Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:48 AM GMT

PDB ID	:	2OA0
Title	:	Crystal structure of Calcium ATPase with bound ADP and cyclopiazonic acid
Authors	:	Young, H.S.; Moncoq, K.A.
Deposited on	:	2006-12-14
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references (i)) 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
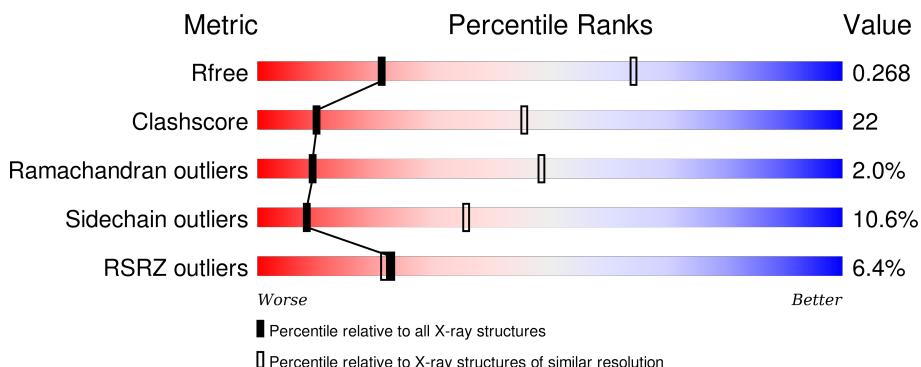
1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
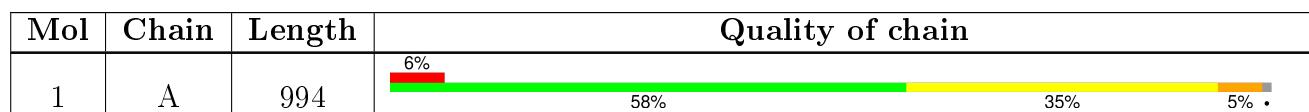
The reported resolution of this entry is 3.40 Å.

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	Percentile Ranks	Value
Rfree		0.268
Clashscore		22
Ramachandran outliers		2.0%
Sidechain outliers		10.6%
RSRZ outliers		6.4%

Worse　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
⫞ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 <=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	6% / 58% / 35% / 5% ·

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
3	CZA	A	1001	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7615 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	980	7562	4806	1270	1430	56	0	0	0
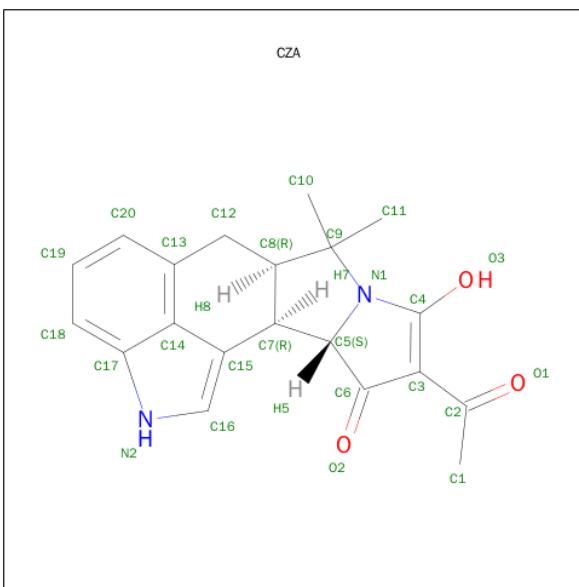
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	variant	UNP P04191

