



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:58 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 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/ValidationPDFNotes.html>

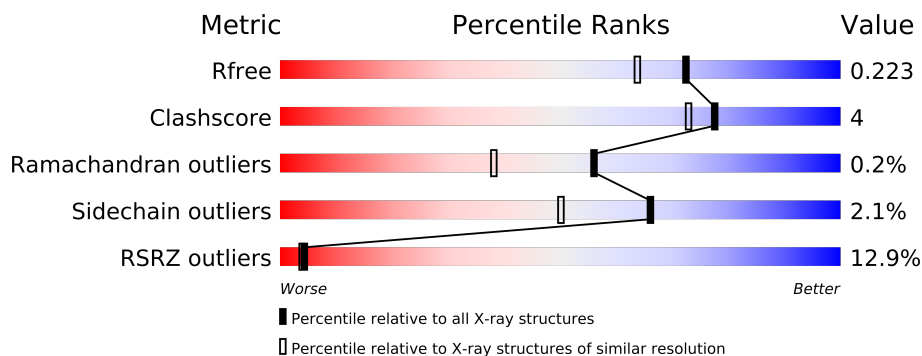
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	287	
1	B	287	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4573 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

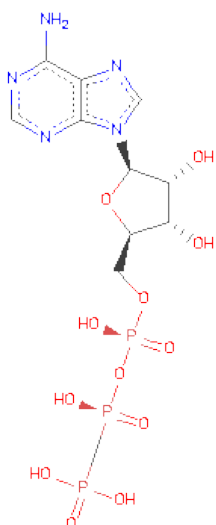
- Molecule 1 is a protein called Probable copper-exporting P-type ATPase A.

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 PHOSPHOMETHYLPHOSPHONICACID 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	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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

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

- Molecule 4 is water.

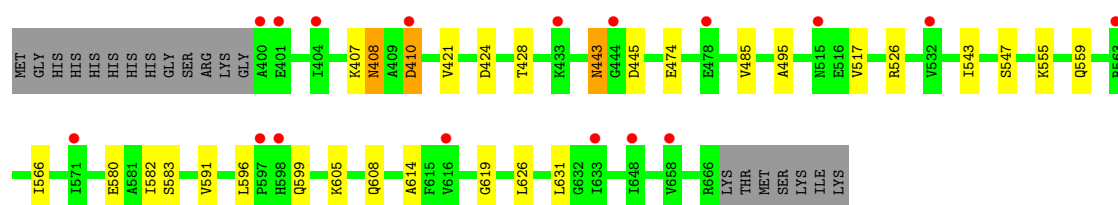
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	262	Total	O	0	0
			262	262		
4	B	211	Total	O	0	0
			211	211		

3 Residue-property plots

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.

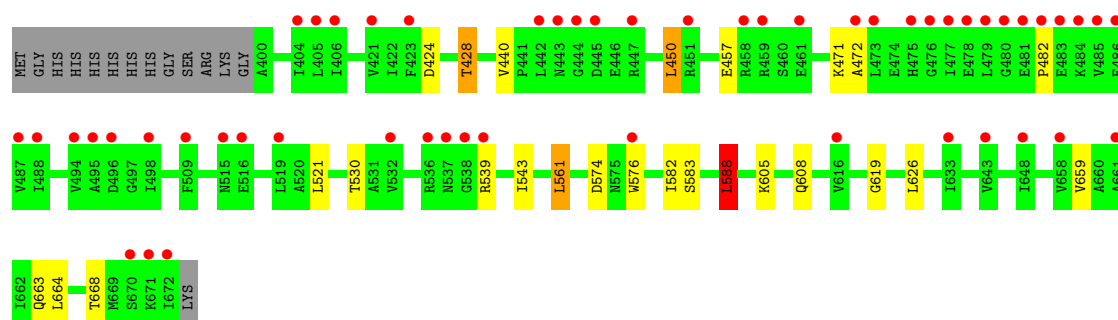
- Molecule 1: Probable copper-exporting P-type ATPase A

Chain A: 



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

Chain B: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	3501 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)	0.38 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 69000 reflections	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	262	0	0	4	0
4	B	211	0	0	2	0
All	All	4573	0	4242	31	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (31) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	265/287 (92%)	262 (99%)	3 (1%)	0	100	100
1	B	271/287 (94%)	264 (97%)	6 (2%)	1 (0%)	43	24
All	All	536/574 (93%)	526 (98%)	9 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	PRO

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	211/228 (92%)	208 (99%)	3 (1%)	78	68
1	B	217/228 (95%)	211 (97%)	6 (3%)	56	37
All	All	428/456 (94%)	419 (98%)	9 (2%)	66	50

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

Mol	Chain	Res	Type
1	A	408	ASN
1	A	410	ASP
1	A	443	ASN
1	B	428	THR
1	B	450	LEU

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 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	33,33,33	1.39	4 (12%)	52,52,52	1.91	12 (23%)
2	ACP	B	997	-	33,33,33	1.71	4 (12%)	52,52,52	1.80	11 (21%)

