:MET:HE2	1.73	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:104:VAL:O	1:A:104:VAL:CG1	2.64	0.45
1:A:288:TRP:C	1:A:290:ARG:N	2.74	0.45
1:A:319:LEU:HG	1:A:339:VAL:HG21	1.99	0.45
1:A:628:ASN:HD21	1:A:631:THR:CB	2.30	0.45
1:A:854:TRP:CZ2	1:A:969:MET:SD	3.09	0.45
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.46	0.45
1:A:76:ALA:HB3	1:A:88:PHE:HZ	1.78	0.45
1:A:775:ILE:HA	1:A:778:THR:HG22	1.97	0.45
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.99	0.45
1:A:907:ILE:HG23	1:A:977:VAL:HG11	1.99	0.45
1:A:924:ARG:O	1:A:926:PRO:HD3	2.17	0.45
1:A:610:SER:OG	1:A:741:SER:HB2	2.17	0.45
1:A:888:CYS:C	1:A:890:ILE:H	2.25	0.45
1:A:50:TRP:O	1:A:54:ILE:HG12	2.17	0.45
1:A:174:ARG:NH1	1:A:188:ILE:HD11	2.32	0.45
1:A:813:ASP:HB3	1:A:815:ASP:OD1	2.17	0.45
1:A:287:SER:C	1:A:290:ARG:HB2	2.42	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:124:PRO:HB3	1:A:158:LYS:CD	2.46	0.45
1:A:133:ASP:O	1:A:134:ARG:HG2	2.17	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: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:42:PRO:O	1:A:120:LYS:NZ	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ILE:HA	1:A:308:PRO:HD3	1.76	0.44
1:A:326:MET:HE1	1:A:339:VAL:HG12	2.00	0.44
1:A:519:GLU:O	1:A:523:ASP:HB2	2.17	0.44
1:A:672:ARG:HH11	1:A:672:ARG:CB	2.29	0.44
1:A:44:GLU:OE2	1:A:46:GLY:HA2	2.18	0.44
1:A:396:LEU:HB2	1:A:400:LYS:H	1.81	0.44
1:A:619:ILE:HD13	1:A:619:ILE:C	2.42	0.44
1:A:648:VAL:HA	1:A:651:ARG:HG3	1.98	0.44
1:A:359:ASN:HD22	1:A:359:ASN:HA	1.48	0.44
1:A:778:THR:OG1	1:A:785:GLU:HA	2.18	0.44
1:A:912:ALA:HB1	1:A:933:LEU:HD11	1.99	0.44
1:A:84:THR:HG23	1:A:84:THR:O	2.17	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:345:THR:HB	1:A:747:VAL:HG21	2.00	0.44
1:A:985:LYS:HB3	1:A:989:ARG:HH21	1.81	0.44
1:A:78:PHE:CG	1:A:79:GLU:N	2.84	0.43
1:A:311:LEU:CB	1:A:312:PRO:CD	2.76	0.43
1:A:361:MET:HA	1:A:600:LEU:O	2.18	0.43
1:A:397:LYS:H	1:A:402:ILE:HG23	1.82	0.43
1:A:962:LEU:HB3	1:A:966:GLN:HB2	2.00	0.43
1:A:141:LYS:O	1:A:142:ALA:C	2.61	0.43
1:A:534:ARG:HG2	1:A:535:VAL:N	2.28	0.43
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.89	0.43
1:A:754:TYR:CD2	1:A:754:TYR:C	2.96	0.43
1:A:467:ARG:HA	1:A:470:ALA:HB2	1.99	0.43
1:A:921:SER:HB3	1:A:924:ARG:NH2	2.32	0.43
1:A:41:LEU:HD23	1:A:236:ARG:HG3	2.00	0.43
1:A:61:LEU:HD12	1:A:61:LEU:HA	1.80	0.43
1:A:201:ASN:HA	1:A:204:LYS:HD2	2.01	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: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:178:SER:O	1:A:179:ILE:C	2.61	0.43
1:A:519:GLU:O	1:A:523:ASP:N	2.35	0.43
1:A:953:LEU:HB2	1:A:954:PRO:HD3	2.01	0.43
1:A:93:VAL:HG12	1:A:793:LEU:HD13	2.01	0.43
1:A:562:LEU:HD13	1:A:599:MET:HE3	2.00	0.43
1:A:563:ALA:O	1:A:564:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLN:H	1:A:177:GLN:HG2	1.70	0.42
1:A:601:ASP:HA	1:A:602:PRO:HD2	1.86	0.42
1:A:987:ILE:C	1:A:989:ARG:N	2.77	0.42
1:A:96:LEU:C	1:A:96:LEU:HD23	2.44	0.42
1:A:337:PRO:C	1:A:339:VAL:H	2.26	0.42
