



Full wwPDB X-ray Structure Validation Report i

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 i symbol.

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

MolProbit	:	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

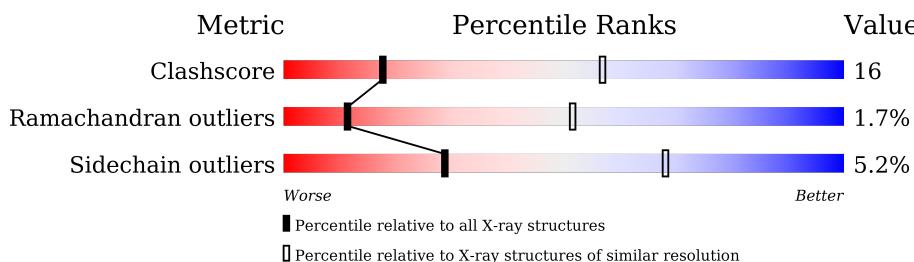
1 Overall quality at a glance

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 $\leq 5\%$. 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.

Note EDS was not executed.

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

2 Entry composition [\(i\)](#)

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 8045	H 4876	N 375	O 1287	S 1450	57	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 4 is water.

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

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:		64%				33%			
V544	T945	M1	I97	E22	A3	A4	H5	S6	S8
A855	A851	A102	V223	R325	I103	G105	K7	S8	T9
L948	L947	V220	T23	V104	V106	V107	V108	V109	V110
V949	V947	A119	A118	A119	I332	I331	I332	I333	I334
D951	V950	M560	C420	V533	D421	D422	S335	S336	S337
P52	P52	C622	B450	A444	L564	L564	A444	A444	A444
L953	F954	E646	E546	A445	L565	L565	P337	I249	A112
V955	V956	E647	E547	I445	T566	T566	S338	E113	E113
T742	T744	V648	V548	I448	R567	R567	K252	M114	F116
A945	A746	N755	N755	V449	P570	P571	I348	V114	G117
A961	A961	N756	N756	E450	E450	E451	D264	V115	V116
E749	V970	N757	N757	T451	P571	P571	D265	M126	V117
V536	R637	N758	N758	V454	V454	V454	P255	P256	P147
A914	V549	A759	A759	V577	V577	V577	F256	F256	T22
V538	V538	T656	T656	E458	E458	E458	S261	S261	G23
T558	T558	E656	E656	L462	L462	L462	I150	I150	I124
G540	G540	A656	A656	V584	V584	V584	V151	V151	T225
F541	F541	E657	E657	P584	P584	P584	E152	E152	F226
M543	M543	N757	N757	V585	V585	V585	V153	V153	D227
E844	E844	T658	T658	E593	E593	E593	I266	I266	O228
D952	D952	E659	E659	F584	F584	F584	L267	L267	V29
V545	V545	N759	N759	V593	V593	V593	V268	V268	R31
E845	E845	T659	T659	E594	E594	E594	A270	A270	R31
V537	V537	E660	E660	N760	N760	N760	V358	V358	R31
V538	V538	E661	E661	A669	A669	A669	N359	N359	R31
V539	V539	R762	R762	E672	E672	E672	V271	V271	R35
V536	V536	N763	N763	E673	E673	E673	N361	N361	I165
V537	V537	N764	N764	E674	E674	E674	S362	S362	I166
V538	V538	T765	T765	E675	E675	E675	V363	V363	I167
V539	V539	N766	N766	E676	E676	E676	C364	C364	I168
V536	V536	T767	T767	E677	E677	E677	I274	I274	I169
V537	V537	N768	N768	E678	E678	E678	V363	V363	I170
V538	V538	T769	T769	E679	E679	E679	C365	C365	I171
V539	V539	N770	N770	E680	E680	E680	V294	V294	I172
V536	V536	T771	T771	E681	E681	E681	K366	K366	I173
V537	V537	N772	N772	E682	E682	E682	V295	V295	R174
V538	V538	T773	T773	E683	E683	E683	V300	V300	V175
V539	V539	N774	N774	E684	E684	E684	V300	V300	V176
V536	V536	T775	T775	E685	E685	E685	V301	V301	V177
V537	V537	N776	N776	E686	E686	E686	V302	V302	V178
V538	V538	T777	T777	E687	E687	E687	V303	V303	V179
V539	V539	N778	N778	E688	E688	E688	V304	V304	V180
V536	V536	T779	T779	E689	E689	E689	V305	V305	V181
