



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

PDB ID : 3J08
EMDB ID: : EMD-5271
Title : High resolution helical reconstruction of the bacterial p-type ATPase copper transporter CopA
Authors : Wu, C.; Allen, G.S.; Cardozo, T.; Stokes, D.L.
Deposited on : 2011-05-09
Resolution : 10.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
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) : trunk27241

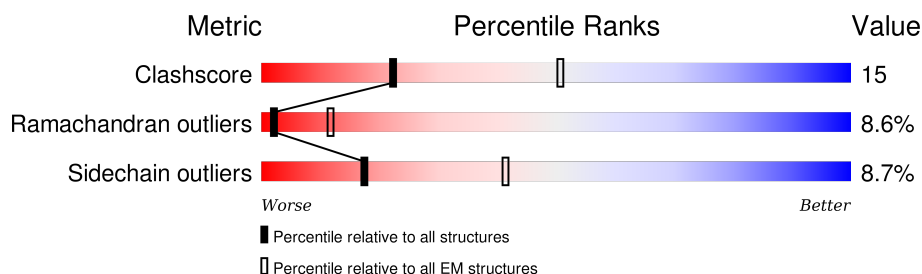
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	645	 70% 20% 7% .
1	B	645	 69% 20% 7% .

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 9734 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

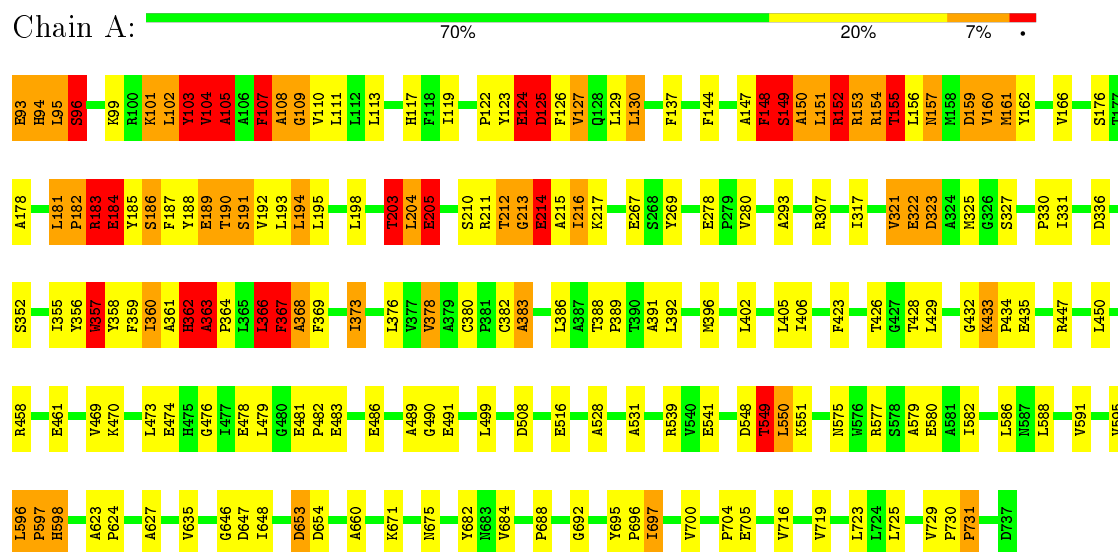
- Molecule 1 is a protein called copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	645	Total	C	N	O	S	0	0
			4867	3139	819	894	15		
1	B	645	Total	C	N	O	S	0	0
			4867	3139	819	894	15		

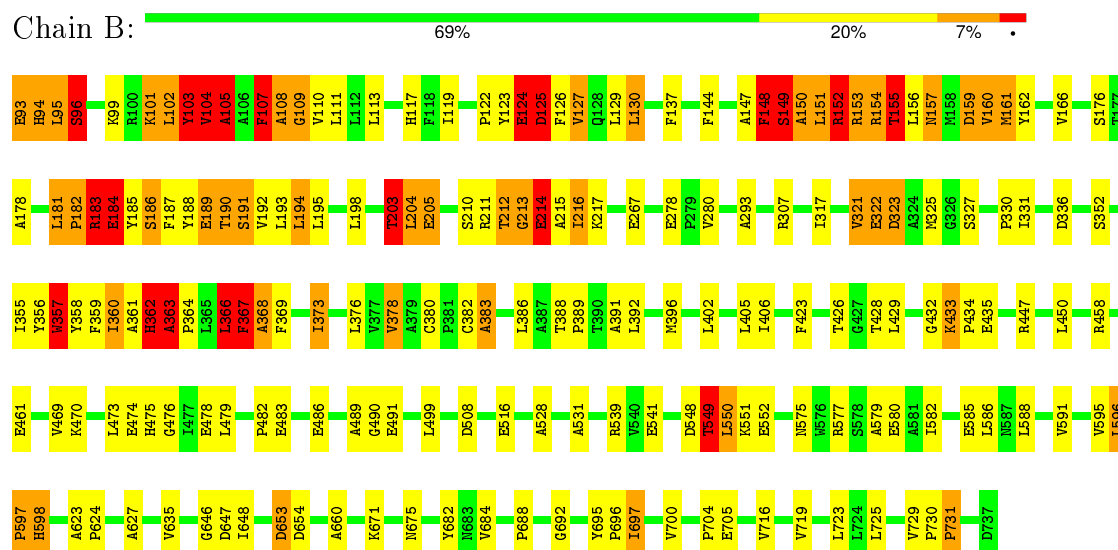
3 Residue-property plots

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. 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. 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: copper-exporting P-type ATPase A