1:A:356:LEU:HA	1:A:607:VAL:HG11	2.01	0.42
1:A:825:LYS:HB2	1:A:825:LYS:HE2	1.80	0.42
1:A:179:ILE:HG13	1:A:180:LEU:HG	2.01	0.42
1:A:349:CYS:HA	1:A:622:ILE:O	2.19	0.42
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.89	0.42
1:A:688:VAL:O	1:A:689:GLU:C	2.62	0.42
1:A:720:MET:HE3	1:A:738:ASP:CB	2.49	0.42
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.33	0.42
1:A:628:ASN:N	1:A:628:ASN:HD22	2.18	0.42
1:A:24:LEU:HG	1:A:149:ASP:HA	2.02	0.42
1:A:352:LYS:HD2	1:A:635:ILE:HG21	2.02	0.42
1:A:924:ARG:NH2	1:A:989:ARG:HH12	2.18	0.42
1:A:124:PRO:HG3	1:A:160:PRO:HA	2.01	0.42
1:A:174:ARG:HH12	1:A:188:ILE:HD11	1.85	0.42
1:A:179:ILE:HG13	1:A:180:LEU:N	2.35	0.42
1:A:249:LEU:HB2	1:A:340:GLU:CD	2.44	0.42
1:A:483:PHE:HE2	1:A:485:LEU:HD21	1.85	0.42
1:A:518:PRO:C	1:A:519:GLU:CD	2.87	0.42
1:A:880:HIS:H	1:A:881:PRO:CD	2.32	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:775:ILE:HG22	1:A:775:ILE:O	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:294:TYR:C	1:A:296:PHE:N	2.77	0.42
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.77	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:130:TYR:HE2	1:A:137:VAL:HG23	1.84	0.41
1:A:337:PRO:C	1:A:339:VAL:N	2.75	0.41
1:A:361:MET:HB2	1:A:361:MET:HE2	1.47	0.41
1:A:366:MET:HE3	1:A:384:ILE:CD1	2.49	0.41
1:A:486:GLU:CD	1:A:486:GLU:H	2.27	0.41
1:A:511:LYS:HA	1:A:570:PRO:HG3	2.02	0.41
1:A:84:THR:O	1:A:86:THR:N	2.53	0.41
1:A:168:ILE:HG23	1:A:173:LEU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PHE:O	1:A:456:ASN:HB2	2.20	0.41
1:A:650:ASP:OD2	1:A:650:ASP:N	2.52	0.41
1:A:109:GLU:O	1:A:111:ASN:CG	2.64	0.41
1:A:389:TYR:HB3	1:A:425:LEU:CD2	2.48	0.41
1:A:377:CYS:HB3	1:A:544:LYS:HG3	2.03	0.41
1:A:463:SER:O	1:A:464:LYS:C	2.63	0.41
1:A:518:PRO:O	1:A:521:VAL:N	2.52	0.41
1:A:808:GLY:C	1:A:809:PHE:CD2	2.99	0.41
1:A:23:GLY:HA3	1:A:130:TYR:O	2.21	0.41
1:A:133:ASP:O	1:A:134:ARG:CG	2.68	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:HD23	1:A:75:LEU:HA	1.82	0.41
1:A:137:VAL:O	1:A:137:VAL:HG22	2.21	0.41
1:A:488:SER:O	1:A:490:ASP:N	2.53	0.41
1:A:109:GLU:O	1:A:111:ASN:ND2	2.54	0.41
1:A:188:ILE:HD13	1:A:486:GLU:HG2	2.02	0.41
1:A:338:SER:O	1:A:342:LEU:HB2	2.21	0.41
1:A:390:ALA:C	1:A:392:GLU:N	2.76	0.41
1:A:612:GLN:OE1	1:A:615:ARG:HD3	2.21	0.41
1:A:175:VAL:HG23	1:A:189:LYS:HG2	2.03	0.40
1:A:298:ILE:O	1:A:302:LEU:HB2	2.21	0.40
1:A:665:GLU:HA	1:A:668:GLU:HB2	2.03	0.40
1:A:161:ALA:C	1:A:210:SER:HB2	2.45	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:487:PHE:HA	1:A:493:SER:O	2.22	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:767:SER:O	1:A:771:GLU:HG3	2.21	0.40
1:A:852:ALA:HB2	1:A:900:ALA:HB2	2.03	0.40
1:A:382:PHE:CE1	1:A:410:LEU:HD11	2.56	0.40
1:A:498:CYS:O	1:A:510:ASN:CB	2.69	0.40
1:A:90:GLU:H	1:A:90:GLU:CD	2.26	0.40
1:A:4:ALA:C	1:A:6:SER:N	2.78	0.40
1:A:32:HIS:C	1:A:34:GLU:H	2.27	0.40
1:A:832:TRP:CZ3	1:A:835:PHE:HD1	2.39	0.40
1:A:904:LEU:O	1:A:905:VAL:C	2.64	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%)	4 25

