Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:14 AM GMT

PDB ID	:	3A1C
Title	:	crystal structure of the P- and N-domains of CopA, a copper-transporting P-type ATPase, bound with AMPPCP-Mg
Authors	:	Tsuda, T.; Toyoshima, C.
Deposited on	:	2009-03-31
Resolution	:	1.85 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 ①) were used in the production of this report:

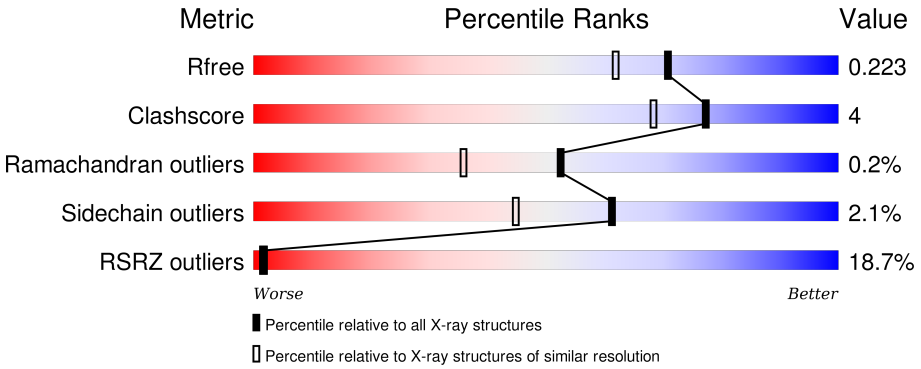
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	287	11% 83% 9% • 7%
1	B	287	24% 86% 8% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4573 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.

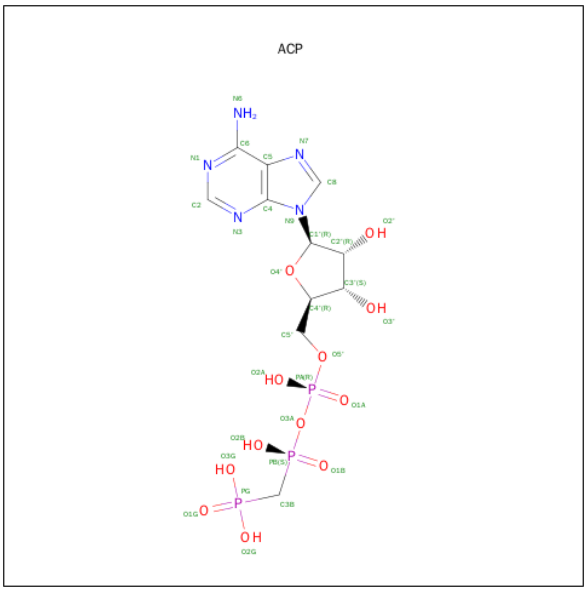
- Molecule 1 is a protein called Probable copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1995	1249	348	395	3			
1	B	273	Total	C	N	O	S	0	0	0
			2042	1279	356	403	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	MET	-	EXPRESSION TAG	UNP O29777
A	388	GLY	-	EXPRESSION TAG	UNP O29777
A	389	HIS	-	EXPRESSION TAG	UNP O29777
A	390	HIS	-	EXPRESSION TAG	UNP O29777
A	391	HIS	-	EXPRESSION TAG	UNP O29777
A	392	HIS	-	EXPRESSION TAG	UNP O29777
A	393	HIS	-	EXPRESSION TAG	UNP O29777
A	394	HIS	-	EXPRESSION TAG	UNP O29777
A	395	GLY	-	EXPRESSION TAG	UNP O29777
A	396	SER	-	EXPRESSION TAG	UNP O29777
A	397	ARG	-	EXPRESSION TAG	UNP O29777
B	387	MET	-	EXPRESSION TAG	UNP O29777
B	388	GLY	-	EXPRESSION TAG	UNP O29777
B	389	HIS	-	EXPRESSION TAG	UNP O29777
B	390	HIS	-	EXPRESSION TAG	UNP O29777
B	391	HIS	-	EXPRESSION TAG	UNP O29777
B	392	HIS	-	EXPRESSION TAG	UNP O29777
B	393	HIS	-	EXPRESSION TAG	UNP O29777
B	394	HIS	-	EXPRESSION TAG	UNP O29777
B	395	GLY	-	EXPRESSION TAG	UNP O29777
B	396	SER	-	EXPRESSION TAG	UNP O29777
B	397	ARG	-	EXPRESSION TAG	UNP O29777