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).
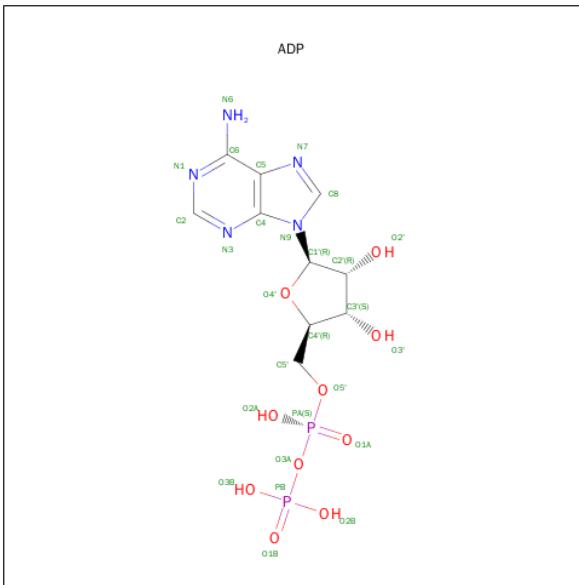
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is (6AR,11AS,11BR)-10-ACETYL-9-HYDROXY-7,7-DIMETHYL-2,6,6A,7,11 A,11B-HEXAHYDRO-11H-PYRROLO[1',2':2,3]ISOINDOLO[4,5,6-CD]INDOL-11-ONE (three-letter code: CZA) (formula: $C_{20}H_{20}N_2O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	20	2	3		
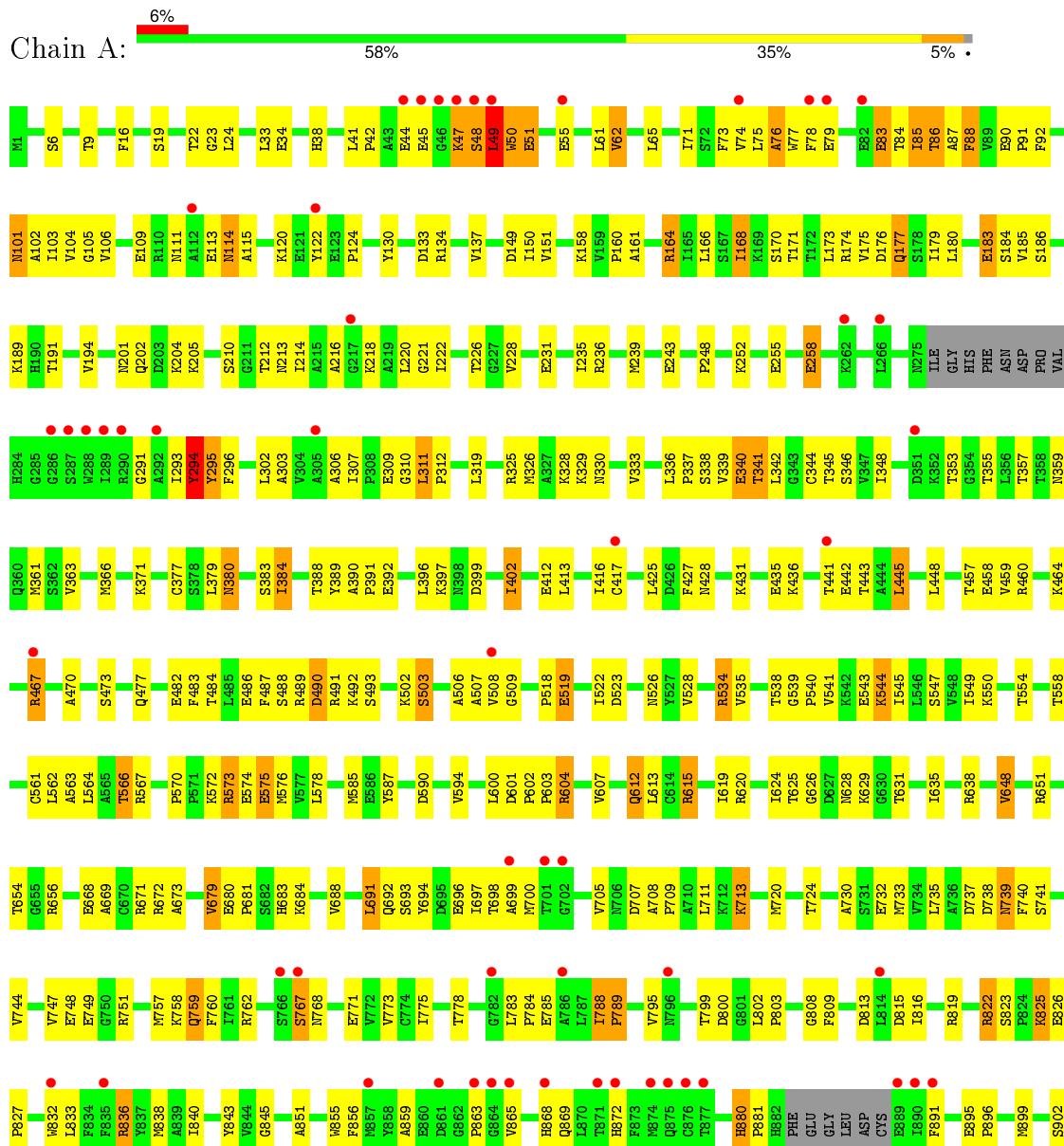
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
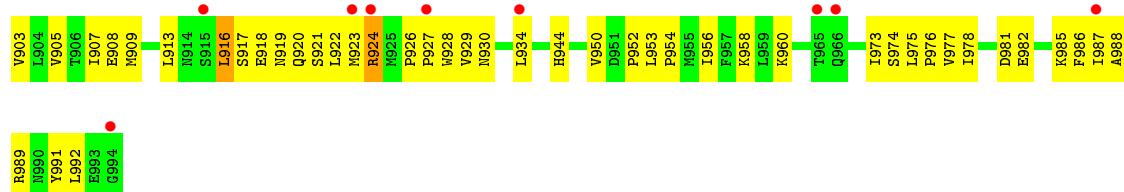
3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.50Å 96.84Å 154.86Å 90.00° 94.83° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.78 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.40) 99.5 (29.78-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.290 , 0.328 0.264 , 0.268	Depositor DCC
R_{free} test set	1293 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	127.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 25372 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7615	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.38	0/7697	0.56	2/10432 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	THR	N-CA-C	5.15	124.91	111.00
1	A	87	ALA	N-CA-C	5.14	124.87	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	GLU	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	7562	0	7670	336	0
2	A	1	0	0	0	0
3	A	25	0	20	13	0
4	A	27	0	12	1	0
All	All	7615	0	7702	336	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 22.