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

Continued on next page...

Continued from previous page...

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 [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%)	699 (83%)	141 (17%)	2 11

All (141) 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	62	VAL
1	A	85	ILE
1	A	86	THR
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	137	VAL
1	A	138	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	VAL
1	A	152	GLU
1	A	158	LYS
1	A	164	ARG
1	A	172	THR
1	A	177	GLN
1	A	179	ILE
1	A	183	GLU
1	A	202	GLN
1	A	205	LYS
1	A	243	GLU
1	A	253	LEU
1	A	258	GLU
1	A	266	LEU
1	A	283	VAL
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	319	LEU
1	A	328	LYS
1	A	340	GLU
1	A	341	THR
1	A	344	CYS
1	A	349	CYS
1	A	353	THR
1	A	359	ASN
1	A	360	GLN
1	A	361	MET
1	A	380	ASN
1	A	384	ILE
1	A	396	LEU
1	A	400	LYS
1	A	402	ILE
1	A	431	LYS
1	A	436	LYS
1	A	441	THR
1	A	445	LEU
1	A	446	THR
1	A	458	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	467	ARG
1	A	473	SER
1	A	478	LEU
1	A	484	THR
1	A	486	GLU
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
1	A	521	VAL
1	A	523	ASP
1	A	528	VAL
1	A	530	VAL
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	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	623	MET
1	A	628	ASN
1	A	635	ILE
1	A	644	GLU
1	A	646	GLU
1	A	663	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	665	GLU
1	A	668	GLU
1	A	682	SER
1	A	688	VAL
1	A	691	LEU
1	A	703	ASP
1	A	705	VAL
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	788	ILE
1	A	809	PHE
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	849	VAL
1	A	865	VAL
1	A	874	MET
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	968	LEU
1	A	981	ASP
1	A	991	TYR
1	A	992	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	111	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	114	ASN
1	A	177	GLN
1	A	190	HIS
1	A	201	ASN
1	A	202	GLN
1	A	275	ASN
1	A	359	ASN
1	A	360	GLN
1	A	380	ASN
1	A	398	ASN
1	A	456	ASN
1	A	510	ASN
1	A	526	ASN
1	A	628	ASN
1	A	739	ASN
1	A	759	GLN
1	A	911	ASN
1	A	914	ASN
1	A	920	GLN
1	A	930	ASN
1	A	944	HIS

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 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	28,29,29	1.54	5 (17%)	29,48,48	1.57	6 (20%)
4	ADP	A	1002	2	28,29,29	1.77	3 (10%)	43,45,45	1.49	9 (20%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CZA	A	1001	2	-	2/4/52/52	0/5/5/5
4	ADP	A	1002	2	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ADP	PA-O3A	-6.65	1.52	1.59
3	A	1001	CZA	C4-N1	-3.91	1.35	1.39
3	A	1001	CZA	C12-C8	3.19	1.58	1.53
4	A	1002	ADP	PB-O1B	2.54	1.58	1.50
3	A	1001	CZA	O3-C4	2.22	1.37	1.31
3	A	1001	CZA	C3-C4	-2.22	1.36	1.40
4	A	1002	ADP	C8-N9	2.16	1.41	1.37
3	A	1001	CZA	C9-N1	-2.15	1.46	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	CZA	C18-C17-N2	3.84	136.89	130.74
4	A	1002	ADP	O3A-PA-O1A	-3.56	99.99	110.70
4	A	1002	ADP	O3B-PB-O3A	3.52	116.44	104.64
3	A	1001	CZA	C17-N2-C16	3.30	112.01	109.08
3	A	1001	CZA	C17-C14-C15	3.26	111.29	107.59
3	A	1001	CZA	C14-C17-N2	-2.92	102.41	106.88
3	A	1001	CZA	C15-C16-N2	-2.62	108.19	110.31
4	A	1002	ADP	O2'-C2'-C3'	-2.48	103.87	111.82
4	A	1002	ADP	C2-N1-C6	-2.35	114.88	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	O2A-PA-O3A	2.18	113.17	107.27
3	A	1001	CZA	O1-C2-C3	2.10	124.14	120.43
4	A	1002	ADP	O2A-PA-O1A	2.09	122.15	112.44
4	A	1002	ADP	N3-C4-N9	2.07	130.69	127.17
4	A	1002	ADP	N9-C8-N7	-2.04	111.04	113.94
4	A	1002	ADP	O3A-PB-O1B	-2.02	100.41	111.04