V537	V537	N779	N779	E690	E690	E690	V306	V306	V182
V538	V538	T780	T780	E691	E691	E691	V307	V307	V183
V539	V539	N781	N781	E692	E692	E692	V308	V308	V184
V536	V536	T782	T782	E693	E693	E693	V309	V309	V185
V537	V537	N783	N783	E694	E694	E694	V310	V310	V186
V538	V538	T784	T784	E695	E695	E695	V311	V311	V187
V539	V539	N785	N785	E696	E696	E696	V312	V312	V188
V536	V536	T786	T786	E697	E697	E697	V313	V313	A68
V537	V537	N787	N787	E698	E698	E698	K388	K388	A69
V538	V538	T788	T788	E699	E699	E699	N510	N510	A69
V539	V539	N789	N789	E700	E700	E700	K511	K511	A69
V536	V536	T789	T789	E701	E701	E701	M620	M620	A70
V537	V537	N790	N790	E702	E702	E702	K512	K512	A70
V538	V538	T791	T791	E703	E703	E703	K513	K513	A71
V539	V539	N792	N792	E704	E704	E704	M621	M621	A71
V536	V536	T793	T793	E705	E705	E705	K514	K514	A72
V537	V537	N794	N794	E706	E706	E706	M622	M622	A72
V538	V538	T795	T795	E707	E707	E707	K515	K515	A73
V539	V539	N796	N796	E708	E708	E708	M623	M623	A73
V536	V536	T797	T797	E709	E709	E709	K516	K516	A74
V537	V537	N798	N798	E710	E710	E710	M624	M624	A74
V538	V538	T799	T799	E711	E711	E711	K517	K517	A75
V539	V539	N800	N800	E712	E712	E712	M625	M625	A75
V536	V536	T801	T801	E713	E713	E713	K518	K518	A76
V537	V537	N802	N802	E714	E714	E714	M626	M626	A76
V538	V538	T803	T803	E715	E715	E715	K519	K519	A77
V539	V539	N804	N804	E716	E716	E716	M627	M627	A77
V536	V536	T805	T805	E717	E717	E717	K520	K520	A78
V537	V537	N806	N806	E718	E718	E718	M628	M628	A78
V538	V538	T807	T807	E719	E719	E719	K521	K521	A79
V539	V539	N808	N808	E720	E720	E720	M629	M629	A79
V536	V536	T809	T809	E721	E721	E721	K522	K522	A80
V537	V537	N809	N809	E722	E722	E722	M630	M630	A80
V538	V538	T810	T810	E723	E723	E723	K523	K523	A81
V539	V539	N810	N810	E724	E724	E724	M631	M631	A81
V536	V536	T811	T811	E725	E725	E725	K524	K524	A82
V537	V537	N812	N812	E726	E726	E726	M632	M632	A82
V538	V538	T813	T813	E727	E727	E727	K525	K525	A83
V539	V539	N813	N813	E728	E728	E728	M633	M633	A83
V536	V536	T814	T814	E729	E729	E729	K526	K526	A84
V537	V537	N815	N815	E730	E730	E730	M634	M634	A84
V538	V538	T816	T816	E731	E731	E731	K527	K527	A85
V539	V539	N816	N816	E732	E732	E732	M635	M635	A85
V536	V536	T817	T817	E733	E733	E733	K528	K528	A86
V537	V537	N817	N817	E734	E734	E734	M636	M636	A86
V538	V538	T818	T818	E735	E735	E735	K529	K529	A87
V539	V539	N818	N818	E736	E736	E736	M637	M637	A87
V536	V536	T819	T819	E737	E737	E737	K530	K530	A88
V537	V537	N819	N819	E738	E738	E738	M638	M638	A88
V538	V538	T820	T820	E739	E739	E739	K531	K531	A89
V539	V539	N820	N820	E740	E740	E740	M639	M639	A89
V536	V536	T821	T821	E741	E741	E741	K532	K532	A90
V537	V537	N821	N821	E742	E742	E742	M640	M640	A90
V538	V538	T822	T822	E743	E743	E743	K533	K533	A91
V539	V539	N822	N822	E744	E744	E744	M641	M641	A91
V536	V536	T823	T823	E745	E745	E745	K534	K534	A92
V537	V537	N823	N823	E746	E746	E746	M642	M642	A92
V538	V538	T824	T824	E747	E747	E747	K535	K535	A93
V539	V539	N824	N824	E748	E748	E748	M643	M643	A93
V536	V536	T825	T825	E749	E749	E749	K536	K536	A94
V537	V537	N825	N825	E750	E750	E750	M644	M644	A94