All (336) 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:924:ARG:HB2	1:A:924:ARG:HH21	1.05	1.13
1:A:573:ARG:HG3	1:A:573:ARG:HH21	0.97	1.06
1:A:62:VAL:HG11	3:A:1001:CZA:H13	1.06	1.05
1:A:615:ARG:HG2	1:A:615:ARG:HH11	1.17	1.04
1:A:924:ARG:HB2	1:A:924:ARG:NH2	1.75	1.02
1:A:201:ASN:HD21	1:A:231:GLU:HG2	1.27	1.00
1:A:291:GLY:O	1:A:294:TYR:HD2	1.43	0.99
1:A:759:GLN:NE2	1:A:759:GLN:HA	1.72	0.98
1:A:62:VAL:HG11	3:A:1001:CZA:C1	1.96	0.96
1:A:575:GLU:HA	1:A:575:GLU:OE2	1.64	0.96
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.45	0.96
1:A:114:ASN:N	1:A:114:ASN:HD22	1.65	0.95
1:A:573:ARG:HH21	1:A:573:ARG:CG	1.80	0.94
1:A:573:ARG:HG3	1:A:573:ARG:NH2	1.78	0.93
1:A:114:ASN:HD22	1:A:114:ASN:H	1.17	0.92
1:A:328:LYS:HA	1:A:328:LYS:HE2	1.55	0.88
1:A:615:ARG:HG2	1:A:615:ARG:NH1	1.77	0.87
1:A:631:THR:O	1:A:635:ILE:HG12	1.74	0.87
1:A:502:LYS:HG3	1:A:503:SER:H	1.40	0.87
1:A:558:THR:HB	1:A:635:ILE:HD13	1.59	0.85
1:A:615:ARG:CG	1:A:615:ARG:HH11	1.90	0.84
1:A:47:LYS:C	1:A:47:LYS:HD3	1.96	0.84
1:A:291:GLY:O	1:A:294:TYR:CD2	2.31	0.83
1:A:759:GLN:HE21	1:A:759:GLN:HA	1.41	0.81
1:A:836:ARG:HB2	1:A:836:ARG:HH21	1.45	0.81
1:A:90:GLU:HG2	1:A:91:PRO:HD3	1.63	0.80
1:A:311:LEU:HB3	1:A:312:PRO:CD	2.11	0.79
1:A:744:VAL:O	1:A:747:VAL:HG12	1.83	0.78
1:A:62:VAL:CG1	3:A:1001:CZA:H13	2.02	0.78
1:A:201:ASN:ND2	1:A:231:GLU:HG2	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HB2	1:A:585:MET:HG3	1.65	0.76
1:A:916:LEU:HD21	1:A:930:ASN:HB2	1.68	0.76
1:A:795:VAL:HA	1:A:799:THR:HB	1.66	0.75
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.69	0.74
1:A:312:PRO:HG3	3:A:1001:CZA:H112	1.67	0.74
1:A:114:ASN:ND2	1:A:114:ASN:H	1.85	0.73
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.70	0.73
1:A:836:ARG:HH21	1:A:836:ARG:CB	2.01	0.72
1:A:978:ILE:O	1:A:982:GLU:HG2	1.89	0.72
1:A:114:ASN:N	1:A:114:ASN:ND2	2.36	0.72
1:A:902:SER:HA	1:A:944:HIS:HE1	1.54	0.72
1:A:47:LYS:O	1:A:48:SER:HB3	1.88	0.71
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.72	0.71
1:A:75:LEU:HD22	1:A:293:ILE:HG23	1.70	0.71
1:A:550:LYS:O	1:A:554:THR:HG22	1.90	0.71
1:A:489:ARG:NH1	1:A:489:ARG:HG3	2.04	0.71
1:A:235:ILE:HG23	1:A:709:PRO:HG3	1.73	0.70
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.21	0.70
1:A:201:ASN:HD21	1:A:231:GLU:CG	2.05	0.69
1:A:47:LYS:HD3	1:A:48:SER:N	2.07	0.69
1:A:357:THR:HG22	1:A:603:PRO:HA	1.74	0.69
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.75	0.69
1:A:574:GLU:HG2	1:A:574:GLU:O	1.91	0.69
1:A:175:VAL:HG12	1:A:212:THR:CG2	2.23	0.69
1:A:102:ALA:HA	3:A:1001:CZA:O1	1.92	0.69
1:A:73:PHE:CE2	1:A:91:PRO:HB2	2.29	0.68
1:A:248:PRO:HD2	1:A:340:GLU:OE2	1.93	0.68
1:A:42:PRO:HG2	1:A:236:ARG:CZ	2.23	0.67
1:A:823:SER:OG	1:A:825:LYS:HG3	1.94	0.67
1:A:783:LEU:HB3	1:A:784:PRO:CD	2.25	0.67
1:A:669:ALA:O	1:A:673:ALA:HB2	1.96	0.66
1:A:692:GLN:C	1:A:694:TYR:H	1.99	0.65
1:A:507:ALA:C	1:A:509:GLY:H	1.98	0.65
1:A:902:SER:HA	1:A:944:HIS:CE1	2.31	0.65
1:A:880:HIS:N	1:A:881:PRO:HD2	2.11	0.65
1:A:102:ALA:HB2	3:A:1001:CZA:H11	1.78	0.65