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 31 11 5 12 3	0	0
2	B	1	Total C N O P 31 11 5 12 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

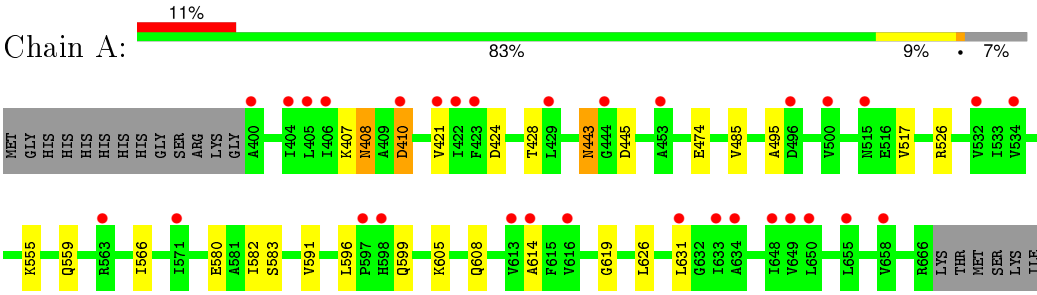
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	262	Total O 262 262	0	0
4	B	211	Total O 211 211	0	0

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.

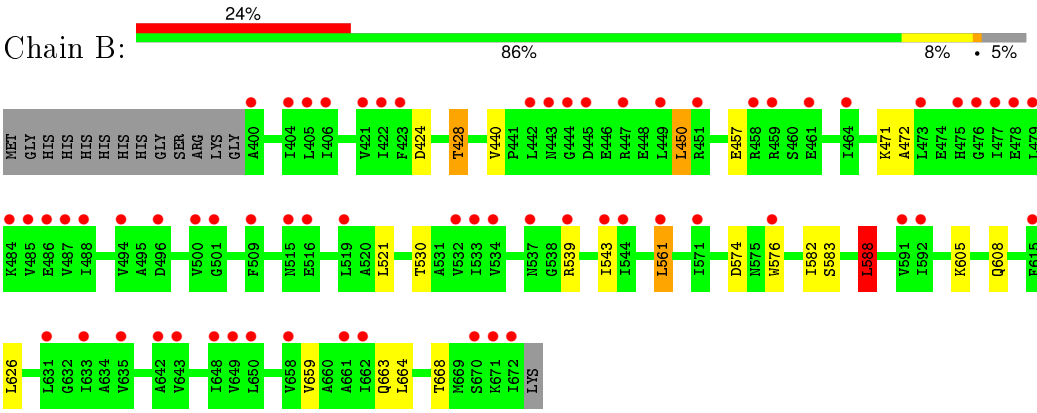
- Molecule 1: Probable copper-exporting P-type ATPase A

Chain A:



- Molecule 1: Probable copper-exporting P-type ATPase A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	90.79Å 90.79Å 191.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 27.35 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.85) 99.7 (27.35-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.225 0.194 , 0.223	Depositor DCC
R_{free} test set	3500 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 69000 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4573	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: MG, ACP

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	0.55	0/2009	0.68	2/2714 (0.1%)
1	B	0.47	0/2056	0.60	1/2775 (0.0%)
All	All	0.51	0/4065	0.64	3/5489 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	526	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	526	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	588	LEU	CB-CG-CD1	5.05	119.59	111.00

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	1995	0	2078	17	0
1	B	2042	0	2136	15	0
2	A	31	0	14	0	0
2	B	31	0	14	1	0
3	A	1	0	0	0	0
4	A	262	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	211	0	0	2	0
All	All	4573	0	4242	31	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 4.