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



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	two-fold phase residual	Depositor
CTF correction method	each tube-crystal	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO-163	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.76	0/4941	1.14	30/6700 (0.4%)
1	B	0.76	0/4941	1.14	31/6700 (0.5%)
All	All	0.76	0/9882	1.14	61/13400 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	30
1	B	0	30
All	All	0	60

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	SER	N-CA-CB	6.87	120.80	110.50
1	A	96	SER	N-CA-CB	6.85	120.77	110.50
1	A	155	THR	N-CA-CB	6.20	122.07	110.30
1	B	155	THR	N-CA-CB	6.18	122.05	110.30
1	B	149	SER	O-C-N	5.95	132.22	122.70
1	A	149	SER	O-C-N	5.94	132.21	122.70
1	A	491	GLU	OE1-CD-OE2	5.72	130.17	123.30
1	B	491	GLU	OE1-CD-OE2	5.70	130.15	123.30
1	A	189	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	B	189	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	357	TRP	CB-CA-C	5.59	121.58	110.40
1	B	435	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	435	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	B	357	TRP	CB-CA-C	5.58	121.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	THR	O-C-N	5.55	131.57	122.70
1	A	203	THR	O-C-N	5.54	131.57	122.70
1	B	184	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	A	184	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	B	705	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	A	705	GLU	OE1-CD-OE2	5.44	129.82	123.30
1	B	598	HIS	N-CA-CB	5.37	120.27	110.60
1	A	598	HIS	N-CA-CB	5.37	120.26	110.60
1	B	461	GLU	OE1-CD-OE2	5.31	129.68	123.30
1	A	93	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	B	93	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	211	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	461	GLU	OE1-CD-OE2	5.27	129.63	123.30
1	B	124	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	B	580	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	A	124	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	B	211	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	580	GLU	OE1-CD-OE2	5.25	129.61	123.30
1	B	267	GLU	OE1-CD-OE2	5.24	129.59	123.30
1	A	267	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	B	125	ASP	CB-CA-C	5.21	120.81	110.40
1	A	125	ASP	CB-CA-C	5.19	120.77	110.40
1	B	486	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	A	278	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	486	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	B	383	ALA	N-CA-CB	5.15	117.31	110.10
1	B	278	GLU	OE1-CD-OE2	5.15	129.47	123.30
1	A	383	ALA	N-CA-CB	5.13	117.29	110.10
1	A	293	ALA	N-CA-CB	5.13	117.29	110.10
1	B	293	ALA	N-CA-CB	5.12	117.27	110.10
1	A	516	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	A	577	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	B	516	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	B	105	ALA	CB-CA-C	5.07	117.71	110.10
1	B	577	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	105	ALA	CB-CA-C	5.06	117.69	110.10
1	B	214	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	B	307	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	214	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	483	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	A	205	GLU	OE1-CD-OE2	5.03	129.33	123.30
1	B	541	GLU	OE1-CD-OE2	5.03	129.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	GLU	OE1-CD-OE2	5.03	129.33	123.30
1	A	307	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	B	552	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	A	541	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	B	585	GLU	OE1-CD-OE2	5.00	129.30	123.30

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	LEU	Peptide
1	A	103	TYR	Peptide
1	A	107	PHE	Peptide
1	A	127	VAL	Peptide
1	A	152	ARG	Peptide
1	A	154	ARG	Peptide
1	A	182	PRO	Peptide
1	A	183	ARG	Peptide
1	A	184	GLU	Peptide
1	A	189	GLU	Peptide
1	A	190	THR	Peptide
1	A	212	THR	Peptide
1	A	213	GLY	Peptide
1	A	323	ASP	Peptide
1	A	355	ILE	Peptide
1	A	361	ALA	Peptide
1	A	362	HIS	Peptide
1	A	363	ALA	Peptide
1	A	433	LYS	Peptide
1	A	434	PRO	Peptide
1	A	549	THR	Peptide
1	A	595	VAL	Peptide
1	A	596	LEU	Peptide
1	A	597	PRO	Peptide
1	A	646	GLY	Peptide
1	A	647	ASP	Peptide
1	A	730	PRO	Peptide
1	A	731	PRO	Peptide
1	A	95	LEU	Peptide
1	A	96	SER	Peptide
1	B	102	LEU	Peptide
1	B	103	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	107	PHE	Peptide
1	B	127	VAL	Peptide
1	B	152	ARG	Peptide
1	B	154	ARG	Peptide
1	B	182	PRO	Peptide
1	B	183	ARG	Peptide
1	B	184	GLU	Peptide
1	B	189	GLU	Peptide
1	B	190	THR	Peptide
1	B	212	THR	Peptide
1	B	213	GLY	Peptide
1	B	323	ASP	Peptide
1	B	355	ILE	Peptide
1	B	361	ALA	Peptide
1	B	362	HIS	Peptide
1	B	363	ALA	Peptide
1	B	433	LYS	Peptide
1	B	434	PRO	Peptide
1	B	549	THR	Peptide
1	B	595	VAL	Peptide
1	B	596	LEU	Peptide
1	B	597	PRO	Peptide
1	B	646	GLY	Peptide
1	B	647	ASP	Peptide
1	B	730	PRO	Peptide
1	B	731	PRO	Peptide
1	B	95	LEU	Peptide
1	B	96	SER	Peptide

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 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	4867	0	5113	188	0
1	B	4867	0	5113	190	0
All	All	9734	0	10226	299	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 15.

