Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2016 – 07:02 PM EDT

PDB ID	:	3J7T
Title	:	Calcium atpase structure with two bound calcium ions determined by electron crystallography of thin 3D crystals
Authors	:	Yonekura, K.; Kato, K.; Ogasawara, M.; Tomita, M.; Toyoshima, C.
Deposited on	:	2014-08-07
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

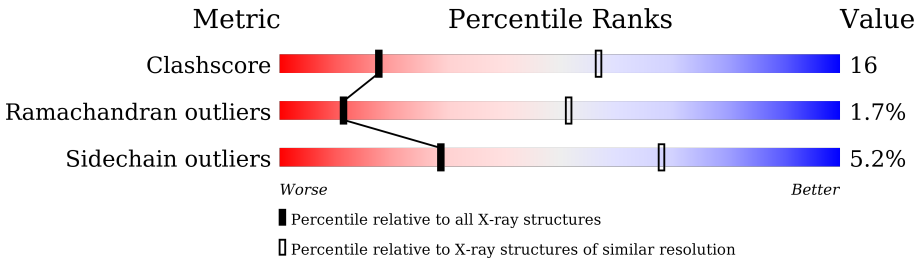
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	64% 33% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8203 atoms, of which 375 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	994	Total	C	H	N	O	S	0	0	0
			8045	4876	375	1287	1450	57			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		

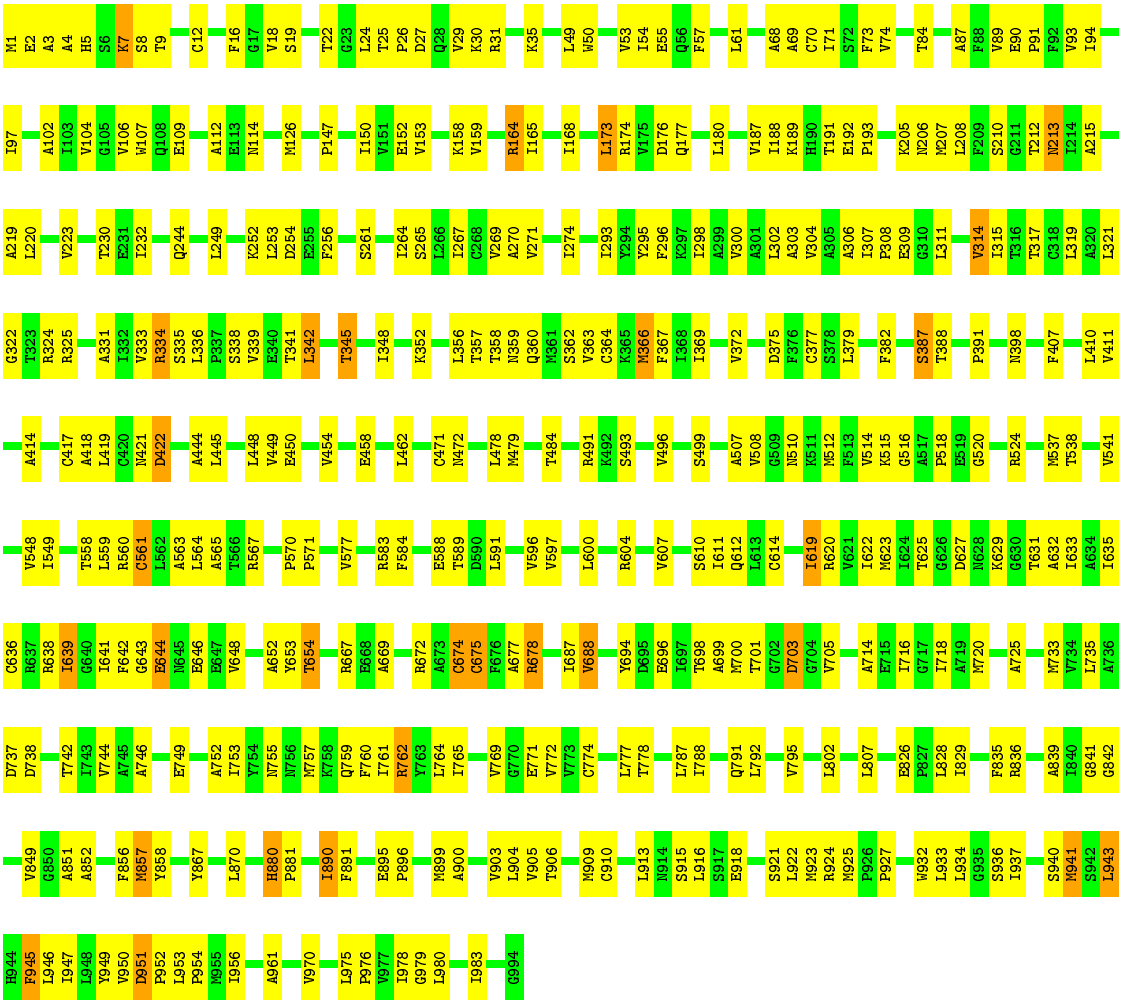
3 Residue-property plots (i)

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.