All (31) 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:B:664:LEU:O	1:B:668:THR:HG23	1.73	0.89
1:B:450:LEU:HD11	1:B:471:LYS:HG3	1.76	0.67
1:A:605:LYS:HA	1:A:608:GLN:HE21	1.62	0.64
1:B:605:LYS:HA	1:B:608:GLN:HE21	1.62	0.62
1:A:424:ASP:O	1:A:428:THR:HB	1.99	0.62
1:B:561:LEU:HD13	1:B:659:VAL:HG22	1.83	0.61
1:A:582:ILE:HD12	4:A:1133:HOH:O	2.03	0.59
1:B:583:SER:HA	1:B:588:LEU:HD22	1.85	0.58
1:B:424:ASP:O	1:B:428:THR:HB	2.04	0.57
1:A:474:GLU:OE1	4:A:1091:HOH:O	2.17	0.57
1:A:407:LYS:HD3	4:A:1075:HOH:O	2.08	0.52
1:A:408:ASN:ND2	1:A:410:ASP:OD1	2.42	0.52
1:A:421:VAL:HG23	1:A:566:ILE:HG21	1.93	0.49
1:A:583:SER:HB2	1:A:591:VAL:HG21	1.93	0.49
1:B:619:GLY:HA2	1:B:626:LEU:CD1	2.42	0.49
1:B:440:VAL:HB	1:B:543:ILE:HG12	1.95	0.48
1:B:530:THR:OG1	1:B:574:ASP:OD2	2.33	0.47
1:A:443:ASN:ND2	1:A:445:ASP:H	2.14	0.46
1:B:582:ILE:HD12	4:B:1428:HOH:O	2.15	0.46
1:B:663:GLN:OE1	4:B:1339:HOH:O	2.21	0.46
1:A:547:SER:HB2	4:A:1106:HOH:O	2.16	0.45
1:A:580:GLU:HG3	1:B:576:TRP:CZ3	2.52	0.45
1:A:555:LYS:O	1:A:559:GLN:HG3	2.17	0.45
1:B:619:GLY:HA2	1:B:626:LEU:HD11	1.99	0.44
1:A:596:LEU:O	1:A:599:GLN:HB2	2.18	0.43
1:A:619:GLY:HA2	1:A:626:LEU:CD1	2.50	0.42
1:A:517:VAL:HG13	1:A:543:ILE:HD11	2.01	0.42
1:A:485:VAL:HG22	1:A:495:ALA:HB2	2.03	0.41
1:B:450:LEU:HD22	1:B:472:ALA:HB2	2.02	0.41
1:A:614:ALA:HA	1:A:631:LEU:O	2.21	0.40
1:B:457:GLU:OE2	2:B:997:ACP:N1	2.54	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	265/287 (92%)	262 (99%)	3 (1%)	0	100 100
1	B	271/287 (94%)	264 (97%)	6 (2%)	1 (0%)	39 22
All	All	536/574 (93%)	526 (98%)	9 (2%)	1 (0%)	52 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	211/228 (92%)	208 (99%)	3 (1%)	74 63
1	B	217/228 (95%)	211 (97%)	6 (3%)	51 33
All	All	428/456 (94%)	419 (98%)	9 (2%)	61 45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	A	410	ASP

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Mol	Chain	Res	Type
1	A	443	ASN
1	B	428	THR
1	B	450	LEU
1	B	521	LEU
1	B	539	ARG
1	B	561	LEU
1	B	588	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	A	443	ASN
1	A	587	ASN
1	A	608	GLN
1	A	628	GLN
1	B	515	ASN
1	B	608	GLN
1	B	621	ASN
1	B	628	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, 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	$\#\|Z\| > 2$
2	ACP	A	997	3	25,33,33	1.40	3 (12%)	31,52,52	2.10	7 (22%)
2	ACP	B	997	-	25,33,33	1.33	3 (12%)	31,52,52	2.02	4 (12%)

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
2	ACP	A	997	3	-	0/15/38/38	0/3/3/3
2	ACP	B	997	-	-	0/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	997	ACP	C2-N3	2.03	1.35	1.32
2	B	997	ACP	O4'-C1'	2.47	1.44	1.41
2	B	997	ACP	PB-O3A	2.98	1.61	1.58
2	A	997	ACP	PB-O3A	3.24	1.62	1.58
2	B	997	ACP	C5-C4	3.35	1.48	1.40
2	A	997	ACP	C5-C4	3.36	1.48	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	997	ACP	N3-C2-N1	-8.13	122.67	128.89
2	B	997	ACP	N3-C2-N1	-7.64	123.04	128.89
2	B	997	ACP	C2'-C1'-N9	-4.44	107.51	114.29
2	A	997	ACP	C2'-C1'-N9	-3.51	108.93	114.29
2	A	997	ACP	PA-O3A-PB	-3.13	123.93	132.73
2	B	997	ACP	O1G-PG-C3B	-2.77	104.81	111.13
2	B	997	ACP	C4-C5-N7	-2.68	107.02	109.48
2	A	997	ACP	O2G-PG-C3B	-2.00	101.54	106.40
2	A	997	ACP	C2-N1-C6	2.08	122.48	118.77
2	A	997	ACP	O2B-PB-O1B	2.48	117.91	110.12
2	A	997	ACP	O3G-PG-O2G	3.65	118.81	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	997	ACP	1	0