All (299) 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:280:VAL:HG11	1:B:474:GLU:CD	1.21	1.48
1:A:458:ARG:NH1	1:B:473:LEU:HG	1.18	1.43
1:A:479:LEU:N	1:B:478:GLU:HA	1.39	1.35
1:A:458:ARG:HH12	1:B:473:LEU:CG	1.39	1.34
1:A:280:VAL:CG1	1:B:474:GLU:CD	2.01	1.27
1:A:458:ARG:NH1	1:B:473:LEU:CG	1.97	1.26
1:A:280:VAL:HG11	1:B:474:GLU:OE2	1.10	1.26
1:A:458:ARG:NH1	1:B:473:LEU:O	1.70	1.24
1:A:478:GLU:HA	1:B:479:LEU:N	1.50	1.20
1:A:280:VAL:CG1	1:B:474:GLU:OE1	1.95	1.14
1:A:478:GLU:CA	1:B:479:LEU:H	1.44	1.12
1:A:478:GLU:HB3	1:B:478:GLU:C	1.72	1.06
1:A:280:VAL:HG21	1:B:470:LYS:NZ	1.71	1.05
1:A:474:GLU:OE2	1:B:280:VAL:HG21	1.52	1.05
1:A:479:LEU:N	1:B:478:GLU:CA	2.20	1.04
1:A:473:LEU:HD11	1:B:469:VAL:CG1	1.89	1.03
1:A:479:LEU:H	1:B:478:GLU:HA	0.93	1.03
1:A:478:GLU:CA	1:B:479:LEU:N	2.02	1.01
1:A:458:ARG:CZ	1:B:473:LEU:HG	1.93	0.99
1:A:280:VAL:HG21	1:B:470:LYS:HZ2	1.23	0.97
1:A:473:LEU:CG	1:B:458:ARG:HH12	1.78	0.96
1:A:473:LEU:HG	1:B:458:ARG:NH1	1.81	0.96
1:A:478:GLU:CB	1:B:478:GLU:C	2.30	0.95
1:A:280:VAL:CG1	1:B:474:GLU:OE2	2.04	0.95
1:A:473:LEU:HG	1:B:458:ARG:HH12	1.32	0.95
1:A:124:GLU:HA	1:A:125:ASP:C	1.90	0.92
1:A:458:ARG:NH1	1:B:473:LEU:C	2.25	0.89
1:B:124:GLU:HA	1:B:125:ASP:C	1.90	0.89
1:A:447:ARG:NH2	1:B:482:PRO:HD3	1.88	0.86
1:A:402:LEU:HD13	1:A:660:ALA:HB1	1.59	0.85
1:A:458:ARG:HH12	1:B:473:LEU:CB	1.91	0.84
1:B:402:LEU:HD13	1:B:660:ALA:HB1	1.59	0.84
1:A:470:LYS:HZ2	1:B:280:VAL:HG21	1.41	0.83
1:A:470:LYS:NZ	1:B:280:VAL:HG21	1.93	0.83
1:A:280:VAL:HG11	1:B:474:GLU:OE1	1.67	0.82
1:A:474:GLU:OE2	1:B:280:VAL:CG2	2.17	0.82
1:A:458:ARG:HH12	1:B:473:LEU:HG	0.72	0.81
1:A:478:GLU:HA	1:B:479:LEU:H	0.68	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:HB3	1:B:478:GLU:HB3	1.61	0.80
1:A:473:LEU:CG	1:B:458:ARG:NH1	2.41	0.79
1:A:362:HIS:HB3	1:A:363:ALA:HB2	1.66	0.78
1:B:362:HIS:HB3	1:B:363:ALA:HB2	1.66	0.78
1:A:458:ARG:NH1	1:B:473:LEU:CD1	2.48	0.76
1:A:473:LEU:HG	1:B:458:ARG:CZ	2.16	0.75
1:A:160:VAL:HA	1:A:161:MET:C	2.06	0.74
1:B:357:TRP:N	1:B:358:TYR:HA	2.03	0.73
1:A:469:VAL:HG13	1:B:473:LEU:HD11	1.69	0.73
1:A:473:LEU:HD11	1:B:469:VAL:HG13	1.69	0.73
1:B:160:VAL:HA	1:B:161:MET:C	2.06	0.73
1:A:357:TRP:N	1:A:358:TYR:HA	2.03	0.72
1:A:478:GLU:HB3	1:B:478:GLU:CB	2.19	0.72
1:A:473:LEU:HG	1:B:458:ARG:NH2	2.05	0.72
1:A:490:GLY:HA3	1:A:596:LEU:HD22	1.72	0.70
1:B:490:GLY:HA3	1:B:596:LEU:HD22	1.72	0.69
1:A:117:HIS:NE2	1:A:373:ILE:HG21	2.08	0.69
1:A:469:VAL:CG1	1:B:473:LEU:HD11	2.22	0.68
1:B:489:ALA:HB1	1:B:596:LEU:HD13	1.75	0.68
1:A:478:GLU:C	1:B:478:GLU:HA	2.13	0.68
