Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:48 AM GMT

PDB ID	:	2O9J
Title	:	Crystal structure of calcium atpase with bound magnesium fluoride and cyclopiazonic acid
Authors	:	Young, H.S.; Moncoq, K.A.
Deposited on	:	2006-12-13
Resolution	:	2.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

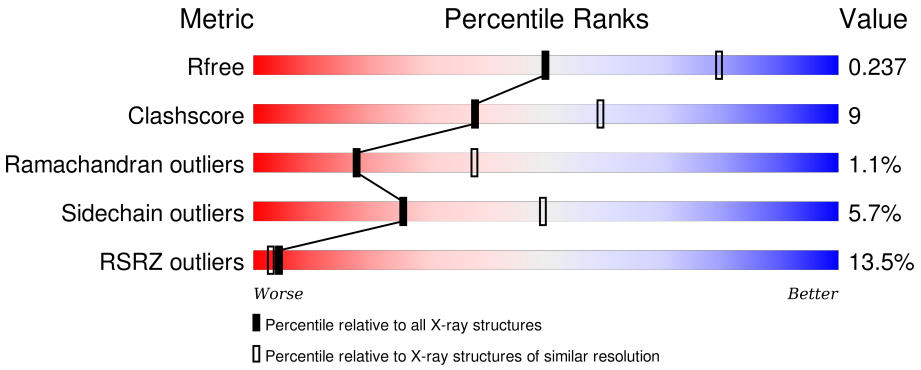
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	13% 78% 18%

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	NA	A	997	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CZA	A	1001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7669 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	980	Total	C	N	O	S	0	0	0
			7562	4805	1267	1433	57			

There is a discrepancy between the modelled and reference sequences:

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

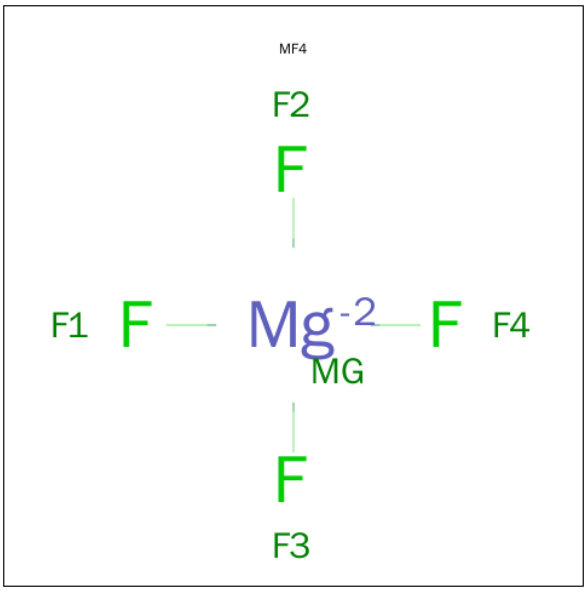
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

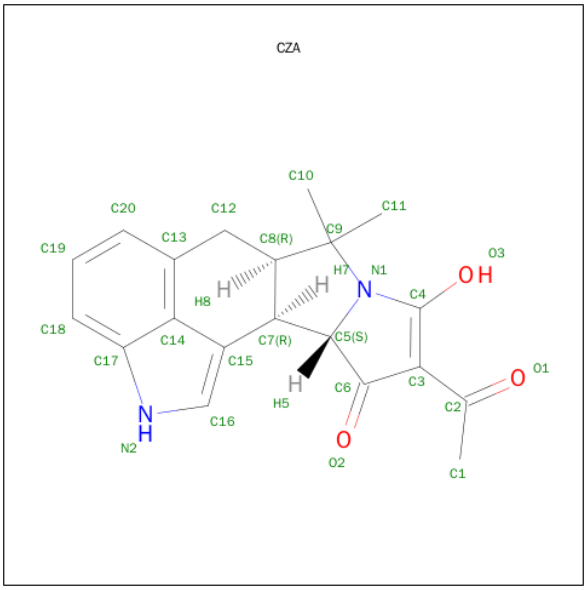
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



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

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



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

- Molecule 6 is water.