Note EDS was not executed.

- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.30Å 64.40Å 147.32Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40	Depositor
% Data completeness (in resolution range)	67.5 (8.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.277 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8203	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA

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	0.34	0/7811	0.55	0/10592

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	7670	375	7763	246	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	155	0	0	5	0
All	All	7828	375	7763	246	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 16.

All (246) 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:180:LEU:HD21	1:A:232:ILE:HD13	1.61	0.83
1:A:623:MET:SD	1:A:636:CYS:SG	2.79	0.81
1:A:173:LEU:HD11	1:A:219:ALA:HB2	1.67	0.77
1:A:701:THR:HB	1:A:720:MET:HE3	1.66	0.76
1:A:165:ILE:HG22	1:A:191:THR:HG22	1.68	0.75
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.67	0.75
1:A:927:PRO:HB2	1:A:934:LEU:HD21	1.70	0.74
1:A:267:ILE:HD12	1:A:772:VAL:HG11	1.71	0.72
1:A:363:VAL:HG23	1:A:444:ALA:HB1	1.71	0.71
1:A:852:ALA:HB2	1:A:900:ALA:HB2	1.72	0.71
1:A:642:PHE:CD2	1:A:648:VAL:HG11	2.26	0.70
1:A:635:ILE:O	1:A:639:ILE:HG12	1.93	0.69
1:A:342:LEU:HD11	1:A:733:MET:HE2	1.75	0.68
1:A:315:ILE:HD11	1:A:757:MET:HG3	1.77	0.67
1:A:633:ILE:HD11	1:A:652:ALA:HB1	1.77	0.67
1:A:653:TYR:OH	1:A:669:ALA:HB1	1.95	0.66
1:A:654:THR:HG23	1:A:677:ALA:HB3	1.77	0.66
1:A:173:LEU:CD1	1:A:219:ALA:HB2	2.26	0.65
1:A:450:GLU:HA	1:A:471:CYS:SG	2.38	0.63
1:A:102:ALA:O	1:A:106:VAL:HG12	1.99	0.62
1:A:8:SER:O	1:A:12:CYS:SG	2.53	0.62
1:A:633:ILE:HD11	1:A:652:ALA:CB	2.30	0.62
1:A:949:TYR:CE2	1:A:961:ALA:HB1	2.35	0.62
1:A:787:LEU:HD13	1:A:792:LEU:HD21	1.83	0.61
1:A:25:THR:O	1:A:29:VAL:HG23	2.01	0.60
1:A:366:MET:CB	1:A:597:VAL:HG12	2.31	0.60
1:A:366:MET:HB3	1:A:597:VAL:HG12	1.82	0.60
1:A:165:ILE:HG13	1:A:207:MET:HA	1.84	0.60
1:A:646:GLU:O	1:A:648:VAL:HG13	2.03	0.59
1:A:364:CYS:HB3	1:A:559:LEU:HD13	1.85	0.59
1:A:210:SER:HB3	1:A:230:THR:HG23	1.84	0.59