1:B:117:HIS:NE2	1:B:373:ILE:HG21	2.08	0.68
1:A:489:ALA:HB1	1:A:596:LEU:HD13	1.75	0.68
1:A:391:ALA:HB2	1:A:723:LEU:HD13	1.76	0.67
1:A:473:LEU:CD1	1:B:458:ARG:NH1	2.57	0.67
1:A:473:LEU:HD12	1:B:458:ARG:NH1	2.10	0.66
1:A:470:LYS:NZ	1:B:280:VAL:CG2	2.58	0.66
1:A:482:PRO:HD3	1:B:447:ARG:NH2	2.11	0.66
1:B:391:ALA:HB2	1:B:723:LEU:HD13	1.76	0.66
1:B:166:VAL:HG11	1:B:203:THR:HG21	1.78	0.65
1:A:280:VAL:HG13	1:B:474:GLU:OE1	1.91	0.65
1:A:478:GLU:C	1:B:478:GLU:CB	2.65	0.65
1:A:479:LEU:N	1:B:478:GLU:CB	2.52	0.65
1:A:280:VAL:CG2	1:B:470:LYS:NZ	2.56	0.65
1:A:166:VAL:HG11	1:A:203:THR:HG21	1.78	0.64
1:A:478:GLU:HB3	1:B:478:GLU:CA	2.27	0.64
1:A:473:LEU:HG	1:B:458:ARG:HH22	1.62	0.64
1:A:478:GLU:CB	1:B:478:GLU:HB3	2.29	0.62
1:A:124:GLU:HA	1:A:126:PHE:N	2.14	0.62
1:B:124:GLU:HA	1:B:126:PHE:N	2.14	0.62
1:A:482:PRO:HD3	1:B:447:ARG:HH21	1.64	0.62
1:A:181:LEU:HD13	1:A:182:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD13	1:B:182:PRO:HD2	1.82	0.61
1:A:151:LEU:O	1:A:152:ARG:C	2.39	0.61
1:A:154:ARG:HA	1:A:155:THR:O	2.01	0.61
1:B:151:LEU:O	1:B:152:ARG:C	2.39	0.61
1:B:154:ARG:HA	1:B:155:THR:O	2.01	0.60
1:A:476:GLY:HA2	1:B:458:ARG:HD3	1.83	0.59
1:A:215:ALA:C	1:A:217:LYS:H	2.06	0.59
1:A:473:LEU:HD11	1:B:469:VAL:HG11	1.81	0.59
1:A:186:SER:H	1:A:187:PHE:CA	2.15	0.59
1:A:124:GLU:CA	1:A:125:ASP:C	2.68	0.58
1:B:550:LEU:HD13	1:B:586:LEU:HD11	1.85	0.58
1:B:215:ALA:C	1:B:217:LYS:H	2.06	0.58
1:A:528:ALA:HB1	1:A:582:ILE:HG13	1.86	0.58
1:A:458:ARG:NH1	1:B:473:LEU:CA	2.67	0.58
1:A:363:ALA:HB3	1:A:364:PRO:HD3	1.86	0.58
1:B:186:SER:H	1:B:187:PHE:CA	2.15	0.58
1:A:321:VAL:HG22	1:A:627:ALA:CB	2.34	0.57
1:B:321:VAL:HG22	1:B:627:ALA:CB	2.34	0.57
1:A:147:ALA:O	1:A:148:PHE:C	2.43	0.57
1:A:550:LEU:HD13	1:A:586:LEU:HD11	1.85	0.57
1:B:356:TYR:O	1:B:357:TRP:C	2.42	0.57
1:A:356:TYR:O	1:A:357:TRP:C	2.42	0.57
1:B:203:THR:O	1:B:205:GLU:N	2.37	0.57
1:A:203:THR:O	1:A:205:GLU:N	2.37	0.57
1:A:478:GLU:C	1:B:478:GLU:CA	2.70	0.56
1:B:363:ALA:HB3	1:B:364:PRO:HD3	1.86	0.56
1:B:528:ALA:HB1	1:B:582:ILE:HG13	1.86	0.56
1:A:458:ARG:HH12	1:B:473:LEU:CA	2.18	0.56
1:B:147:ALA:O	1:B:148:PHE:C	2.43	0.56
1:A:478:GLU:C	1:B:478:GLU:HB3	2.25	0.56
1:B:187:PHE:CE2	1:B:188:TYR:HB2	2.41	0.56
1:B:392:LEU:O	1:B:396:MET:N	2.39	0.55
1:A:447:ARG:HH21	1:B:482:PRO:HD3	1.69	0.55
1:A:187:PHE:CE2	1:A:188:TYR:HB2	2.41	0.55
1:B:149:SER:O	1:B:150:ALA:C	2.45	0.55
1:A:392:LEU:O	1:A:396:MET:N	2.39	0.55
1:A:458:ARG:CZ	1:B:473:LEU:O	2.48	0.55
1:B:186:SER:N	1:B:187:PHE:HA	2.22	0.55
1:A:684:VAL:O	1:A:688:PRO:HD2	2.07	0.55
1:A:186:SER:N	1:A:187:PHE:HA	2.22	0.54