1:A:180:LEU:HA	1:A:705:VAL:HG22	1.79	0.65
1:A:397:LYS:HB3	1:A:402:ILE:HG21	1.79	0.64
1:A:183:GLU:O	1:A:185:VAL:N	2.30	0.64
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.78	0.64
1:A:950:VAL:O	1:A:954:PRO:HD2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLY:O	1:A:543:GLU:HG2	1.97	0.64
1:A:489:ARG:HG3	1:A:489:ARG:HH11	1.63	0.63
1:A:62:VAL:HG22	3:A:1001:CZA:H7	1.81	0.63
1:A:624:ILE:HD12	1:A:684:LYS:HE2	1.80	0.63
1:A:604:ARG:O	1:A:607:VAL:HG22	1.99	0.62
1:A:161:ALA:CA	1:A:210:SER:HB2	2.29	0.62
1:A:759:GLN:NE2	1:A:759:GLN:CA	2.58	0.62
1:A:255:GLU:HA	1:A:258:GLU:CG	2.30	0.61
1:A:985:LYS:O	1:A:989:ARG:HB2	2.01	0.61
1:A:688:VAL:HG11	1:A:713:LYS:HB3	1.83	0.61
1:A:856:PHE:HZ	1:A:891:PHE:HA	1.65	0.61
1:A:33:LEU:HD11	1:A:38:HIS:CE1	2.36	0.61
1:A:975:LEU:N	1:A:976:PRO:HD2	2.15	0.61
1:A:344:CYS:SG	1:A:822:ARG:NH1	2.75	0.60
1:A:380:ASN:HD21	1:A:397:LYS:HE3	1.67	0.60
1:A:255:GLU:HA	1:A:258:GLU:HG2	1.85	0.59
1:A:49:LEU:HD12	1:A:50:TRP:CE3	2.38	0.59
1:A:179:ILE:HG13	1:A:180:LEU:H	1.67	0.59
1:A:161:ALA:HA	1:A:210:SER:HB2	1.84	0.58
1:A:759:GLN:HE21	1:A:759:GLN:CA	2.16	0.58
1:A:175:VAL:HG12	1:A:212:THR:HG22	1.86	0.58
1:A:952:PRO:O	1:A:956:ILE:HG13	2.04	0.58
1:A:366:MET:CE	1:A:448:LEU:HD11	2.33	0.58
1:A:735:LEU:HD13	1:A:739:ASN:O	2.03	0.58
1:A:880:HIS:H	1:A:881:PRO:HD2	1.66	0.58
1:A:174:ARG:HB2	1:A:216:ALA:HB3	1.86	0.58
1:A:924:ARG:CB	1:A:924:ARG:HH21	1.97	0.58
1:A:47:LYS:C	1:A:47:LYS:CD	2.69	0.58
1:A:762:ARG:HH11	1:A:833:LEU:HD21	1.69	0.57
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.03	0.57
1:A:22:THR:OG1	1:A:23:GLY:N	2.36	0.57
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.86	0.57
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.87	0.57
1:A:483:PHE:CE2	1:A:578:LEU:HD21	2.39	0.57
1:A:303:ALA:O	1:A:307:ILE:HG12	2.05	0.56
1:A:201:ASN:HA	1:A:204:LYS:HD2	1.87	0.56
1:A:248:PRO:HB2	1:A:822:ARG:HH22	1.71	0.56
1:A:757:MET:HA	1:A:760:PHE:CE2	2.40	0.56
1:A:417:CYS:SG	1:A:445:LEU:HG	2.45	0.56
1:A:390:ALA:C	1:A:392:GLU:H	2.08	0.56
1:A:502:LYS:HG3	1:A:503:SER:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.88	0.55
1:A:76:ALA:HB3	1:A:88:PHE:CZ	2.42	0.55
1:A:326:MET:CE	1:A:333:VAL:HG21	2.37	0.55
1:A:539:GLY:N	1:A:540:PRO:HD2	2.21	0.55
1:A:921:SER:HB2	1:A:989:ARG:HH22	1.72	0.55
1:A:71:ILE:O	1:A:75:LEU:HG	2.06	0.55
1:A:739:ASN:HD22	1:A:741:SER:H	1.53	0.55
1:A:73:PHE:HE2	1:A:91:PRO:HB2	1.72	0.55
1:A:49:LEU:HD12	1:A:50:TRP:HE3	1.72	0.55
1:A:346:SER:OG	1:A:696:GLU:HG2	2.07	0.55
1:A:487:PHE:HA	1:A:493:SER:O	2.07	0.55
1:A:534:ARG:HG2	1:A:535:VAL:N	2.21	0.54
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.88	0.54
1:A:856:PHE:CZ	1:A:891:PHE:HA	2.42	0.54
1:A:672:ARG:CZ	1:A:672:ARG:HB2	2.37	0.54
1:A:325:ARG:HD2	1:A:749:GLU:OE2	2.08	0.54
1:A:762:ARG:NH1	1:A:833:LEU:HD21	2.22	0.54
1:A:338:SER:HA	1:A:341:THR:CG2	2.37	0.54
1:A:918:GLU:HG2	1:A:919:ASN:HD22	1.72	0.54
1:A:175:VAL:HG12	1:A:212:THR:HG21	1.89	0.54
1:A:575:GLU:OE2	1:A:575:GLU:CA	2.46	0.54
1:A:692:GLN:C	1:A:694:TYR:N	2.60	0.54
