



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 12:32 AM JST

PDB ID : 9V53 / pdb_00009v53
EMDB ID : EMD-64785
Title : Structure of TolC, YbjP, and AcrABZ complex
Authors : Ge, X.F.; Gu, Z.W.; Wang, J.W.
Deposited on : 2025-05-25
Resolution : 3.39 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

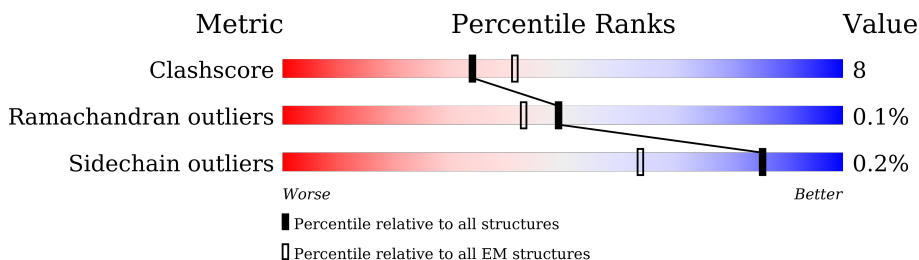
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.39 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.











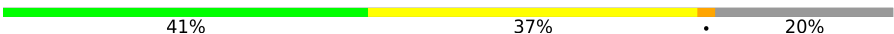
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	C1	493	74% 14% 12%
1	C2	493	69% 19% 12%
1	C3	493	73% 14% 12%
2	P1	171	63% 26% 11%
2	P2	171	63% 25% • 11%
2	P3	171	60% 29% • 11%
3	A1	397	74% 13% 13%
3	A2	397	76% 10% 13%
3	A3	397	76% 11% 13%

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Mol	Chain	Length	Quality of chain
3	a1	397	 76%11%13%
3	a2	397	 76%11%13%
3	a3	397	 78%8%13%
4	BL	1049	 77%21%.
4	BO	1049	 77%21%.
4	BT	1049	 78%21%.
5	ZL	49	 49%31%20%
5	ZO	49	 49%31%20%
5	ZT	49	 41%37%.20%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 53464 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 Outer membrane protein TolC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		
1	C2	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		
1	C3	432	Total	C	N	O	S	0	0
			3331	2054	591	681	5		

- Molecule 2 is a protein called Uncharacterized lipoprotein YbjP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P1	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		
2	P2	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		
2	P3	152	Total	C	N	O	S	0	0
			1182	722	218	238	4		

- Molecule 3 is a protein called Multidrug efflux pump subunit AcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	A2	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	A3	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a2	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a1	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		
3	a3	344	Total	C	N	O	S	0	0
			2587	1617	456	512	2		

- Molecule 4 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BL	1036	Total	C	N	O	S	0	0
			7847	5050	1296	1457	44		
4	BT	1034	Total	C	N	O	S	0	0
			7837	5044	1294	1455	44		
4	BO	1034	Total	C	N	O	S	0	0
			7837	5044	1294	1455	44		

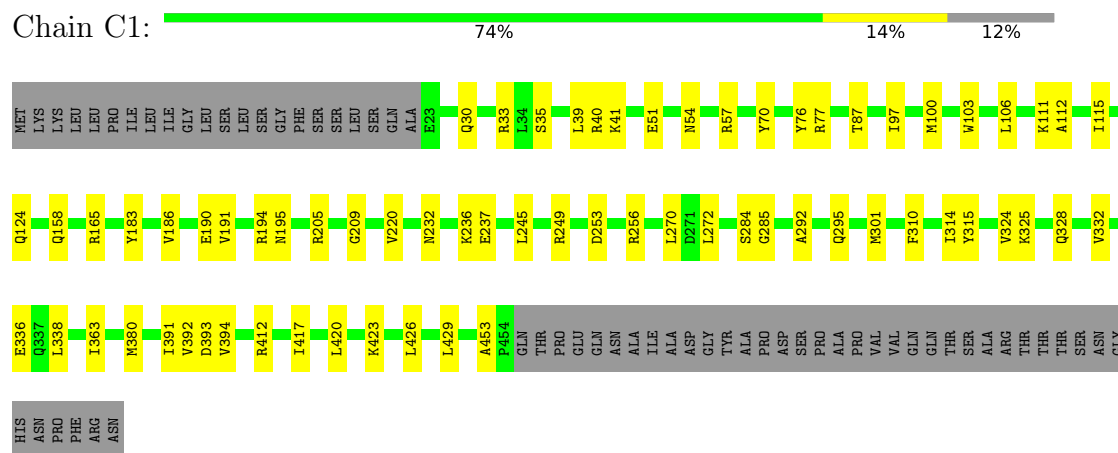
- Molecule 5 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	ZL	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
5	ZT	39	Total	C	N	O	S	0	0
			294	203	41	47	3		
5	ZO	39	Total	C	N	O	S	0	0
			294	203	41	47	3		