1:B:103:TYR:O	1:B:104:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:CD1	1:A:428:THR:HG21	2.43	0.54
1:A:103:TYR:O	1:A:104:VAL:HG12	2.07	0.54
1:A:186:SER:H	1:A:187:PHE:HA	1.73	0.54
1:B:684:VAL:O	1:B:688:PRO:HD2	2.07	0.54
1:A:149:SER:O	1:A:150:ALA:C	2.45	0.54
1:A:186:SER:CB	1:A:187:PHE:HA	2.38	0.54
1:A:107:PHE:C	1:A:109:GLY:H	2.11	0.53
1:B:423:PHE:CD1	1:B:428:THR:HG21	2.43	0.53
1:B:215:ALA:C	1:B:217:LYS:N	2.62	0.53
1:B:194:LEU:HD11	1:B:704:PRO:HB2	1.91	0.53
1:A:280:VAL:HG21	1:B:470:LYS:HZ1	1.70	0.53
1:A:317:ILE:O	1:A:321:VAL:HG23	2.09	0.53
1:A:194:LEU:HD11	1:A:704:PRO:HB2	1.91	0.53
1:B:186:SER:H	1:B:187:PHE:HA	1.73	0.53
1:B:129:LEU:C	1:B:129:LEU:HD23	2.29	0.53
1:A:215:ALA:C	1:A:217:LYS:N	2.62	0.53
1:B:428:THR:HA	1:B:635:VAL:HG11	1.91	0.53
1:B:317:ILE:O	1:B:321:VAL:HG23	2.09	0.52
1:A:129:LEU:C	1:A:129:LEU:HD23	2.29	0.52
1:B:124:GLU:CA	1:B:125:ASP:C	2.68	0.52
1:B:550:LEU:HD11	1:B:582:ILE:HG23	1.92	0.52
1:B:107:PHE:C	1:B:109:GLY:H	2.11	0.52
1:A:550:LEU:HD11	1:A:582:ILE:HG23	1.92	0.52
1:B:186:SER:CB	1:B:187:PHE:HA	2.38	0.52
1:B:203:THR:O	1:B:204:LEU:C	2.47	0.52
1:A:203:THR:O	1:A:204:LEU:C	2.47	0.52
1:A:107:PHE:C	1:A:109:GLY:N	2.63	0.51
1:B:635:VAL:HG13	1:B:653:ASP:OD1	2.10	0.51
1:A:376:LEU:O	1:A:380:CYS:N	2.40	0.51
1:B:107:PHE:C	1:B:109:GLY:N	2.63	0.51
1:A:428:THR:HA	1:A:635:VAL:HG11	1.90	0.51
1:A:280:VAL:HG12	1:B:474:GLU:OE1	2.02	0.51
1:B:186:SER:N	1:B:187:PHE:CA	2.74	0.51
1:B:376:LEU:O	1:B:380:CYS:N	2.40	0.51
1:A:149:SER:O	1:A:151:LEU:N	2.44	0.51
1:B:148:PHE:O	1:B:149:SER:HB3	2.11	0.51
1:A:148:PHE:O	1:A:149:SER:HB3	2.11	0.50
1:B:149:SER:O	1:B:151:LEU:N	2.44	0.50
1:A:458:ARG:HH12	1:B:473:LEU:C	2.03	0.50
1:A:635:VAL:HG13	1:A:653:ASP:OD1	2.10	0.50
1:B:156:LEU:O	1:B:157:ASN:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:CA	1:B:478:GLU:C	2.74	0.50
1:A:186:SER:N	1:A:187:PHE:CA	2.74	0.50
1:B:104:VAL:O	1:B:104:VAL:HG13	2.12	0.50
1:A:152:ARG:N	1:A:153:ARG:HA	2.27	0.49
1:A:478:GLU:CA	1:B:478:GLU:CA	2.91	0.49
1:A:104:VAL:HG13	1:A:104:VAL:O	2.12	0.49
1:A:95:LEU:CB	1:A:96:SER:HB2	2.42	0.49
1:B:95:LEU:CB	1:B:96:SER:HB2	2.42	0.49
1:A:156:LEU:O	1:A:157:ASN:C	2.50	0.49
1:B:321:VAL:HG22	1:B:627:ALA:HB1	1.95	0.48
1:A:479:LEU:O	1:B:478:GLU:N	2.40	0.48
1:A:321:VAL:HG22	1:A:627:ALA:HB1	1.95	0.48
1:B:104:VAL:O	1:B:105:ALA:HB3	2.13	0.48
1:A:692:GLY:O	1:A:696:PRO:HD2	2.14	0.48
1:B:152:ARG:N	1:B:153:ARG:HA	2.27	0.47
1:B:186:SER:H	1:B:187:PHE:CB	2.27	0.47
1:A:579:ALA:HB1	1:A:591:VAL:CG2	2.44	0.47
1:B:366:LEU:O	1:B:367:PHE:C	2.52	0.47
1:B:579:ALA:HB1	1:B:591:VAL:CG2	2.44	0.47