1:A:83:GLU:HB3	1:A:85:ILE:HG13	1.89	0.54
1:A:294:TYR:CG	1:A:295:TYR:N	2.75	0.53
1:A:175:VAL:HG21	1:A:189:LYS:HE3	1.90	0.53
1:A:168:ILE:CG2	1:A:173:LEU:HB2	2.39	0.53
1:A:366:MET:HE1	1:A:448:LEU:HD11	1.90	0.53
1:A:986:PHE:HD1	1:A:989:ARG:CZ	2.22	0.52
1:A:880:HIS:N	1:A:881:PRO:CD	2.73	0.52
1:A:73:PHE:CD2	1:A:91:PRO:HB2	2.44	0.52
1:A:916:LEU:HD21	1:A:930:ASN:CB	2.37	0.52
1:A:311:LEU:HB3	1:A:312:PRO:HD2	1.90	0.52
1:A:836:ARG:NH2	1:A:836:ARG:CB	2.72	0.52
1:A:671:ARG:HD2	1:A:694:TYR:CE1	2.44	0.52
1:A:6:SER:HA	1:A:194:VAL:O	2.08	0.52
1:A:319:LEU:HG	1:A:339:VAL:HG21	1.92	0.52
1:A:124:PRO:HB3	1:A:158:LYS:HD2	1.90	0.52
1:A:130:TYR:CZ	1:A:137:VAL:HB	2.44	0.52
1:A:648:VAL:HA	1:A:651:ARG:HG3	1.92	0.52
1:A:312:PRO:CG	3:A:1001:CZA:H112	2.38	0.51
1:A:795:VAL:HA	1:A:799:THR:CB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:SER:C	1:A:976:PRO:HD2	2.30	0.51
1:A:235:ILE:O	1:A:239:MET:HG3	2.11	0.51
1:A:65:LEU:HD12	3:A:1001:CZA:C10	2.41	0.51
1:A:507:ALA:O	1:A:509:GLY:N	2.42	0.51
1:A:214:ILE:HG22	1:A:216:ALA:O	2.11	0.51
1:A:528:VAL:HG21	1:A:541:VAL:HG11	1.91	0.51
1:A:558:THR:HB	1:A:635:ILE:CD1	2.38	0.51
1:A:758:LYS:HG2	1:A:762:ARG:CZ	2.41	0.51
1:A:757:MET:HG2	1:A:760:PHE:CE2	2.46	0.51
1:A:895:GLU:N	1:A:896:PRO:HD2	2.25	0.51
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.91	0.51
1:A:836:ARG:O	1:A:840:ILE:HG12	2.11	0.50
1:A:361:MET:HA	1:A:600:LEU:O	2.12	0.50
1:A:170:SER:OG	1:A:218:LYS:N	2.42	0.50
1:A:47:LYS:O	1:A:48:SER:CB	2.57	0.50
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.93	0.50
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.93	0.50
1:A:561:CYS:C	1:A:562:LEU:HD12	2.31	0.50
1:A:576:MET:HE3	1:A:587:TYR:HB3	1.93	0.50
1:A:688:VAL:HG23	1:A:700:MET:HE3	1.94	0.50
1:A:708:ALA:N	1:A:709:PRO:CD	2.74	0.50
1:A:345:THR:HB	1:A:747:VAL:CG2	2.41	0.50
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.93	0.50
1:A:179:ILE:HG13	1:A:180:LEU:N	2.27	0.49
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.93	0.49
1:A:688:VAL:HG23	1:A:700:MET:CE	2.42	0.49
1:A:357:THR:HG22	1:A:603:PRO:CA	2.42	0.49
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.94	0.49
1:A:905:VAL:O	1:A:909:MET:HG2	2.13	0.49
1:A:757:MET:HG2	1:A:760:PHE:HE2	1.78	0.48
1:A:899:MET:O	1:A:903:VAL:HG23	2.14	0.48
1:A:16:PHE:CD2	1:A:222:ILE:HD11	2.48	0.48
1:A:563:ALA:O	1:A:564:LEU:HD23	2.13	0.48
1:A:377:CYS:SG	1:A:541:VAL:HA	2.53	0.48
1:A:428:ASN:HB2	1:A:435:GLU:HG2	1.95	0.48
1:A:164:ARG:NH2	1:A:191:THR:O	2.45	0.48
1:A:491:ARG:CB	1:A:585:MET:HG3	2.40	0.48
1:A:65:LEU:HD11	1:A:307:ILE:HG21	1.96	0.48
1:A:467:ARG:HA	1:A:470:ALA:HB2	1.94	0.48
1:A:856:PHE:HE1	1:A:896:PRO:HG3	1.79	0.47
1:A:326:MET:HE1	1:A:333:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.97	0.47
1:A:84:THR:HG23	1:A:84:THR:O	2.14	0.47
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.96	0.47
1:A:319:LEU:HG	1:A:339:VAL:CG2	2.44	0.47
1:A:427:PHE:CD2	1:A:464:LYS:HB3	2.49	0.47
1:A:921:SER:HB3	1:A:924:ARG:NH2	2.29	0.47
1:A:518:PRO:O	1:A:522:ILE:HG13	2.15	0.47