There are no chirality outliers.

All (6) torsion outliers are listed below:

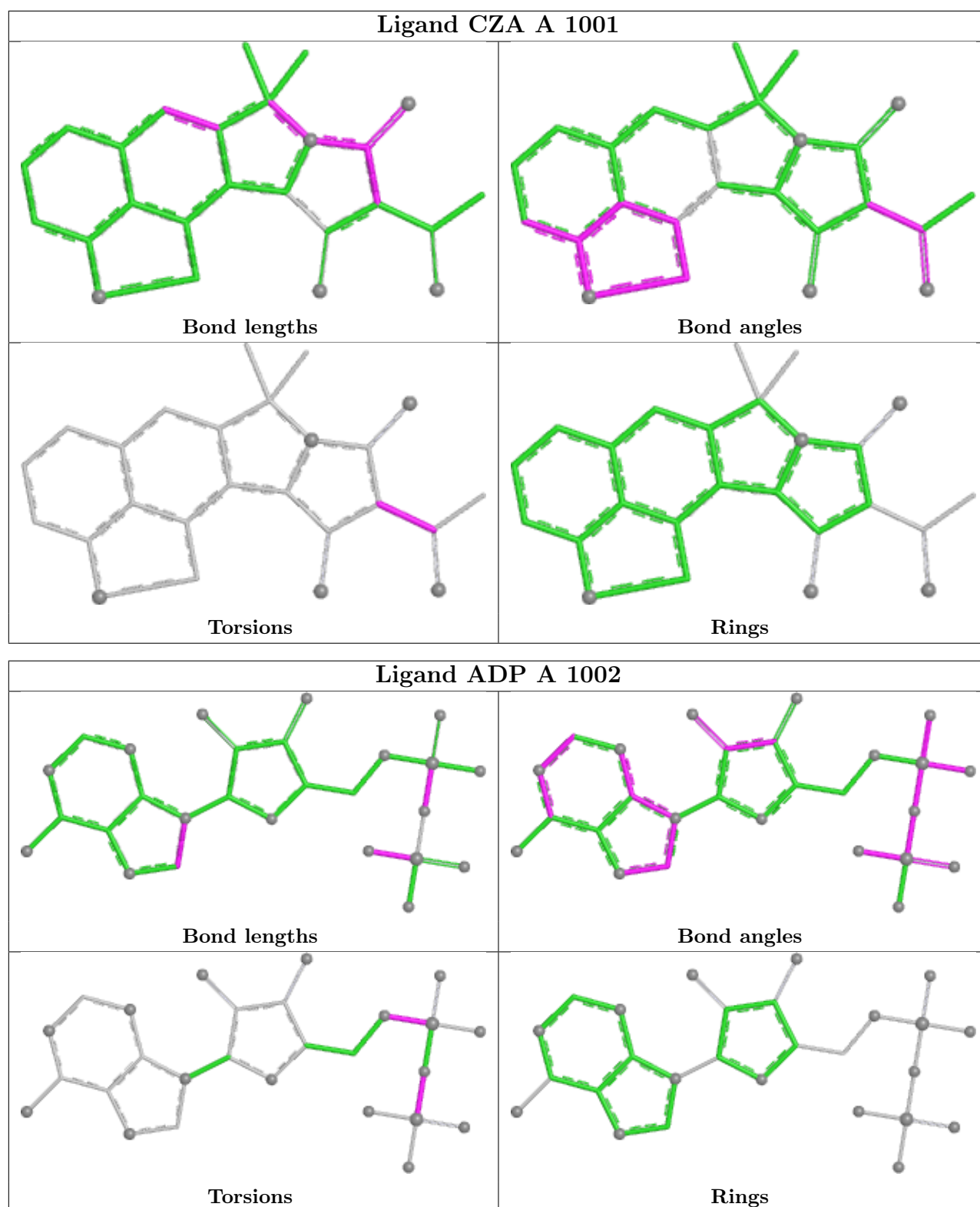
Mol	Chain	Res	Type	Atoms
4	A	1002	ADP	PA-O3A-PB-O2B
4	A	1002	ADP	C5'-O5'-PA-O1A
4	A	1002	ADP	C5'-O5'-PA-O3A
3	A	1001	CZA	O1-C2-C3-C6
3	A	1001	CZA	C1-C2-C3-C6
4	A	1002	ADP	PA-O3A-PB-O1B