1:A:186:SER:H	1:A:187:PHE:CB	2.27	0.47
1:A:104:VAL:O	1:A:105:ALA:HB3	2.13	0.47
1:B:117:HIS:CE1	1:B:373:ILE:HG12	2.50	0.47
1:B:376:LEU:C	1:B:378:VAL:N	2.68	0.47
1:A:366:LEU:O	1:A:367:PHE:C	2.52	0.47
1:B:489:ALA:HB1	1:B:596:LEU:CD1	2.43	0.47
1:A:117:HIS:CE1	1:A:373:ILE:HG12	2.50	0.47
1:B:692:GLY:O	1:B:696:PRO:HD2	2.14	0.47
1:A:376:LEU:C	1:A:378:VAL:N	2.68	0.46
1:A:321:VAL:O	1:A:322:GLU:C	2.53	0.46
1:B:321:VAL:O	1:B:322:GLU:C	2.53	0.46
1:A:482:PRO:HG3	1:B:476:GLY:HA3	1.97	0.46
1:A:321:VAL:O	1:A:323:ASP:N	2.48	0.46
1:B:321:VAL:O	1:B:323:ASP:N	2.48	0.46
1:B:653:ASP:O	1:B:654:ASP:C	2.54	0.46
1:A:368:ALA:O	1:A:369:PHE:CB	2.64	0.46
1:A:388:THR:N	1:A:389:PRO:HD2	2.31	0.46
1:B:105:ALA:O	1:B:107:PHE:O	2.34	0.46
1:A:357:TRP:CB	1:A:358:TYR:HA	2.45	0.45
1:A:93:GLU:CB	1:A:150:ALA:HB2	2.47	0.45
1:B:104:VAL:O	1:B:105:ALA:CB	2.64	0.45
1:A:104:VAL:O	1:A:105:ALA:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG21	1:B:470:LYS:CE	2.43	0.45
1:A:101:LYS:O	1:A:103:TYR:N	2.49	0.45
1:A:458:ARG:NH1	1:B:473:LEU:HD12	2.30	0.45
1:A:105:ALA:O	1:A:107:PHE:O	2.34	0.45
1:B:101:LYS:O	1:B:103:TYR:N	2.49	0.45
1:A:405:LEU:O	1:A:648:ILE:HG23	2.17	0.45
1:B:405:LEU:O	1:B:648:ILE:HG23	2.17	0.45
1:A:653:ASP:O	1:A:654:ASP:C	2.54	0.45
1:A:489:ALA:HB1	1:A:596:LEU:CD1	2.43	0.45
1:B:388:THR:N	1:B:389:PRO:HD2	2.31	0.45
1:B:95:LEU:HB3	1:B:96:SER:HB2	1.99	0.45
1:A:96:SER:HB3	1:A:99:LYS:HB2	1.98	0.45
1:B:117:HIS:CD2	1:B:191:SER:HA	2.52	0.44
1:B:684:VAL:O	1:B:688:PRO:CD	2.66	0.44
1:B:623:ALA:N	1:B:624:PRO:CD	2.80	0.44
1:B:579:ALA:HB1	1:B:591:VAL:HG21	2.00	0.44
1:A:357:TRP:N	1:A:357:TRP:CD1	2.86	0.44
1:B:93:GLU:CB	1:B:150:ALA:HB2	2.47	0.44
1:A:623:ALA:N	1:A:624:PRO:CD	2.80	0.44
1:A:117:HIS:CD2	1:A:191:SER:HA	2.53	0.44
1:A:181:LEU:HD11	1:A:187:PHE:CE2	2.53	0.44
1:B:181:LEU:HD11	1:B:187:PHE:CE2	2.53	0.44
1:B:113:LEU:HD21	1:B:376:LEU:HD12	2.00	0.44
1:A:684:VAL:O	1:A:688:PRO:CD	2.66	0.44
1:A:113:LEU:HD21	1:A:376:LEU:HD12	2.00	0.43
1:B:368:ALA:O	1:B:369:PHE:CB	2.64	0.43
1:A:579:ALA:HB1	1:A:591:VAL:HG21	2.00	0.43
1:A:352:SER:O	1:A:356:TYR:CB	2.66	0.43
1:A:549:THR:C	1:A:550:LEU:HG	2.38	0.43
1:A:426:THR:HG22	1:A:426:THR:O	2.19	0.43
1:B:388:THR:O	1:B:391:ALA:HB3	2.19	0.43
1:B:549:THR:C	1:B:550:LEU:HG	2.38	0.43
1:A:95:LEU:HB3	1:A:96:SER:HB2	1.99	0.43
1:A:470:LYS:HZ1	1:B:280:VAL:CG2	2.30	0.43
1:B:352:SER:O	1:B:356:TYR:CB	2.67	0.43
1:A:117:HIS:CE1	1:A:373:ILE:HG21	2.53	0.43
1:B:96:SER:HB3	1:B:99:LYS:HB2	1.99	0.43
1:A:729:VAL:O	1:A:731:PRO:CD	2.67	0.42
1:B:357:TRP:N	1:B:357:TRP:CD1	2.86	0.42