1:A:737:ASP:O	1:A:738:ASP:HB2	2.03	0.59
1:A:84:THR:HG21	1:A:87:ALA:HB3	1.83	0.58
1:A:975:LEU:N	1:A:976:PRO:HD2	2.18	0.58
1:A:625:THR:HG21	1:A:632:ALA:HB1	1.85	0.58
1:A:174:ARG:HA	1:A:187:VAL:O	2.04	0.58
1:A:642:PHE:CE2	1:A:648:VAL:HG11	2.39	0.57
1:A:895:GLU:HB2	1:A:896:PRO:HD3	1.86	0.57
1:A:264:ILE:HD13	1:A:307:ILE:HG13	1.86	0.57
1:A:3:ALA:HB1	1:A:5:HIS:CE1	2.40	0.57
1:A:677:ALA:O	1:A:678:ARG:C	2.42	0.57
1:A:718:ILE:HA	1:A:733:MET:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:CD1	1:A:91:PRO:HG2	2.39	0.57
1:A:614:CYS:HB3	1:A:619:ILE:HG21	1.86	0.56
1:A:317:THR:O	1:A:321:LEU:HB2	2.04	0.56
1:A:979:GLY:O	1:A:983:ILE:HG12	2.06	0.56
1:A:109:GLU:O	1:A:112:ALA:HB3	2.06	0.56
1:A:192:GLU:HB3	1:A:193:PRO:HD2	1.88	0.56
1:A:319:LEU:HD13	1:A:339:VAL:HG21	1.88	0.55
1:A:524:ARG:HB3	1:A:589:THR:HA	1.89	0.55
1:A:620:ARG:CZ	1:A:622:ILE:HD11	2.37	0.55
1:A:755:ASN:O	1:A:759:GLN:NE2	2.40	0.55
1:A:69:ALA:O	1:A:73:PHE:HB2	2.07	0.55
1:A:980:LEU:HD23	4:A:1230:HOH:O	2.07	0.55
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.89	0.54
1:A:314:VAL:HG21	1:A:760:PHE:CE2	2.42	0.54
1:A:165:ILE:HG22	1:A:191:THR:CG2	2.37	0.54
1:A:623:MET:SD	1:A:675:CYS:SG	3.06	0.53
1:A:856:PHE:CZ	1:A:896:PRO:HG2	2.43	0.53
1:A:333:VAL:HG21	1:A:342:LEU:CD1	2.38	0.53
1:A:308:PRO:CB	1:A:764:LEU:HD23	2.39	0.53
1:A:795:VAL:HG21	1:A:904:LEU:HD23	1.90	0.53
1:A:765:ILE:O	1:A:769:VAL:HG23	2.09	0.53
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.91	0.53
1:A:947:ILE:HD12	1:A:953:LEU:HB3	1.90	0.52
1:A:777:LEU:HD22	1:A:849:VAL:HG21	1.91	0.52
1:A:360:GLN:NE2	1:A:388:THR:HG22	2.24	0.52
1:A:627:ASP:O	1:A:677:ALA:HB1	2.09	0.52
1:A:906:THR:HG21	1:A:970:VAL:HG12	1.92	0.52
1:A:150:ILE:CG2	1:A:220:LEU:HG	2.40	0.51
1:A:322:GLY:HA3	1:A:753:ILE:HD11	1.92	0.51
1:A:338:SER:O	1:A:342:LEU:HB2	2.11	0.51
1:A:419:LEU:O	1:A:421:ASN:N	2.43	0.51
1:A:189:LYS:HZ3	1:A:205:LYS:HA	1.75	0.51
1:A:600:LEU:HD12	1:A:638:ARG:NE	2.25	0.51
1:A:760:PHE:HA	1:A:807:LEU:HD23	1.91	0.51
1:A:50:TRP:HA	1:A:54:ILE:HD13	1.91	0.51
1:A:688:VAL:HG22	1:A:698:THR:HG21	1.91	0.51
1:A:176:ASP:HB2	1:A:215:ALA:HB2	1.93	0.51
1:A:698:THR:HB	1:A:714:ALA:HB1	1.93	0.51