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	-	0/20/38/38	0/1/3/3
2	ACP	B	997	-	-	0/20/38/38	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	ACP	PG-C3B	5.70	1.84	1.79
2	B	997	ACP	PB-C3B	4.50	1.83	1.79
2	A	997	ACP	C5-C4	3.36	1.48	1.40
2	B	997	ACP	C5-C4	3.35	1.48	1.40
2	A	997	ACP	PG-C3B	3.05	1.82	1.79
2	A	997	ACP	C4-N9	-2.72	1.33	1.37
2	B	997	ACP	C4-N9	-2.45	1.34	1.37
2	A	997	ACP	PG-O2G	-2.22	1.50	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	997	ACP	N3-C2-N1	-7.22	122.67	128.71
2	B	997	ACP	N3-C2-N1	-6.78	123.04	128.71
2	A	997	ACP	N3-C4-N9	5.44	135.25	125.43
2	B	997	ACP	N3-C4-N9	5.25	134.91	125.43
2	A	997	ACP	PB-C3B-PG	-3.54	112.53	117.62
2	B	997	ACP	O1G-PG-C3B	-3.33	104.81	110.79
2	A	997	ACP	O3G-PG-O2G	3.30	118.81	108.35
2	B	997	ACP	C5-C4-N3	-3.10	118.94	125.70
2	A	997	ACP	C8-N9-C4	3.02	109.21	106.90
2	B	997	ACP	C4-C5-N7	-2.93	107.02	109.52
2	A	997	ACP	C5-C4-N3	-2.83	119.53	125.70
2	A	997	ACP	O3A-PB-O1B	-2.76	105.67	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	997	ACP	PA-O3A-PB	-2.60	123.93	131.74
2	B	997	ACP	O2B-PB-C3B	2.56	112.51	106.61
2	B	997	ACP	C2-N3-C4	2.42	120.90	114.01
2	A	997	ACP	C2-N3-C4	2.34	120.67	114.01
2	B	997	ACP	C8-N9-C4	2.27	108.63	106.90
2	A	997	ACP	O2B-PB-O1B	2.24	117.91	110.93
2	B	997	ACP	C2'-C1'-N9	-2.24	107.51	113.27
2	B	997	ACP	O3A-PB-O1B	-2.21	106.83	111.51
2	B	997	ACP	O4'-C1'-N9	2.11	110.40	108.44
2	A	997	ACP	C2-N1-C6	2.05	122.48	118.77
2	A	997	ACP	O2G-PG-C3B	-2.00	101.54	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/287 (93%)	0.49	17 (6%) 19 18	28, 39, 50, 56	0
1	B	273/287 (95%)	1.15	53 (19%) 2 1	31, 44, 67, 75	0
All	All	540/574 (94%)	0.82	70 (12%) 4 4	28, 40, 63, 75	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	ILE	9.6
1	B	480	GLY	7.6
1	B	481	GLU	7.2
1	B	643	VAL	6.7
1	B	494	VAL	6.0
1	B	482	PRO	5.9
1	B	670	SER	5.4
1	B	473	LEU	5.3
1	B	496	ASP	5.2
1	B	479	LEU	5.1
1	B	539	ARG	5.0
1	B	485	VAL	4.8
1	B	509	PHE	4.7
1	B	671	LYS	4.5
1	B	444	GLY	4.4
1	B	478	GLU	4.3
1	B	459	ARG	4.3
1	B	484	LYS	3.8
1	B	443	ASN	3.8
1	B	442	LEU	3.8
1	A	400	ALA	3.7
1	B	487	VAL	3.6
1	B	458	ARG	3.6
1	B	537	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	483	GLU	3.6
1	B	488	ILE	3.5
1	A	563	ARG	3.4
1	B	486	GLU	3.3
1	B	538	GLY	3.3
1	B	451	ARG	3.2
1	B	495	ALA	3.2
1	B	532	VAL	3.1
1	B	519	LEU	3.1
1	B	476	GLY	3.0
1	B	536	ARG	3.0
1	A	444	GLY	3.0
1	A	648	ILE	3.0
1	A	616	VAL	2.9
1	B	445	ASP	2.9
1	A	598	HIS	2.8
1	B	461	GLU	2.7
1	A	633	ILE	2.7
1	B	516	GLU	2.5
1	B	406	ILE	2.5
1	B	658	VAL	2.5
1	B	404	ILE	2.5
1	B	515	ASN	2.5
1	B	648	ILE	2.4
1	B	475	HIS	2.4
1	A	658	VAL	2.4
1	A	597	PRO	2.3
1	A	515	ASN	2.3
1	B	498	ILE	2.3
1	B	405	LEU	2.3
1	B	472	ALA	2.2
1	A	401	GLU	2.2
1	B	661	ALA	2.2
1	A	532	VAL	2.1
1	B	423	PHE	2.1
1	A	410	ASP	2.1
1	A	571	ILE	2.1
1	A	478	GLU	2.1
1	B	477	ILE	2.1
1	A	433	LYS	2.1
1	B	616	VAL	2.1
1	B	576	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	404	ILE	2.1
1	B	421	VAL	2.1
1	B	447	ARG	2.1
1	B	633	ILE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ACP	A	997	31/31	0.13	-0.33	34,38,54,56	0
2	ACP	B	997	31/31	0.11	-1.13	44,49,52,54	0
3	MG	A	998	1/1	0.10	-1.51	74,74,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.