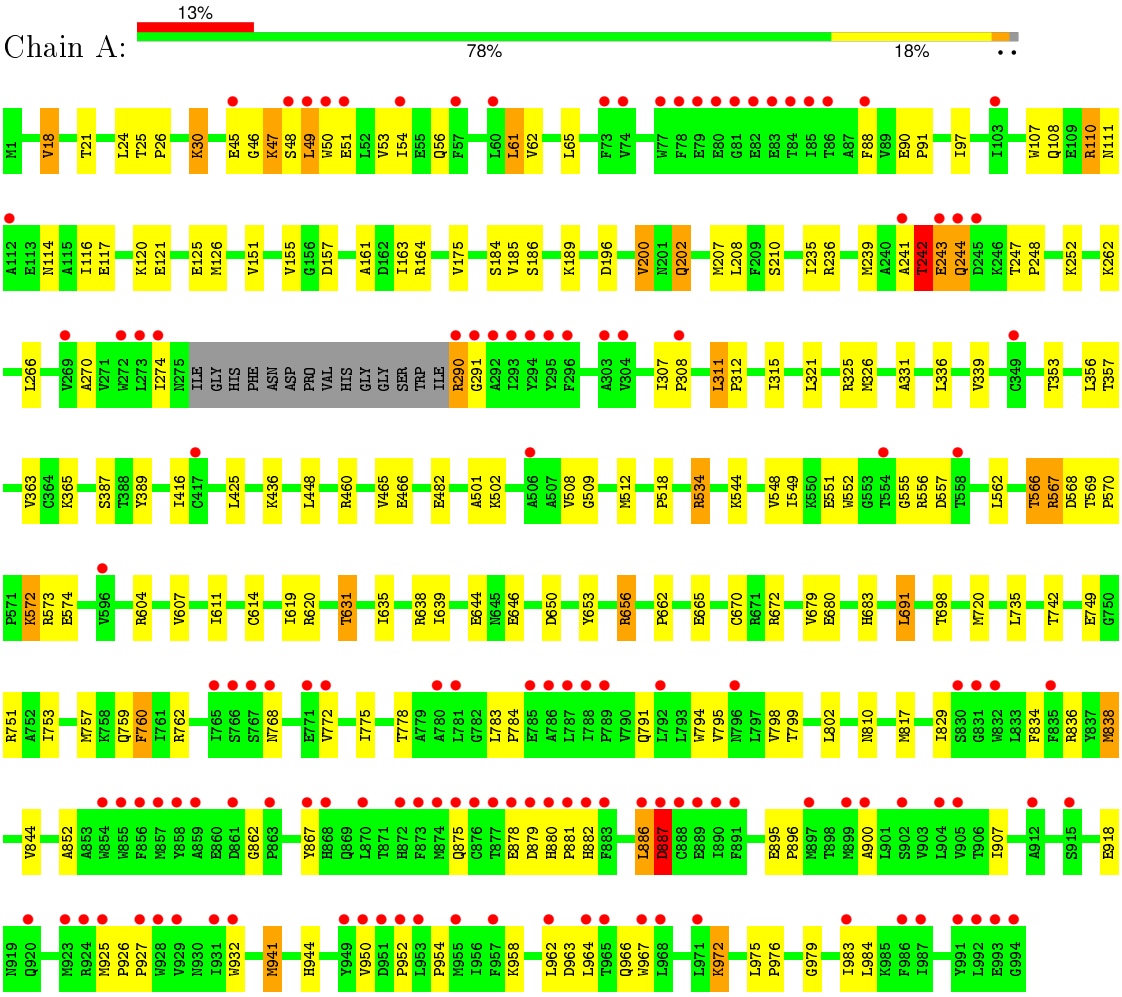
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.38Å 69.88Å 143.41Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	29.10 – 2.65 28.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.10-2.65) 99.7 (28.99-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.246 , 0.287 0.240 , 0.237	Depositor DCC
R_{free} test set	2458 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	63.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 48429 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7669	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: NA, MG, CZA, MF4

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	0.33	0/7696	0.52	0/10431

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7562	0	7668	140	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	25	0	20	10	0
6	A	75	0	0	7	0
All	All	7669	0	7688	141	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 9.