1:A:899:MET:O	1:A:903:VAL:HG23	2.10	0.51
1:A:319:LEU:HA	1:A:753:ILE:HG21	1.92	0.51
1:A:835:PHE:O	1:A:839:ALA:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.91	0.51
1:A:880:HIS:N	1:A:881:PRO:CD	2.74	0.51
1:A:93:VAL:HG21	1:A:956:ILE:CG2	2.41	0.51
1:A:611:ILE:HD12	4:A:1246:HOH:O	2.10	0.51
1:A:311:LEU:CD2	1:A:761:ILE:HD11	2.41	0.50
1:A:667:ARG:HG2	1:A:694:TYR:OH	2.12	0.50
1:A:725:ALA:N	4:A:1121:HOH:O	2.40	0.50
1:A:295:TYR:CD2	1:A:298:ILE:HD12	2.46	0.50
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.42	0.50
1:A:857:MET:HG2	1:A:870:LEU:HD11	1.93	0.50
1:A:382:PHE:CZ	1:A:410:LEU:HD11	2.47	0.49
1:A:629:LYS:O	1:A:633:ILE:HD13	2.12	0.49
1:A:514:VAL:HG21	1:A:591:LEU:HD11	1.93	0.49
1:A:348:ILE:HA	1:A:699:ALA:HB3	1.94	0.49
1:A:774:CYS:SG	1:A:849:VAL:HG13	2.52	0.49
1:A:267:ILE:O	1:A:271:VAL:HG23	2.13	0.49
1:A:319:LEU:HD21	1:A:336:LEU:HB3	1.95	0.49
1:A:331:ALA:HB1	1:A:746:ALA:HB2	1.95	0.49
1:A:910:CYS:HB3	1:A:978:ILE:HD11	1.94	0.49
1:A:358:THR:HA	1:A:604:ARG:HD3	1.94	0.49
1:A:417:CYS:SG	1:A:564:LEU:HD13	2.53	0.48
1:A:600:LEU:HD12	1:A:638:ARG:CZ	2.43	0.48
1:A:174:ARG:NH1	1:A:188:ILE:HG12	2.28	0.48
1:A:249:LEU:HD23	1:A:252:LYS:HD2	1.95	0.48
1:A:414:ALA:HB1	1:A:449:VAL:HG12	1.94	0.48
1:A:342:LEU:HD11	1:A:733:MET:CE	2.41	0.48
1:A:331:ALA:CB	1:A:746:ALA:HB2	2.44	0.48
1:A:641:ILE:HD13	4:A:1152:HOH:O	2.14	0.48
1:A:921:SER:O	1:A:925:MET:N	2.32	0.48
1:A:159:VAL:HG11	1:A:208:LEU:HB3	1.95	0.48
1:A:382:PHE:CE1	1:A:410:LEU:HD11	2.48	0.48
1:A:252:LYS:NZ	1:A:826:GLU:O	2.45	0.48
1:A:909:MET:HE3	1:A:937:ILE:HA	1.95	0.48
1:A:762:ARG:NH2	1:A:915:SER:HA	2.27	0.48
1:A:951:ASP:HB3	1:A:952:PRO:HD3	1.96	0.48
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.95	0.48
1:A:379:LEU:HD12	1:A:548:VAL:HG21	1.96	0.48
1:A:512:MET:SD	1:A:571:PRO:HD2	2.54	0.48
1:A:950:VAL:O	1:A:954:PRO:HD2	2.13	0.48
1:A:147:PRO:HA	1:A:223:VAL:HB	1.94	0.47
1:A:49:LEU:HB3	1:A:254:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:MET:HG3	1:A:570:PRO:HB3	1.96	0.47
1:A:89:VAL:HG11	1:A:956:ILE:HD12	1.95	0.47
1:A:159:VAL:HG21	1:A:208:LEU:HB3	1.97	0.47
1:A:491:ARG:NH1	1:A:493:SER:O	2.48	0.47