1:A:775:ILE:HA	1:A:778:THR:HG22	1.96	0.47
1:A:457:THR:O	1:A:459:VAL:HG13	2.14	0.47
1:A:19:SER:HB3	1:A:22:THR:OG1	2.15	0.47
1:A:767:SER:O	1:A:771:GLU:HG3	2.14	0.47
1:A:489:ARG:O	1:A:492:LYS:HD2	2.15	0.47
1:A:672:ARG:NH1	1:A:672:ARG:CB	2.78	0.47
1:A:809:PHE:HD2	1:A:809:PHE:N	2.13	0.47
1:A:679:VAL:HG22	1:A:683:HIS:CG	2.51	0.46
1:A:294:TYR:O	1:A:296:PHE:N	2.48	0.46
1:A:175:VAL:HG12	1:A:176:ASP:H	1.81	0.46
1:A:921:SER:HB3	1:A:924:ARG:HH22	1.81	0.46
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.46	0.46
1:A:545:ILE:O	1:A:549:ILE:HG13	2.16	0.46
1:A:808:GLY:C	1:A:809:PHE:HD2	2.19	0.46
1:A:41:LEU:HD23	1:A:236:ARG:HG3	1.98	0.46
1:A:338:SER:O	1:A:342:LEU:HB2	2.16	0.46
1:A:177:GLN:H	1:A:177:GLN:HG2	1.65	0.46
1:A:526:ASN:HD22	1:A:590:ASP:HA	1.80	0.46
1:A:809:PHE:N	1:A:809:PHE:CD2	2.83	0.46
1:A:679:VAL:HG22	1:A:683:HIS:ND1	2.30	0.46
1:A:78:PHE:CG	1:A:79:GLU:N	2.83	0.46
1:A:101:ASN:OD1	3:A:1001:CZA:H111	2.16	0.46
1:A:345:THR:HA	1:A:697:ILE:HG22	1.97	0.46
1:A:436:LYS:HB2	1:A:443:THR:HG21	1.98	0.45
1:A:800:ASP:C	1:A:803:PRO:HD2	2.36	0.45
1:A:248:PRO:CB	1:A:822:ARG:HH12	2.29	0.45
1:A:212:THR:HG22	1:A:213:ASN:N	2.31	0.45
1:A:42:PRO:O	1:A:120:LYS:NZ	2.49	0.45
1:A:115:ALA:HB2	1:A:730:ALA:HA	1.98	0.45
1:A:600:LEU:HG	1:A:601:ASP:N	2.31	0.45
1:A:329:LYS:O	1:A:330:ASN:HB2	2.17	0.45
1:A:489:ARG:HH11	1:A:489:ARG:CG	2.25	0.45
1:A:917:SER:OG	1:A:920:GLN:HB2	2.17	0.45
1:A:502:LYS:CG	1:A:503:SER:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PRO:HA	1:A:563:ALA:HB2	1.99	0.44
1:A:33:LEU:HD23	1:A:33:LEU:O	2.17	0.44
1:A:428:ASN:HB2	1:A:435:GLU:CG	2.47	0.44
1:A:519:GLU:OE1	1:A:519:GLU:HA	2.18	0.44
1:A:851:ALA:HB2	1:A:973:ILE:HG21	1.99	0.44
1:A:309:GLU:HA	3:A:1001:CZA:H113	1.98	0.44
1:A:388:THR:HG23	1:A:390:ALA:H	1.83	0.44
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.98	0.44
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.95	0.44
1:A:868:HIS:O	1:A:869:GLN:C	2.56	0.44
1:A:612:GLN:HA	1:A:615:ARG:HD2	1.99	0.44
1:A:880:HIS:ND1	1:A:881:PRO:HD3	2.33	0.44
1:A:255:GLU:HA	1:A:258:GLU:HG3	1.97	0.44
1:A:625:THR:OG1	1:A:626:GLY:N	2.50	0.44
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.88	0.44
1:A:161:ALA:HB1	1:A:226:THR:HG22	2.00	0.44
1:A:612:GLN:O	1:A:615:ARG:HB2	2.18	0.44
1:A:71:ILE:HA	1:A:74:VAL:HG12	1.99	0.44
1:A:507:ALA:C	1:A:509:GLY:N	2.67	0.44
1:A:707:ASP:O	1:A:711:LEU:HG	2.18	0.43
1:A:492:LYS:NZ	4:A:1002:ADP:H2	2.16	0.43
1:A:953:LEU:HB2	1:A:954:PRO:CD	2.47	0.43
1:A:161:ALA:C	1:A:210:SER:HB2	2.38	0.43
1:A:412:GLU:OE1	1:A:594:VAL:HG21	2.18	0.43
1:A:833:LEU:HD12	1:A:836:ARG:HG2	2.00	0.43
1:A:783:LEU:CB	1:A:784:PRO:CD	2.95	0.43
1:A:672:ARG:NH1	1:A:672:ARG:HB2	2.32	0.43
1:A:336:LEU:HB2	1:A:337:PRO:HD3	2.00	0.43
1:A:720:MET:HE1	1:A:738:ASP:O	2.19	0.43
1:A:988:ALA:HA	1:A:992:LEU:HB2	2.01	0.43
1:A:65:LEU:HD12	3:A:1001:CZA:H103	2.00	0.43
1:A:692:GLN:O	1:A:694:TYR:N	2.51	0.43
1:A:975:LEU:HD23	1:A:975:LEU:C	2.38	0.43
1:A:24:LEU:HG	1:A:149:ASP:HA	2.01	0.43
1:A:51:GLU:O	1:A:55:GLU:HG3	2.19	0.43