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

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.02	17 (1%) 69 49	56, 115, 268, 410	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	863	PRO	7.0
1	A	865	VAL	3.9
1	A	580	ASP	3.6
1	A	498	CYS	3.2
1	A	853	ALA	2.9
1	A	986	PHE	2.7
1	A	2	GLU	2.7
1	A	786	ALA	2.6
1	A	587	TYR	2.5
1	A	868	HIS	2.4
1	A	956	ILE	2.3
1	A	656	ARG	2.3
1	A	881	PRO	2.2
1	A	576	MET	2.2
1	A	918	GLU	2.2
1	A	660	ASP	2.1
1	A	439	GLU	2.1

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](#)

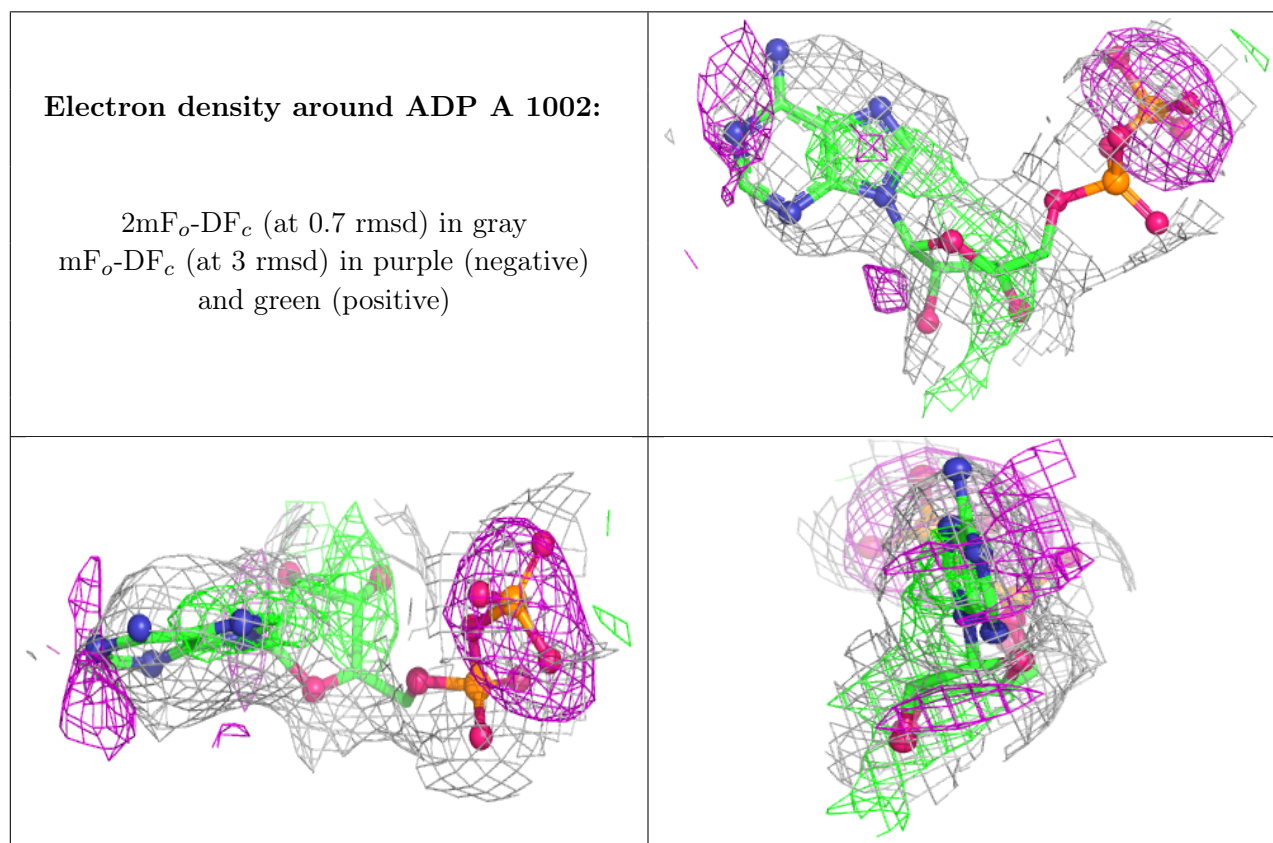
There are no oligosaccharides in this entry.