1:A:27:ASP:O	1:A:30:LYS:HB3	2.14	0.47
1:A:514:VAL:HG12	1:A:515:LYS:N	2.30	0.47
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.48	0.47
1:A:68:ALA:HA	1:A:71:ILE:HG12	1.98	0.47
1:A:4:ALA:HA	1:A:7:LYS:HG3	1.96	0.47
1:A:905:VAL:O	1:A:909:MET:HG2	2.15	0.47
1:A:159:VAL:HG21	1:A:208:LEU:HD22	1.96	0.46
1:A:362:SER:OG	1:A:387:SER:O	2.33	0.46
1:A:308:PRO:HB2	1:A:764:LEU:HD23	1.97	0.46
1:A:771:GLU:O	1:A:774:CYS:HB3	2.15	0.46
1:A:369:ILE:CG2	1:A:372:VAL:HG23	2.45	0.46
1:A:407:PHE:O	1:A:411:VAL:HG23	2.15	0.46
1:A:311:LEU:HD22	1:A:761:ILE:HD11	1.98	0.46
1:A:735:LEU:HD22	1:A:742:THR:HB	1.97	0.46
1:A:31:ARG:HH11	1:A:35:LYS:HE2	1.81	0.46
1:A:516:GLY:O	1:A:563:ALA:N	2.49	0.46
1:A:341:THR:HB	1:A:716:ILE:HD11	1.98	0.46
1:A:909:MET:HG3	1:A:941:MET:HE1	1.96	0.46
1:A:300:VAL:O	1:A:303:ALA:HB3	2.16	0.46
1:A:499:SER:HB3	1:A:510:ASN:OD1	2.15	0.46
1:A:213:ASN:N	1:A:213:ASN:OD1	2.48	0.46
1:A:2:GLU:O	1:A:3:ALA:C	2.55	0.45
1:A:333:VAL:HG21	1:A:342:LEU:HD11	1.99	0.45
1:A:50:TRP:HD1	1:A:55:GLU:HG3	1.81	0.45
1:A:940:SER:HA	1:A:943:LEU:HD22	1.98	0.45
1:A:70:CYS:O	1:A:74:VAL:HG23	2.15	0.45
1:A:168:ILE:CD1	1:A:191:THR:HG23	2.46	0.45
1:A:164:ARG:NH1	1:A:206:ASN:HD22	2.15	0.45
1:A:577:VAL:HG21	1:A:583:ARG:HD2	1.99	0.45
1:A:941:MET:O	1:A:945:PHE:HB2	2.16	0.45
1:A:759:GLN:NE2	1:A:918:GLU:HB2	2.32	0.45
1:A:499:SER:HA	1:A:510:ASN:HA	1.98	0.45
1:A:422:ASP:OD1	1:A:422:ASP:N	2.50	0.45
1:A:418:ALA:HB2	1:A:449:VAL:HG11	1.97	0.45
1:A:950:VAL:HB	1:A:953:LEU:HD22	1.99	0.45
1:A:458:GLU:O	1:A:462:LEU:HD12	2.17	0.44
1:A:352:LYS:HA	1:A:356:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLU:OE2	1:A:472:ASN:ND2	2.50	0.44
1:A:104:VAL:HG22	1:A:802:LEU:HD21	1.99	0.44
1:A:687:ILE:O	1:A:688:VAL:C	2.55	0.44
1:A:858:TYR:CE2	1:A:867:TYR:HB2	2.52	0.44
1:A:890:ILE:O	1:A:890:ILE:HD13	2.18	0.44
1:A:265:SER:O	1:A:269:VAL:HG23	2.18	0.44
1:A:152:GLU:HA	1:A:220:LEU:HD12	2.00	0.44
1:A:315:ILE:O	1:A:319:LEU:HB3	2.17	0.44
1:A:358:THR:O	1:A:359:ASN:HB3	2.16	0.44
1:A:559:LEU:HD23	1:A:600:LEU:HD13	1.99	0.44
1:A:5:HIS:HB3	1:A:207:MET:CE	2.48	0.44
1:A:270:ALA:O	1:A:274:ILE:HG23	2.17	0.44