1:A:357:THR:HB	1:A:602:PRO:O	2.19	0.43
1:A:987:ILE:C	1:A:989:ARG:N	2.72	0.43
1:A:388:THR:HG23	1:A:390:ALA:HB3	2.01	0.43
1:A:104:VAL:CG1	1:A:104:VAL:O	2.66	0.43
1:A:310:GLY:O	1:A:311:LEU:C	2.57	0.42
1:A:822:ARG:O	1:A:822:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:HD21	1:A:397:LYS:CE	2.32	0.42
1:A:109:GLU:O	1:A:111:ASN:ND2	2.52	0.42
1:A:629:LYS:HB2	1:A:654:THR:CG2	2.49	0.42
1:A:573:ARG:NH2	1:A:573:ARG:CG	2.49	0.42
1:A:294:TYR:C	1:A:296:PHE:H	2.23	0.42
1:A:488:SER:C	1:A:490:ASP:N	2.71	0.42
1:A:442:GLU:O	1:A:445:LEU:HB2	2.20	0.42
1:A:458:GLU:OE2	1:A:460:ARG:HG2	2.20	0.42
1:A:558:THR:CB	1:A:635:ILE:HD13	2.37	0.42
1:A:122:TYR:CE1	1:A:179:ILE:HG22	2.54	0.42
1:A:85:ILE:HD12	1:A:85:ILE:H	1.84	0.42
1:A:379:LEU:HG	1:A:544:LYS:HD3	2.01	0.42
1:A:672:ARG:HH11	1:A:672:ARG:HB3	1.84	0.42
1:A:506:ALA:O	1:A:507:ALA:HB2	2.20	0.42
1:A:312:PRO:HG3	3:A:1001:CZA:C11	2.43	0.42
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.46	0.42
1:A:333:VAL:HG22	1:A:733:MET:HG3	2.02	0.42
1:A:348:ILE:HG12	1:A:699:ALA:HB3	2.02	0.42
1:A:826:GLU:HA	1:A:827:PRO:HD3	1.81	0.42
1:A:601:ASP:HA	1:A:602:PRO:HD2	1.85	0.41
1:A:357:THR:HA	1:A:603:PRO:HA	2.02	0.41
1:A:802:LEU:N	1:A:803:PRO:CD	2.83	0.41
1:A:105:GLY:HA2	1:A:109:GLU:HG3	2.02	0.41
1:A:137:VAL:HG22	1:A:137:VAL:O	2.19	0.41
1:A:491:ARG:HG3	1:A:493:SER:OG	2.20	0.41
1:A:88:PHE:HA	1:A:88:PHE:HD2	1.69	0.41
1:A:124:PRO:HG3	1:A:160:PRO:HA	2.02	0.41
1:A:680:GLU:HG3	1:A:681:PRO:HD2	2.01	0.41
1:A:168:ILE:HG21	1:A:173:LEU:HB2	2.02	0.41
1:A:105:GLY:C	1:A:109:GLU:HB2	2.40	0.41
1:A:383:SER:C	1:A:384:ILE:HD13	2.40	0.41
1:A:773:VAL:HG12	1:A:845:GLY:HA3	2.02	0.41
1:A:604:ARG:HH11	1:A:604:ARG:HG3	1.84	0.41
1:A:748:GLU:O	1:A:751:ARG:HB2	2.20	0.41
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.91	0.41
1:A:825:LYS:HE2	1:A:825:LYS:HB2	1.86	0.41
1:A:926:PRO:O	1:A:929:VAL:HG23	2.21	0.41
1:A:800:ASP:OD1	1:A:908:GLU:HG3	2.20	0.41
1:A:924:ARG:NH2	1:A:989:ARG:HH12	2.19	0.41
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.86	0.41
1:A:832:TRP:CD1	1:A:988:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HA	1:A:255:GLU:HG2	2.03	0.41
1:A:76:ALA:HB1	1:A:77:TRP:CE3	2.56	0.41
1:A:813:ASP:HB3	1:A:815:ASP:OD1	2.20	0.41
1:A:390:ALA:C	1:A:392:GLU:N	2.73	0.41
1:A:488:SER:O	1:A:490:ASP:N	2.54	0.41
1:A:306:ALA:HA	1:A:768:ASN:HB3	2.03	0.41
1:A:133:ASP:O	1:A:134:ARG:HD3	2.21	0.41
1:A:907:ILE:HG23	1:A:977:VAL:HG11	2.03	0.40
1:A:166:LEU:HG	1:A:221:GLY:HA2	2.03	0.40
1:A:175:VAL:O	1:A:186:SER:HB2	2.21	0.40
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.57	0.40
1:A:737:ASP:O	1:A:738:ASP:HB2	2.21	0.40
1:A:85:ILE:HD12	1:A:85:ILE:N	2.36	0.40
1:A:470:ALA:O	1:A:473:SER:HB2	2.21	0.40
1:A:473:SER:O	1:A:477:GLN:HG2	2.21	0.40
1:A:363:VAL:HG12	1:A:384:ILE:HG13	2.04	0.40
1:A:691:LEU:HD23	1:A:698:THR:HG21	2.03	0.40
1:A:651:ARG:HH21	1:A:651:ARG:HG3	1.87	0.40
1:A:150:ILE:CG2	1:A:220:LEU:HD11	2.51	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	974/994 (98%)	856 (88%)	99 (10%)	19 (2%)	9	48