All (141) 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:290:ARG:HD2	1:A:291:GLY:H	1.11	1.06
1:A:202:GLN:HE21	1:A:202:GLN:H	1.04	0.98
1:A:290:ARG:CD	1:A:291:GLY:H	1.83	0.91
1:A:202:GLN:HE21	1:A:202:GLN:N	1.71	0.88
1:A:631:THR:HG21	6:A:2070:HOH:O	1.77	0.84
1:A:795:VAL:HA	1:A:799:THR:HG22	1.58	0.84
1:A:290:ARG:HD2	1:A:291:GLY:N	1.91	0.83
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.60	0.82
1:A:460:ARG:HD2	6:A:2050:HOH:O	1.85	0.75
1:A:751:ARG:HD2	1:A:817:MET:CE	2.17	0.74
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.70	0.73
1:A:18:VAL:CG1	1:A:24:LEU:HD23	2.20	0.72
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.22	0.70
1:A:202:GLN:NE2	1:A:202:GLN:H	1.86	0.70
1:A:775:ILE:HA	1:A:778:THR:HG22	1.73	0.69
1:A:751:ARG:HD2	1:A:817:MET:HE1	1.75	0.68
1:A:312:PRO:CG	5:A:1001:CZA:H112	2.23	0.68
1:A:311:LEU:HD22	1:A:315:ILE:HG13	1.75	0.67
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.76	0.67
1:A:880:HIS:N	1:A:881:PRO:HD2	2.10	0.66
1:A:604:ARG:HB2	1:A:607:VAL:HG23	1.76	0.66
1:A:555:GLY:N	6:A:2036:HOH:O	2.22	0.65
1:A:312:PRO:CD	5:A:1001:CZA:C11	2.75	0.65
1:A:312:PRO:CD	5:A:1001:CZA:H112	2.27	0.64
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.81	0.63
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.82	0.62
1:A:108:GLN:HB2	1:A:336:LEU:HB2	1.82	0.61
1:A:61:LEU:HD12	5:A:1001:CZA:H8	1.84	0.60
1:A:321:LEU:O	1:A:325:ARG:HB2	2.02	0.60
1:A:950:VAL:O	1:A:954:PRO:HD3	2.03	0.59
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.84	0.58
1:A:18:VAL:HG11	1:A:24:LEU:HD23	1.86	0.58
1:A:963:ASP:H	1:A:966:GLN:HG3	1.69	0.57
1:A:875:GLN:HB3	1:A:879:ASP:HB2	1.85	0.57
1:A:834:PHE:O	1:A:838:MET:HB2	2.05	0.57
1:A:880:HIS:N	1:A:881:PRO:CD	2.68	0.57
1:A:336:LEU:O	1:A:339:VAL:HG12	2.04	0.57
1:A:501:ALA:O	1:A:502:LYS:HB2	2.05	0.57
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.85	0.57
1:A:653:TYR:OH	1:A:672:ARG:NH2	2.38	0.56
1:A:312:PRO:CG	5:A:1001:CZA:C11	2.83	0.56
1:A:312:PRO:HG2	5:A:1001:CZA:C11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD11	1:A:307:ILE:HD12	1.89	0.55
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.88	0.55
1:A:331:ALA:HB2	1:A:742:THR:HG21	1.90	0.54
1:A:247:THR:HB	1:A:248:PRO:HD2	1.90	0.54
1:A:829:ILE:O	1:A:829:ILE:HD12	2.08	0.54
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.90	0.53
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.91	0.53
1:A:62:VAL:HG13	5:A:1001:CZA:H7	1.91	0.53
1:A:548:VAL:HA	1:A:551:GLU:HG2	1.91	0.53
1:A:720:MET:CE	1:A:735:LEU:HD12	2.39	0.52
1:A:312:PRO:HG2	5:A:1001:CZA:H111	1.92	0.52
1:A:326:MET:HG3	1:A:331:ALA:HB3	1.91	0.52
1:A:551:GLU:HG3	1:A:552:TRP:N	2.24	0.51
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.91	0.51
1:A:962:LEU:HB3	1:A:966:GLN:HB3	1.90	0.51
1:A:18:VAL:HG13	1:A:24:LEU:HD23	1.92	0.51
1:A:607:VAL:O	1:A:611:ILE:HG12	2.11	0.51
1:A:508:VAL:HG12	1:A:509:GLY:N	2.26	0.51
1:A:557:ASP:HA	1:A:638:ARG:NH2	2.25	0.50
1:A:670:CYS:HB3	1:A:691:LEU:HD13	1.93	0.50
1:A:944:HIS:HE1	1:A:967:TRP:HH2	1.60	0.50
1:A:508:VAL:CG1	1:A:509:GLY:N	2.74	0.50
1:A:574:GLU:H	1:A:574:GLU:CD	2.15	0.50
1:A:720:MET:HE1	1:A:735:LEU:HD12	1.93	0.50
1:A:114:ASN:O	1:A:117:GLU:HG3	2.12	0.49
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.13	0.49
1:A:567:ARG:HD3	1:A:569:THR:O	2.12	0.49
1:A:768:ASN:O	1:A:772:VAL:HG23	2.12	0.49