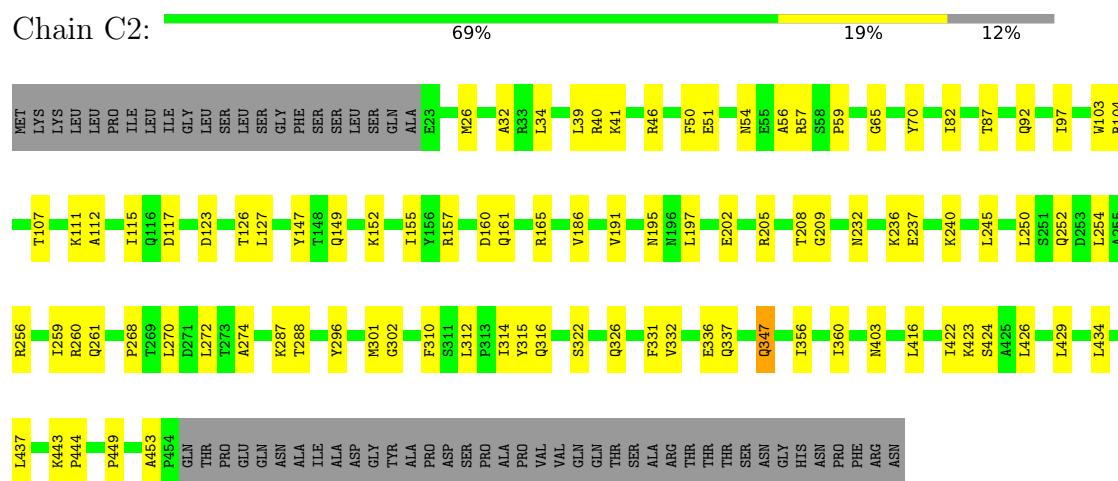
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

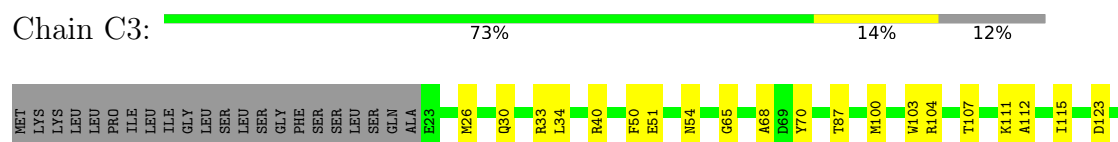
- Molecule 1: Outer membrane protein TolC

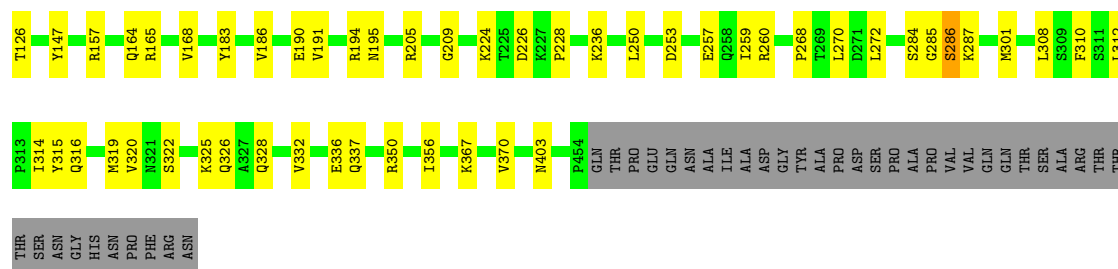


- Molecule 1: Outer membrane protein TolC



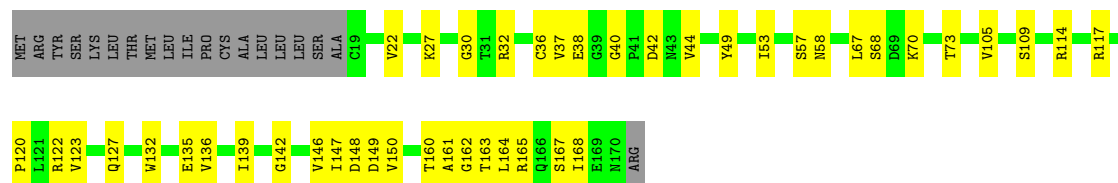
- Molecule 1: Outer membrane protein TolC