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	85	ILE

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Mol	Chain	Res	Type
1	A	184	SER
1	A	295	TYR
1	A	508	VAL
1	A	76	ALA
1	A	482	GLU
1	A	503	SER
1	A	648	VAL
1	A	693	SER
1	A	311	LEU
1	A	916	LEU
1	A	49	LEU
1	A	86	THR
1	A	294	TYR
1	A	391	PRO
1	A	863	PRO
1	A	789	PRO
1	A	106	VAL

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	828/840 (99%)	740 (89%)	88 (11%)	8	36

All (88) 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

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Mol	Chain	Res	Type
1	A	62	VAL
1	A	88	PHE
1	A	92	PHE
1	A	101	ASN
1	A	103	ILE
1	A	113	GLU
1	A	114	ASN
1	A	151	VAL
1	A	164	ARG
1	A	168	ILE
1	A	171	THR
1	A	177	GLN
1	A	183	GLU
1	A	202	GLN
1	A	205	LYS
1	A	228	VAL
1	A	243	GLU
1	A	258	GLU
1	A	294	TYR
1	A	302	LEU
1	A	340	GLU
1	A	341	THR
1	A	353	THR
1	A	359	ASN
1	A	371	LYS
1	A	380	ASN
1	A	384	ILE
1	A	396	LEU
1	A	399	ASP
1	A	402	ILE
1	A	431	LYS
1	A	441	THR
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	490	ASP
1	A	519	GLU
1	A	523	ASP
1	A	534	ARG
1	A	538	THR
1	A	544	LYS

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Mol	Chain	Res	Type
1	A	547	SER
1	A	566	THR
1	A	572	LYS
1	A	573	ARG
1	A	575	GLU
1	A	604	ARG
1	A	612	GLN
1	A	613	LEU
1	A	615	ARG
1	A	619	ILE
1	A	620	ARG
1	A	628	ASN
1	A	638	ARG
1	A	668	GLU
1	A	679	VAL
1	A	691	LEU
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	785	GLU
1	A	788	ILE
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	880	HIS
1	A	923	MET
1	A	924	ARG
1	A	958	LYS
1	A	960	LYS
1	A	981	ASP
1	A	991	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN

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Mol	Chain	Res	Type
1	A	138	GLN
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	526	ASN
1	A	628	ASN
1	A	739	ASN
1	A	756	ASN
1	A	759	GLN
1	A	914	ASN
1	A	919	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	-	25,29,29	2.33	6 (24%)	22,48,48	2.24	5 (22%)
4	ADP	A	1002	2	22,29,29	1.10	3 (13%)	27,45,45	1.94	3 (11%)

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	-	-	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	C15-C14	-3.83	1.36	1.40
3	A	1001	CZA	C4-N1	-3.71	1.34	1.39
3	A	1001	CZA	C13-C14	-3.12	1.37	1.44
4	A	1002	ADP	C2-N3	2.21	1.36	1.32
4	A	1002	ADP	O4'-C1'	2.50	1.44	1.41
4	A	1002	ADP	C5-C4	2.71	1.46	1.40
3	A	1001	CZA	O2-C6	4.12	1.29	1.22
3	A	1001	CZA	C3-C4	4.95	1.48	1.40
3	A	1001	CZA	O3-C4	6.40	1.48	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	PA-O3A-PB	-6.02	112.47	132.67
4	A	1002	ADP	N3-C2-N1	-5.49	124.69	128.89
4	A	1002	ADP	C4-C5-N7	-3.66	106.11	109.48
3	A	1001	CZA	O2-C6-C3	-2.88	120.59	128.37
3	A	1001	CZA	C15-C16-N2	-2.78	103.49	108.79
3	A	1001	CZA	C12-C13-C14	-2.66	117.17	119.49
3	A	1001	CZA	C7-C5-C6	2.78	125.47	116.02
3	A	1001	CZA	C13-C14-C15	7.86	130.98	123.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	CZA	13	0
4	A	1002	ADP	1	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 (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	980/994 (98%)	0.19	63 (6%)	23	21	66, 112, 175, 204	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	863	PRO	6.4
1	A	875	GLN	6.2
1	A	865	VAL	5.7
1	A	289	ILE	5.4
1	A	868	HIS	5.3
1	A	864	GLY	5.2
1	A	288	TRP	4.8
1	A	290	ARG	4.8
1	A	508	VAL	4.7
1	A	872	HIS	4.5
1	A	46	GLY	4.5
1	A	835	PHE	4.4
1	A	994	GLY	4.3
1	A	78	PHE	4.0
1	A	832	TRP	4.0
1	A	112	ALA	4.0
1	A	122	TYR	3.9
1	A	857	MET	3.9
1	A	796	ASN	3.8
1	A	987	ILE	3.6
1	A	876	CYS	3.6
1	A	874	MET	3.5
1	A	889	GLU	3.5
1	A	287	SER	3.4
1	A	923	MET	3.4
1	A	890	ILE	3.3
1	A	924	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	766	SER	3.0
1	A	965	THR	2.9
1	A	47	LYS	2.9
1	A	871	THR	2.9
1	A	266	LEU	2.9
1	A	82	GLU	2.9
1	A	292	ALA	2.9
1	A	786	ALA	2.8
1	A	891	PHE	2.8
1	A	934	LEU	2.8
1	A	767	SER	2.7
1	A	79	GLU	2.6
1	A	467	ARG	2.6
1	A	48	SER	2.6
1	A	217	GLY	2.5
1	A	45	GLU	2.5
1	A	286	GLY	2.5
1	A	927	PRO	2.5
1	A	305	ALA	2.3
1	A	55	GLU	2.2
1	A	417	CYS	2.2
1	A	782	GLY	2.2
1	A	861	ASP	2.2
1	A	74	VAL	2.2
1	A	966	GLN	2.1
1	A	44	GLU	2.1
1	A	814	LEU	2.1
1	A	262	LYS	2.1
1	A	699	ALA	2.0
1	A	351	ASP	2.0
1	A	877	THR	2.0
1	A	441	THR	2.0
1	A	701	THR	2.0
1	A	49	LEU	2.0
1	A	702	GLY	2.0
1	A	915	SER	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.

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6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.82	0.27	0.45	91,98,117,118	0
3	CZA	A	1001	25/25	0.88	0.20	-0.21	110,110,113,115	0
2	MG	A	995	1/1	0.87	1.05	-	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.