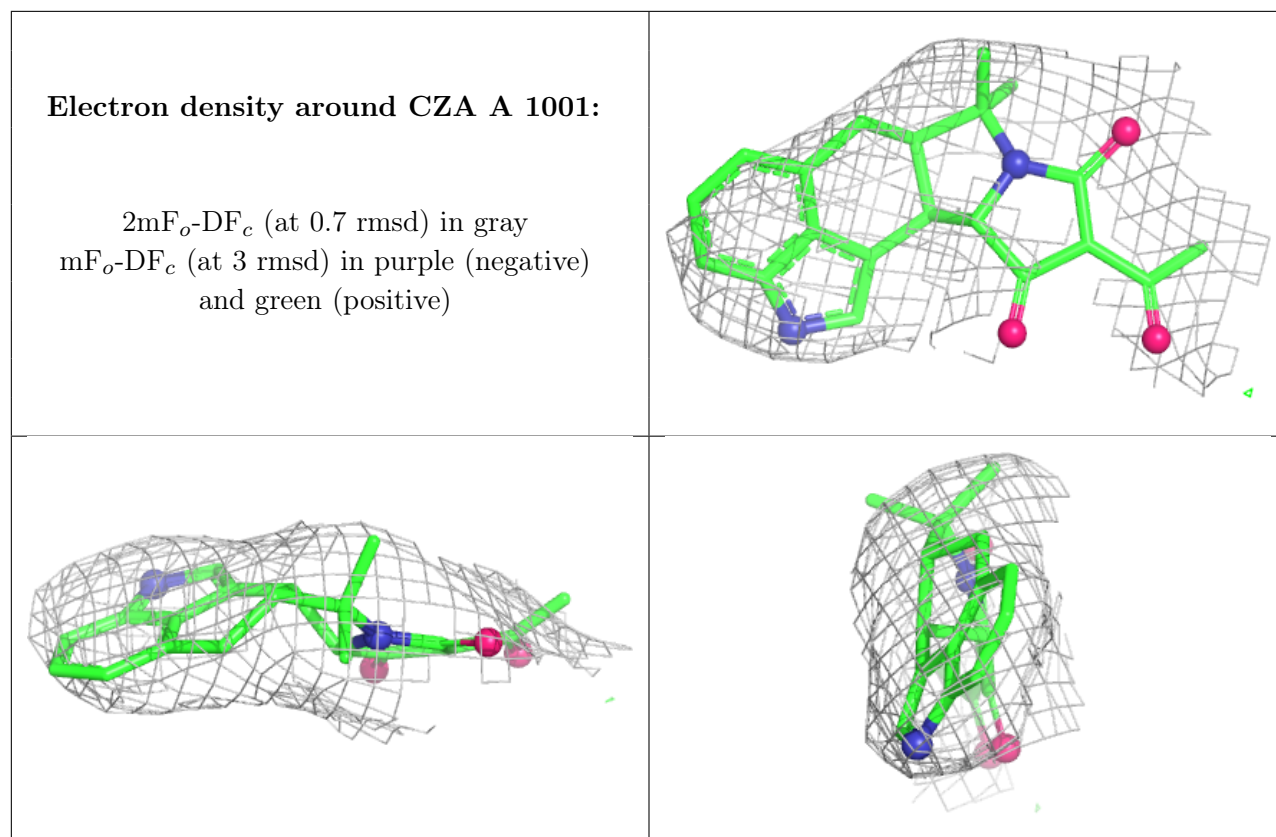
6.4 Ligands [i](#)

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
2	MG	A	995	1/1	0.70	0.16	61,61,61,61	0
4	ADP	A	1002	27/27	0.80	0.16	110,110,110,110	0
2	MG	A	996	1/1	0.86	0.12	117,117,117,117	0
3	CZA	A	1001	25/25	0.95	0.11	154,154,154,154	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.