1:A:157:ASP:HA	6:A:2008:HOH:O	2.13	0.49
1:A:241:ALA:C	1:A:243:GLU:H	2.15	0.49
1:A:46:GLY:O	1:A:47:LYS:O	2.31	0.48
1:A:312:PRO:HD3	5:A:1001:CZA:H112	1.95	0.48
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.95	0.48
1:A:290:ARG:CD	1:A:291:GLY:N	2.63	0.48
1:A:895:GLU:N	1:A:896:PRO:HD2	2.28	0.47
1:A:798:VAL:O	1:A:802:LEU:HD23	2.15	0.47
1:A:482:GLU:OE2	1:A:573:ARG:NE	2.43	0.47
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.95	0.47
1:A:544:LYS:HE2	6:A:2058:HOH:O	2.14	0.47
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.49	0.47
1:A:638:ARG:HD3	6:A:2041:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ARG:HH11	1:A:568:ASP:HB2	1.81	0.46
1:A:972:LYS:NZ	1:A:972:LYS:HA	2.31	0.46
1:A:50:TRP:O	1:A:54:ILE:HG13	2.16	0.46
1:A:557:ASP:HA	1:A:638:ARG:HH22	1.81	0.45
1:A:196:ASP:OD2	1:A:656:ARG:NE	2.49	0.45
1:A:175:VAL:O	1:A:186:SER:HA	2.17	0.45
1:A:944:HIS:CE1	1:A:967:TRP:HH2	2.35	0.45
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.72	0.45
1:A:572:LYS:HB3	1:A:574:GLU:OE1	2.16	0.45
1:A:48:SER:C	1:A:50:TRP:H	2.19	0.45
1:A:189:LYS:NZ	1:A:207:MET:O	2.50	0.45
1:A:353:THR:HA	1:A:357:THR:OG1	2.17	0.44
1:A:836:ARG:HG3	1:A:984:LEU:HD13	1.99	0.44
1:A:116:ILE:CD1	1:A:239:MET:HB2	2.48	0.44
1:A:979:GLY:O	1:A:983:ILE:HG12	2.18	0.44
1:A:116:ILE:HD11	1:A:239:MET:HB2	1.99	0.44
1:A:795:VAL:CA	1:A:799:THR:HG22	2.39	0.43
1:A:242:THR:O	1:A:244:GLN:N	2.51	0.43
1:A:200:VAL:HG22	1:A:680:GLU:CG	2.48	0.43
1:A:161:ALA:HA	1:A:210:SER:HB2	2.00	0.43
1:A:25:THR:HB	1:A:26:PRO:HD2	2.00	0.43
1:A:556:ARG:NH2	1:A:644:GLU:OE2	2.44	0.43
1:A:635:ILE:O	1:A:639:ILE:HG12	2.18	0.43
1:A:762:ARG:HH22	1:A:918:GLU:HG3	1.83	0.43
1:A:557:ASP:HB2	6:A:2036:HOH:O	2.19	0.43
1:A:886:LEU:HB2	1:A:887:ASP:H	1.56	0.43
1:A:662:PRO:HG2	1:A:665:GLU:HG3	1.99	0.43
5:A:1001:CZA:H101	5:A:1001:CZA:HO3	1.84	0.43
1:A:650:ASP:O	1:A:672:ARG:HD2	2.19	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.82	0.43
1:A:757:MET:HA	1:A:760:PHE:CE2	2.54	0.43
1:A:795:VAL:HA	1:A:799:THR:CG2	2.38	0.42
1:A:270:ALA:O	1:A:274:ILE:HG13	2.19	0.42
1:A:941:MET:HA	1:A:941:MET:CE	2.49	0.42
1:A:116:ILE:O	1:A:120:LYS:HG3	2.20	0.42
1:A:760:PHE:CD1	1:A:760:PHE:C	2.93	0.42
1:A:252:LYS:HA	1:A:252:LYS:HD3	1.83	0.42
1:A:241:ALA:O	1:A:243:GLU:N	2.51	0.42
1:A:925:MET:HA	1:A:926:PRO:HD2	1.77	0.42
1:A:107:TRP:O	1:A:110:ARG:HD3	2.19	0.42
1:A:163:ILE:HB	1:A:208:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HD13	1:A:97:ILE:HA	1.89	0.41
1:A:556:ARG:HD3	1:A:638:ARG:HG3	2.01	0.41
1:A:614:CYS:HB3	1:A:619:ILE:HB	2.03	0.41
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.85	0.41
1:A:363:VAL:HG11	1:A:448:LEU:HD22	2.02	0.41
1:A:975:LEU:N	1:A:976:PRO:HD2	2.36	0.41
1:A:184:SER:O	1:A:185:VAL:C	2.59	0.41
1:A:791:GLN:O	1:A:795:VAL:HG23	2.21	0.41
1:A:794:TRP:CZ3	1:A:799:THR:HB	2.56	0.41
1:A:875:GLN:HA	1:A:878:GLU:HB3	2.03	0.41
1:A:572:LYS:O	1:A:573:ARG:C	2.59	0.41
1:A:110:ARG:HB2	1:A:110:ARG:HE	1.68	0.41
1:A:783:LEU:HB3	1:A:784:PRO:HD2	2.02	0.41
1:A:53:VAL:O	1:A:56:GLN:HB2	2.21	0.41
1:A:88:PHE:O	1:A:91:PRO:HD2	2.20	0.41
1:A:235:ILE:O	1:A:239:MET:HG2	2.21	0.40
1:A:749:GLU:O	1:A:753:ILE:HG12	2.22	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	976/994 (98%)	897 (92%)	68 (7%)	11 (1%)	17 38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	111	ASN
1	A	243	GLU
1	A	862	GLY