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

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	267/287 (93%)	0.67	32 (11%)	6 6	28, 39, 50, 56	0
1	B	273/287 (95%)	1.16	69 (25%)	1 0	31, 44, 67, 75	0
All	All	540/574 (94%)	0.92	101 (18%)	2 1	28, 40, 63, 75	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	ILE	10.2
1	B	480	GLY	7.5
1	B	481	GLU	7.0
1	B	643	VAL	6.8
1	B	670	SER	6.4
1	B	482	PRO	5.4
1	B	485	VAL	5.2
1	B	443	ASN	4.7
1	B	533	ILE	4.6
1	B	532	VAL	4.6
1	B	473	LEU	4.5
1	B	459	ARG	4.3
1	B	671	LYS	4.2
1	A	616	VAL	4.2
1	B	484	LYS	4.1
1	B	496	ASP	4.1
1	B	539	ARG	4.1
1	B	478	GLU	4.0
1	B	494	VAL	3.8
1	B	519	LEU	3.8
1	A	400	ALA	3.7
1	B	509	PHE	3.6
1	B	658	VAL	3.6
1	B	444	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	3.5
1	B	534	VAL	3.5
1	A	658	VAL	3.4
1	B	544	ILE	3.3
1	A	633	ILE	3.3
1	A	423	PHE	3.3
1	A	648	ILE	3.3
1	B	479	LEU	3.2
1	A	563	ARG	3.2
1	B	404	ILE	3.2
1	B	442	LEU	3.2
1	A	444	GLY	3.2
1	B	476	GLY	3.1
1	A	598	HIS	3.1
1	B	483	GLU	3.0
1	B	648	ILE	3.0
1	B	421	VAL	3.0
1	B	405	LEU	3.0
1	B	423	PHE	3.0
1	A	422	ILE	2.9
1	B	650	LEU	2.9
1	B	458	ARG	2.8
1	B	616	VAL	2.8
1	A	571	ILE	2.7
1	A	404	ILE	2.7
1	A	597	PRO	2.7
1	A	614	ALA	2.7
1	A	421	VAL	2.7
1	B	661	ALA	2.6
1	A	515	ASN	2.6
1	B	543	ILE	2.6
1	A	405	LEU	2.6
1	A	410	ASP	2.6
1	A	532	VAL	2.6
1	B	633	ILE	2.6
1	A	534	VAL	2.6
1	B	406	ILE	2.6
1	B	592	ILE	2.6
1	B	615	PHE	2.5
1	B	449	LEU	2.5
1	B	576	TRP	2.5
1	B	662	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	451	ARG	2.5
1	B	642	ALA	2.5
1	B	561	LEU	2.4
1	B	591	VAL	2.4
1	A	406	ILE	2.4
1	B	486	GLU	2.4
1	B	501	GLY	2.4
1	B	631	LEU	2.4
1	B	635	VAL	2.4
1	B	464	ILE	2.3
1	B	445	ASP	2.3
1	B	477	ILE	2.3
1	A	429	LEU	2.3
1	A	500	VAL	2.3
1	B	487	VAL	2.3
1	A	655	LEU	2.3
1	B	516	GLU	2.3
1	B	649	VAL	2.2
1	A	496	ASP	2.2
1	B	571	ILE	2.2
1	B	537	ASN	2.2
1	B	447	ARG	2.2
1	B	400	ALA	2.1
1	A	544	ILE	2.1
1	B	488	ILE	2.1
1	B	461	GLU	2.1
1	A	631	LEU	2.1
1	A	634	ALA	2.1
1	A	650	LEU	2.1
1	B	515	ASN	2.0
1	B	422	ILE	2.0
1	A	613	VAL	2.0
1	A	649	VAL	2.0
1	A	453	ALA	2.0
1	B	475	HIS	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
2	ACP	B	997	31/31	0.94	0.12	-0.69	44,49,52,54	0
2	ACP	A	997	31/31	0.94	0.10	-1.29	34,38,54,56	0
3	MG	A	998	1/1	0.76	0.13	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.