1:B:95:LEU:HB2	1:B:96:SER:HB2	2.01	0.42
1:A:695:TYR:C	1:A:697:ILE:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:CA	1:B:478:GLU:HA	2.49	0.42
1:A:95:LEU:CB	1:A:96:SER:CB	2.97	0.42
1:A:269:TYR:CE1	1:B:475:HIS:HD2	2.29	0.42
1:B:429:LEU:O	1:B:550:LEU:C	2.57	0.42
1:B:729:VAL:O	1:B:731:PRO:CD	2.67	0.42
1:A:388:THR:O	1:A:391:ALA:HB3	2.19	0.42
1:A:108:ALA:O	1:A:111:LEU:N	2.52	0.42
1:B:190:THR:O	1:B:193:LEU:N	2.53	0.42
1:B:204:LEU:O	1:B:205:GLU:C	2.58	0.42
1:B:108:ALA:O	1:B:111:LEU:N	2.52	0.42
1:A:531:ALA:O	1:A:575:ASN:ND2	2.53	0.42
1:B:357:TRP:N	1:B:358:TYR:CA	2.79	0.42
1:A:429:LEU:O	1:A:550:LEU:C	2.57	0.42
1:B:129:LEU:HD23	1:B:130:LEU:N	2.35	0.42
1:A:129:LEU:HD23	1:A:130:LEU:N	2.35	0.42
1:B:426:THR:O	1:B:426:THR:HG22	2.19	0.42
1:A:481:GLU:HG2	1:B:447:ARG:NH1	2.35	0.42
1:A:95:LEU:HB2	1:A:96:SER:HB2	2.01	0.42
1:B:95:LEU:CB	1:B:96:SER:CB	2.97	0.42
1:A:190:THR:O	1:A:193:LEU:N	2.53	0.42
1:B:382:CYS:O	1:B:383:ALA:HB3	2.20	0.42
1:A:458:ARG:NH2	1:B:473:LEU:HG	2.29	0.41
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.97	0.41
1:A:382:CYS:O	1:A:383:ALA:HB3	2.20	0.41
1:B:357:TRP:CB	1:B:358:TYR:HA	2.44	0.41
1:B:117:HIS:CE1	1:B:373:ILE:HG21	2.53	0.41
1:B:695:TYR:C	1:B:697:ILE:H	2.22	0.41
1:A:183:ARG:O	1:A:184:GLU:O	2.38	0.41
1:B:362:HIS:HA	1:B:363:ALA:HA	1.80	0.41
1:B:528:ALA:HB1	1:B:582:ILE:CG1	2.50	0.41
1:B:160:VAL:HG13	1:B:161:MET:O	2.21	0.41
1:B:635:VAL:HG13	1:B:653:ASP:CG	2.41	0.41
1:A:123:TYR:O	1:A:124:GLU:C	2.59	0.41
1:A:160:VAL:HG13	1:A:161:MET:O	2.21	0.41
1:A:357:TRP:N	1:A:358:TYR:CA	2.79	0.41
1:A:113:LEU:HD11	1:A:376:LEU:HB2	2.03	0.41
1:A:94:HIS:O	1:A:95:LEU:C	2.58	0.41
1:B:94:HIS:O	1:B:95:LEU:C	2.58	0.41
1:B:531:ALA:O	1:B:575:ASN:ND2	2.53	0.41
1:B:183:ARG:O	1:B:184:GLU:O	2.38	0.41
1:A:213:GLY:O	1:A:214:GLU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LYS:CE	1:B:280:VAL:HG21	2.51	0.41
1:A:93:GLU:HB2	1:A:150:ALA:HB2	2.03	0.41
1:A:113:LEU:HD21	1:A:376:LEU:HB2	2.03	0.41
1:B:113:LEU:HD11	1:B:376:LEU:HB2	2.03	0.41
1:B:213:GLY:O	1:B:214:GLU:CB	2.69	0.41
1:A:204:LEU:O	1:A:205:GLU:C	2.58	0.40
1:A:729:VAL:O	1:A:731:PRO:HD3	2.21	0.40
1:B:729:VAL:O	1:B:731:PRO:HD3	2.21	0.40
1:B:671:LYS:CE	1:B:725:LEU:O	2.69	0.40
1:A:671:LYS:CE	1:A:725:LEU:O	2.69	0.40
1:B:635:VAL:HG22	1:B:653:ASP:OD1	2.22	0.40
1:B:113:LEU:HD21	1:B:376:LEU:HB2	2.03	0.40
1:B:123:TYR:O	1:B:124:GLU:C	2.59	0.40
1:A:321:VAL:O	1:A:323:ASP:HB2	2.22	0.40
1:A:130:LEU:HD23	1:A:130:LEU:HA	2.00	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 PDB entries followed by that with respect to all EM entries.