1:A:377:CYS:SG	1:A:541:VAL:HA	2.58	0.44
1:A:565:ALA:CB	1:A:591:LEU:HD13	2.47	0.44
1:A:749:GLU:O	1:A:752:ALA:N	2.51	0.44
1:A:419:LEU:HD11	1:A:479:MET:HG3	2.00	0.44
1:A:952:PRO:O	1:A:956:ILE:HG12	2.17	0.44
1:A:417:CYS:O	1:A:445:LEU:O	2.36	0.43
1:A:559:LEU:HD22	1:A:600:LEU:HD22	1.99	0.43
1:A:448:LEU:O	1:A:448:LEU:HD12	2.18	0.43
1:A:153:VAL:HG23	1:A:153:VAL:O	2.17	0.43
1:A:16:PHE:O	1:A:18:VAL:HG13	2.18	0.43
1:A:177:GLN:HA	1:A:212:THR:OG1	2.19	0.43
1:A:700:MET:O	1:A:718:ILE:N	2.43	0.43
1:A:916:LEU:HD21	1:A:933:LEU:HD23	1.99	0.43
1:A:303:ALA:O	1:A:304:VAL:C	2.56	0.43
1:A:788:ILE:O	1:A:791:GLN:N	2.49	0.43
1:A:484:THR:HG23	1:A:496:VAL:HG12	2.01	0.43
1:A:382:PHE:CE2	1:A:410:LEU:HD11	2.54	0.43
1:A:356:LEU:HD23	1:A:607:VAL:HG11	2.00	0.43
1:A:643:GLY:O	1:A:644:GLU:C	2.56	0.43
1:A:807:LEU:HD11	1:A:915:SER:O	2.18	0.43
1:A:366:MET:HB2	1:A:597:VAL:HG12	2.00	0.43
1:A:807:LEU:HD21	1:A:915:SER:HB3	2.00	0.43
1:A:293:ILE:O	1:A:296:PHE:HB3	2.19	0.42
1:A:93:VAL:O	1:A:97:ILE:HG12	2.19	0.42
1:A:321:LEU:HB3	1:A:325:ARG:HH21	1.84	0.42
1:A:319:LEU:HA	1:A:753:ILE:HD13	2.00	0.42
1:A:24:LEU:HD12	1:A:24:LEU:N	2.35	0.42
1:A:417:CYS:SG	1:A:564:LEU:CD1	3.07	0.42
1:A:382:PHE:CD1	1:A:410:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LYS:HB2	1:A:623:MET:HE2	2.01	0.42
1:A:565:ALA:HB3	1:A:591:LEU:HD13	2.01	0.42
1:A:922:LEU:HD12	1:A:978:ILE:HG23	2.01	0.42
1:A:150:ILE:HG22	1:A:220:LEU:HG	2.02	0.42
1:A:57:PHE:CZ	1:A:61:LEU:HD21	2.54	0.42
1:A:584:PHE:CD2	1:A:584:PHE:N	2.88	0.42
1:A:641:ILE:HG23	1:A:674:CYS:SG	2.60	0.42
1:A:367:PHE:CE2	1:A:379:LEU:HD13	2.55	0.42
1:A:561:CYS:HA	1:A:597:VAL:O	2.20	0.42
1:A:153:VAL:HG11	1:A:208:LEU:CD1	2.50	0.41
1:A:334:ARG:O	1:A:335:SER:C	2.58	0.41
1:A:507:ALA:HA	1:A:510:ASN:ND2	2.35	0.41
1:A:520:GLY:O	1:A:524:ARG:NH1	2.53	0.41
1:A:762:ARG:CZ	1:A:915:SER:HA	2.51	0.41
1:A:345:THR:HG21	1:A:699:ALA:HB2	2.02	0.41
1:A:906:THR:HG21	1:A:970:VAL:CG1	2.51	0.41
1:A:302:LEU:HD21	1:A:772:VAL:HA	2.02	0.41
1:A:1:MET:SD	1:A:16:PHE:HE1	2.44	0.41
1:A:356:LEU:CD2	1:A:607:VAL:HG11	2.51	0.41
1:A:778:THR:HG23	1:A:849:VAL:HG11	2.01	0.41
1:A:315:ILE:CD1	1:A:757:MET:HG3	2.49	0.41