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Mol	Chain	Res	Type
1	A	887	ASP
1	A	49	LEU
1	A	242	THR
1	A	155	VAL
1	A	244	GLN
1	A	958	LYS
1	A	882	HIS

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	829/840 (99%)	782 (94%)	47 (6%)	25 49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	VAL
1	A	21	THR
1	A	30	LYS
1	A	45	GLU
1	A	49	LEU
1	A	51	GLU
1	A	61	LEU
1	A	65	LEU
1	A	110	ARG
1	A	121	GLU
1	A	125	GLU
1	A	126	MET
1	A	151	VAL
1	A	164	ARG
1	A	200	VAL
1	A	202	GLN
1	A	236	ARG
1	A	242	THR
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	290	ARG
1	A	311	LEU
1	A	356	LEU
1	A	387	SER
1	A	436	LYS
1	A	465	VAL
1	A	466	GLU
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	572	LYS
1	A	620	ARG
1	A	631	THR
1	A	646	GLU
1	A	656	ARG
1	A	691	LEU
1	A	759	GLN
1	A	760	PHE
1	A	810	ASN
1	A	838	MET
1	A	867	TYR
1	A	886	LEU
1	A	887	ASP
1	A	932	TRP
1	A	941	MET
1	A	964	LEU
1	A	972	LYS

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

Mol	Chain	Res	Type
1	A	108	GLN
1	A	114	ASN
1	A	138	GLN
1	A	202	GLN
1	A	250	GLN
1	A	359	ASN
1	A	360	GLN
1	A	477	GLN
1	A	755	ASN
1	A	759	GLN

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Mol	Chain	Res	Type
1	A	810	ASN
1	A	875	GLN
1	A	914	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	$\#\|Z\| > 2$
5	CZA	A	1001	-	25,29,29	2.34	6 (24%)	22,48,48	2.34	6 (27%)
4	MF4	A	996	1,2	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CZA	A	1001	-	-	0/4/52/52	0/5/5/5
4	MF4	A	996	1,2	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	CZA	C4-N1	-4.08	1.34	1.39
5	A	1001	CZA	C15-C14	-4.04	1.35	1.40
5	A	1001	CZA	C13-C14	-3.23	1.37	1.44
5	A	1001	CZA	O2-C6	3.97	1.29	1.22
5	A	1001	CZA	C3-C4	4.95	1.48	1.40
5	A	1001	CZA	O3-C4	6.37	1.48	1.31