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	643/645 (100%)	518 (81%)	70 (11%)	55 (9%)	1	17
1	B	643/645 (100%)	518 (81%)	70 (11%)	55 (9%)	1	17
All	All	1286/1290 (100%)	1036 (81%)	140 (11%)	110 (9%)	2	17

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	101	LYS
1	A	103	TYR

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Mol	Chain	Res	Type
1	A	104	VAL
1	A	105	ALA
1	A	107	PHE
1	A	127	VAL
1	A	130	LEU
1	A	148	PHE
1	A	150	ALA
1	A	151	LEU
1	A	152	ARG
1	A	176	SER
1	A	178	ALA
1	A	185	TYR
1	A	191	SER
1	A	203	THR
1	A	204	LEU
1	A	214	GLU
1	A	322	GLU
1	A	363	ALA
1	A	433	LYS
1	A	550	LEU
1	A	598	HIS
1	A	653	ASP
1	B	96	SER
1	B	101	LYS
1	B	103	TYR
1	B	104	VAL
1	B	105	ALA
1	B	107	PHE
1	B	127	VAL
1	B	130	LEU
1	B	148	PHE
1	B	150	ALA
1	B	151	LEU
1	B	152	ARG
1	B	176	SER
1	B	178	ALA
1	B	185	TYR
1	B	191	SER
1	B	203	THR
1	B	204	LEU
1	B	214	GLU
1	B	322	GLU

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Mol	Chain	Res	Type
1	B	363	ALA
1	B	433	LYS
1	B	550	LEU
1	B	598	HIS
1	B	653	ASP
1	A	102	LEU
1	A	109	GLY
1	A	119	ILE
1	A	124	GLU
1	A	149	SER
1	A	184	GLU
1	A	216	ILE
1	A	357	TRP
1	A	362	HIS
1	A	368	ALA
1	A	432	GLY
1	A	551	LYS
1	B	102	LEU
1	B	109	GLY
1	B	119	ILE
1	B	124	GLU
1	B	149	SER
1	B	184	GLU
1	B	216	ILE
1	B	357	TRP
1	B	362	HIS
1	B	368	ALA
1	B	432	GLY
1	B	551	LYS
1	A	155	THR
1	A	160	VAL
1	A	321	VAL
1	A	325	MET
1	A	597	PRO
1	B	155	THR
1	B	160	VAL
1	B	321	VAL
1	B	325	MET
1	B	597	PRO
1	A	108	ALA
1	A	122	PRO
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	205	GLU
1	A	210	SER
1	A	360	ILE
1	A	367	PHE
1	A	549	THR
1	B	108	ALA
1	B	122	PRO
1	B	157	ASN
1	B	205	GLU
1	B	210	SER
1	B	360	ILE
1	B	367	PHE
1	B	549	THR
1	A	359	PHE
1	A	366	LEU
1	B	359	PHE
1	B	366	LEU
1	A	159	ASP
1	A	327	SER
1	B	159	ASP
1	B	327	SER
1	A	330	PRO
1	B	330	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 PDB entries followed by that with respect to all EM entries.

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	515/515 (100%)	470 (91%)	45 (9%)	13	45
1	B	515/515 (100%)	470 (91%)	45 (9%)	13	45
All	All	1030/1030 (100%)	940 (91%)	90 (9%)	17	45

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	104	VAL
1	A	110	VAL
1	A	124	GLU
1	A	125	ASP
1	A	137	PHE
1	A	144	PHE
1	A	148	PHE
1	A	152	ARG
1	A	153	ARG
1	A	155	THR
1	A	159	ASP
1	A	161	MET
1	A	162	TYR
1	A	181	LEU
1	A	183	ARG
1	A	186	SER
1	A	192	VAL
1	A	194	LEU
1	A	195	LEU
1	A	198	LEU
1	A	212	THR
1	A	216	ILE
1	A	331	ILE
1	A	336	ASP
1	A	357	TRP
1	A	360	ILE
1	A	366	LEU
1	A	367	PHE
1	A	373	ILE
1	A	378	VAL
1	A	386	LEU
1	A	406	ILE
1	A	450	LEU
1	A	499	LEU
1	A	508	ASP
1	A	539	ARG
1	A	548	ASP
1	A	588	LEU
1	A	675	ASN
1	A	682	TYR
1	A	697	ILE
1	A	700	VAL

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Mol	Chain	Res	Type
1	A	716	VAL
1	A	719	VAL
1	B	94	HIS
1	B	104	VAL
1	B	110	VAL
1	B	124	GLU
1	B	125	ASP
1	B	137	PHE
1	B	144	PHE
1	B	148	PHE
1	B	152	ARG
1	B	153	ARG
1	B	155	THR
1	B	159	ASP
1	B	161	MET
1	B	162	TYR
1	B	181	LEU
1	B	183	ARG
1	B	186	SER
1	B	192	VAL
1	B	194	LEU
1	B	195	LEU
1	B	198	LEU
1	B	212	THR
1	B	216	ILE
1	B	331	ILE
1	B	336	ASP
1	B	357	TRP
1	B	360	ILE
1	B	366	LEU
1	B	367	PHE
1	B	373	ILE
1	B	378	VAL
1	B	386	LEU
1	B	406	ILE
1	B	450	LEU
1	B	499	LEU
1	B	508	ASP
1	B	539	ARG
1	B	548	ASP
1	B	588	LEU
1	B	675	ASN

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Mol	Chain	Res	Type
1	B	682	TYR
1	B	697	ILE
1	B	700	VAL
1	B	716	VAL
1	B	719	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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.