1:A:256:PHE:CE1	1:A:829:ILE:HD13	2.56	0.41
1:A:303:ALA:O	1:A:306:ALA:N	2.54	0.41
1:A:153:VAL:HG21	1:A:208:LEU:HD11	2.02	0.41
1:A:264:ILE:HG21	1:A:307:ILE:HD11	2.02	0.41
1:A:25:THR:HB	1:A:26:PRO:HD2	2.03	0.41
1:A:757:MET:HE3	1:A:828:LEU:HD11	2.03	0.41
1:A:841:GLY:O	1:A:842:GLY:C	2.59	0.41
1:A:298:ILE:O	1:A:302:LEU:HB2	2.20	0.40
1:A:375:ASP:O	1:A:541:VAL:HG23	2.21	0.40
1:A:5:HIS:HB3	1:A:207:MET:SD	2.60	0.40
1:A:631:THR:O	1:A:635:ILE:HD13	2.21	0.40
1:A:932:TRP:O	1:A:936:SER:OG	2.38	0.40
1:A:559:LEU:CD2	1:A:600:LEU:HD13	2.51	0.40
1:A:607:VAL:HG12	4:A:1246:HOH:O	2.22	0.40
1:A:934:LEU:HA	1:A:937:ILE:HD12	2.04	0.40
1:A:49:LEU:HD23	1:A:254:ASP:HB3	2.04	0.40
1:A:53:VAL:CG1	1:A:261:SER:HB2	2.51	0.40
1:A:558:THR:O	1:A:558:THR:HG22	2.22	0.40
1:A:267:ILE:CD1	1:A:772:VAL:HG11	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	842 (85%)	133 (13%)	17 (2%)	11 51

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	ARG
1	A	951	ASP
1	A	387	SER
1	A	518	PRO
1	A	678	ARG
1	A	705	VAL
1	A	22	THR
1	A	857	MET
1	A	644	GLU
1	A	703	ASP
1	A	345	THR
1	A	560	ARG
1	A	508	VAL
1	A	391	PRO
1	A	880	HIS
1	A	94	ILE
1	A	688	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	840/840 (100%)	796 (95%)	44 (5%)	29 68

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	9	THR
1	A	19	SER
1	A	107	TRP
1	A	114	ASN
1	A	126	MET
1	A	158	LYS
1	A	164	ARG
1	A	173	LEU
1	A	213	ASN
1	A	244	GLN
1	A	253	LEU
1	A	309	GLU
1	A	314	VAL
1	A	324	ARG
1	A	342	LEU
1	A	357	THR
1	A	366	MET
1	A	398	ASN
1	A	422	ASP
1	A	454	VAL
1	A	478	LEU
1	A	537	MET
1	A	538	THR
1	A	561	CYS
1	A	612	GLN
1	A	619	ILE
1	A	639	ILE
1	A	654	THR
1	A	672	ARG
1	A	674	CYS
1	A	675	CYS
1	A	696	GLU
1	A	703	ASP
1	A	762	ARG
1	A	836	ARG
1	A	890	ILE
1	A	891	PHE

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Mol	Chain	Res	Type
1	A	923	MET
1	A	924	ARG
1	A	941	MET
1	A	943	LEU
1	A	945	PHE
1	A	946	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	32	HIS
1	A	101	ASN
1	A	108	GLN
1	A	111	ASN
1	A	114	ASN
1	A	244	GLN
1	A	280	ASN
1	A	359	ASN
1	A	477	GLN
1	A	612	GLN
1	A	759	GLN
1	A	920	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.