V538	V538	T826	T826	E751	E751	E751	K537	K537	A95
V539	V539	N826	N826	E752	E752	E752	M645	M645	A95
V536	V536	T827	T827	E753	E753	E753	K538	K538	A96
V537	V537	N827	N827	E754	E754	E754	M646	M646	A96
V538	V538	T828	T828	E755	E755	E755	K539	K539	A97
V539	V539	N828	N828	E756	E756	E756	M647	M647	A97
V536	V536	T829	T829	E757	E757	E757	K540	K540	A98
V537	V537	N829	N829	E758	E758	E758	M648	M648	A98
V538	V538	T830	T830	E759	E759	E759	K541	K541	A99
V539	V539	N830	N830	E760	E760	E760	M649	M649	A99
V536	V536	T831	T831	E761	E761	E761	K542	K542	A100
V537	V537	N831	N831	E762	E762	E762	M650	M650	A100
V538	V538	T832	T832	E763	E763	E763	K543	K543	A101
V539	V539	N832	N832	E764	E764	E764	M651	M651	A101
V536	V536	T833	T833	E765	E765	E765	K544	K544	A102
V537	V537	N833	N833	E766	E766	E766	M652	M652	A102
V538	V538	T834	T834	E767	E767	E767	K545	K545	A103
V539	V539	N834	N834	E768	E768	E768	M653	M653	A103
V536	V536	T835	T835	E769	E769	E769	K546	K546	A104
V537	V537	N835	N835	E770	E770	E770	M654	M654	A104
V538	V538	T836	T836	E771	E771	E771	K547	K547	A105
V539	V539	N836	N836	E772	E772	E772	M655	M655	A105
V536	V536	T837	T837	E773	E773	E773	K548	K548	A106
V537	V537	N837	N837	E774	E774	E774	M656	M656	A106
V538	V538	T838	T838	E775	E775	E775	K549	K549	A107
V539	V539	N838	N838	E776	E776	E776	M657	M657	A107
V536	V536	T839	T839	E777	E777	E777	K550	K550	A108
V537	V537	N839	N839	E778	E778	E778	M658	M658	A108
V538	V538	T840	T840	E779	E779	E779	K551	K551	A109
V539	V539	N840	N840	E780	E780	E780	M659	M659	A109
V536	V536	T841	T841	E781	E781	E781	K552	K552	A110
V537	V537	N841	N841	E782	E782	E782	M660	M660	A110
V538	V538	T842	T842	E783	E783	E783	K553	K553	A111
V539	V539	N842	N842	E784	E784	E784	M661	M661	A111
V536	V536	T843	T843	E785	E785	E785	K554	K554	A112
V537	V537	N843	N843	E786	E786	E786	M662	M662	A112
V538	V538	T844	T844	E787	E787	E787	K555	K555	A113
V539	V539	N844	N844	E788	E788	E788	M663	M663	A113
V536	V536	T845	T845	E789	E789	E789	K556	K556	A114
V537	V537	N845	N845	E790	E790	E790	M664	M664	A114
V538									

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	166.30 Å 90.00°	64.40 Å 98.30°	147.32 Å 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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

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 [\(i\)](#)

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 MolProbit. 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 (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%)	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 (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%)	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 [\(i\)](#)

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 [\(i\)](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

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

6.4 Ligands [\(i\)](#)

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

6.5 Other polymers [\(i\)](#)

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