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1001	CZA	O2-C6-C3	-3.08	120.04	128.37
5	A	1001	CZA	C15-C16-N2	-2.83	103.38	108.79
5	A	1001	CZA	C12-C13-C14	-2.81	117.05	119.49
5	A	1001	CZA	C18-C17-C14	-2.07	117.56	121.11
5	A	1001	CZA	C7-C5-C6	2.62	124.92	116.02
5	A	1001	CZA	C13-C14-C15	8.23	131.34	123.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	CZA	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.58	132 (13%)	4	3	38, 64, 145, 164	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	TRP	10.0
1	A	890	ILE	9.7
1	A	867	TYR	9.5
1	A	85	ILE	7.4
1	A	84	THR	7.0
1	A	881	PRO	7.0
1	A	887	ASP	6.5
1	A	877	THR	6.3
1	A	86	THR	6.2
1	A	868	HIS	5.9
1	A	78	PHE	5.8
1	A	891	PHE	5.8
1	A	929	VAL	5.7
1	A	889	GLU	5.6
1	A	81	GLY	5.4
1	A	951	ASP	5.4
1	A	965	THR	5.4
1	A	112	ALA	5.4
1	A	835	PHE	5.2
1	A	874	MET	5.2
1	A	855	TRP	4.9
1	A	876	CYS	4.7
1	A	923	MET	4.4
1	A	60	LEU	4.4
1	A	964	LEU	4.4
1	A	241	ALA	4.4
1	A	883	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	788	ILE	4.0
1	A	928	TRP	4.0
1	A	987	ILE	4.0
1	A	244	GLN	4.0
1	A	856	PHE	3.9
1	A	780	ALA	3.9
1	A	882	HIS	3.6
1	A	88	PHE	3.6
1	A	83	GLU	3.6
1	A	932	TRP	3.5
1	A	888	CYS	3.5
1	A	830	SER	3.4
1	A	994	GLY	3.4
1	A	897	MET	3.4
1	A	993	GLU	3.4
1	A	971	LEU	3.4
1	A	900	ALA	3.4
1	A	992	LEU	3.3
1	A	875	GLN	3.2
1	A	771	GLU	3.2
1	A	968	LEU	3.2
1	A	295	TYR	3.2
1	A	858	TYR	3.2
1	A	983	ILE	3.1
1	A	789	PRO	3.1
1	A	50	TRP	3.1
1	A	245	ASP	3.1
1	A	861	ASP	3.1
1	A	880	HIS	3.0
1	A	291	GLY	3.0
1	A	886	LEU	2.9
1	A	349	CYS	2.9
1	A	991	TYR	2.9
1	A	296	PHE	2.9
1	A	103	ILE	2.9
1	A	854	TRP	2.9
1	A	785	GLU	2.8
1	A	554	THR	2.8
1	A	931	ILE	2.8
1	A	925	MET	2.7
1	A	831	GLY	2.7
1	A	949	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	904	LEU	2.7
1	A	243	GLU	2.7
1	A	558	THR	2.6
1	A	79	GLU	2.6
1	A	859	ALA	2.6
1	A	49	LEU	2.6
1	A	82	GLU	2.6
1	A	294	TYR	2.6
1	A	781	LEU	2.5
1	A	832	TRP	2.5
1	A	274	ILE	2.5
1	A	879	ASP	2.5
1	A	292	ALA	2.5
1	A	304	VAL	2.5
1	A	796	ASN	2.5
1	A	899	MET	2.5
1	A	786	ALA	2.5
1	A	787	LEU	2.5
1	A	308	PRO	2.5
1	A	768	ASN	2.5
1	A	273	LEU	2.4
1	A	967	TRP	2.4
1	A	74	VAL	2.4
1	A	952	PRO	2.4
1	A	915	SER	2.4
1	A	962	LEU	2.3
1	A	293	ILE	2.3
1	A	290	ARG	2.3
1	A	986	PHE	2.3
1	A	269	VAL	2.3
1	A	303	ALA	2.3
1	A	905	VAL	2.3
1	A	950	VAL	2.3
1	A	57	PHE	2.3
1	A	872	HIS	2.3
1	A	54	ILE	2.3
1	A	953	LEU	2.3
1	A	927	PRO	2.2
1	A	506	ALA	2.2
1	A	766	SER	2.2
1	A	873	PHE	2.2
1	A	902	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLU	2.2
1	A	955	MET	2.2
1	A	80	GLU	2.2
1	A	863	PRO	2.2
1	A	767	SER	2.2
1	A	73	PHE	2.2
1	A	924	ARG	2.1
1	A	272	TRP	2.1
1	A	765	ILE	2.1
1	A	912	ALA	2.1
1	A	45	GLU	2.1
1	A	920	GLN	2.1
1	A	48	SER	2.1
1	A	792	LEU	2.1
1	A	878	GLU	2.1
1	A	870	LEU	2.1
1	A	772	VAL	2.1
1	A	596	VAL	2.0
1	A	857	MET	2.0
1	A	417	CYS	2.0
1	A	957	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
3	NA	A	997	1/1	0.91	0.35	3.29	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CZA	A	1001	25/25	0.85	0.23	0.03	89,89,91,92	0
4	MF4	A	996	5/5	0.95	0.16	-0.22	32,34,35,35	0
2	MG	A	995	1/1	0.98	0.09	-2.77	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.