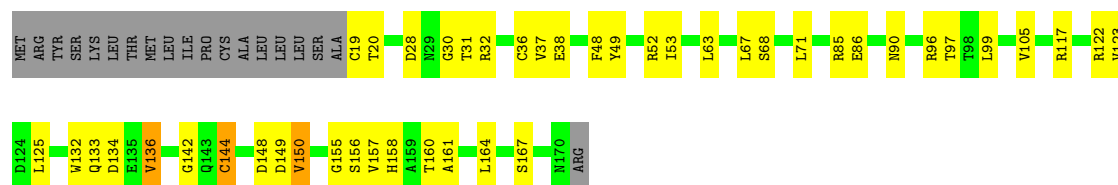
• Molecule 2: Uncharacterized lipoprotein YbjP

Chain P1: 63% 26% 11%



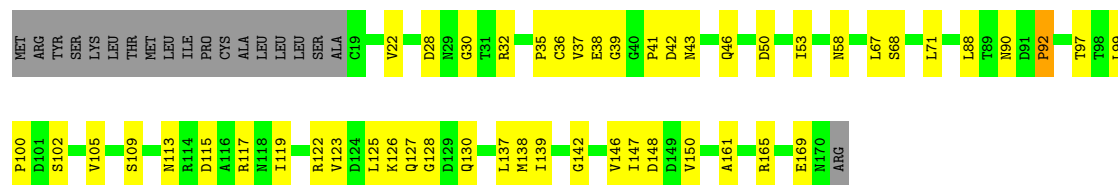
• Molecule 2: Uncharacterized lipoprotein YbjP

Chain P2: 63% 25% 11%



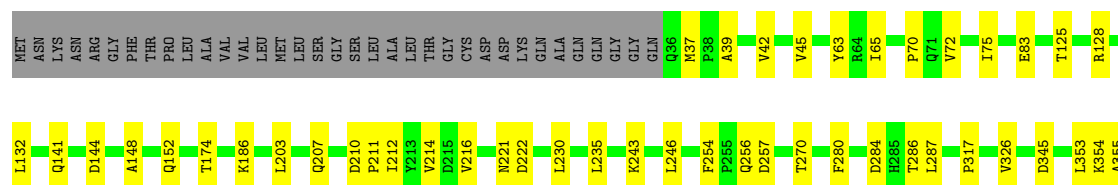
• Molecule 2: Uncharacterized lipoprotein YbjP

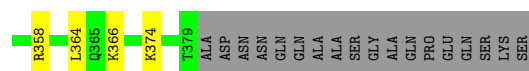
Chain P3: 60% 29% 11%



• Molecule 3: Multidrug efflux pump subunit AcrA

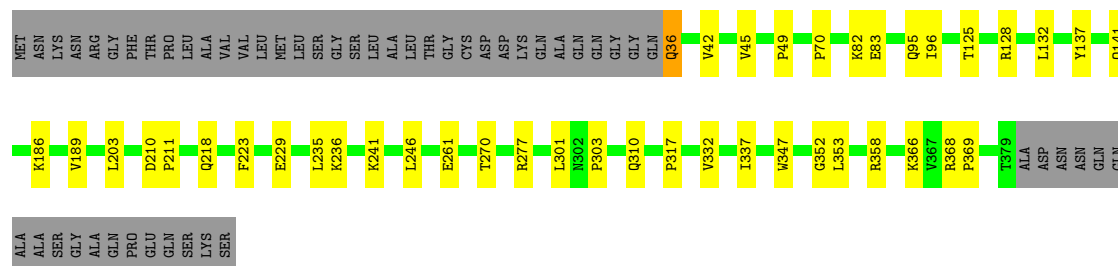
Chain A1: 74% 13% 13%





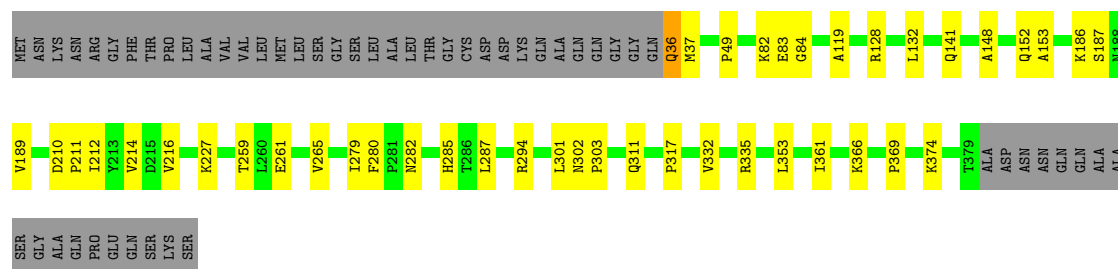
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A2: 76% 10% 13%



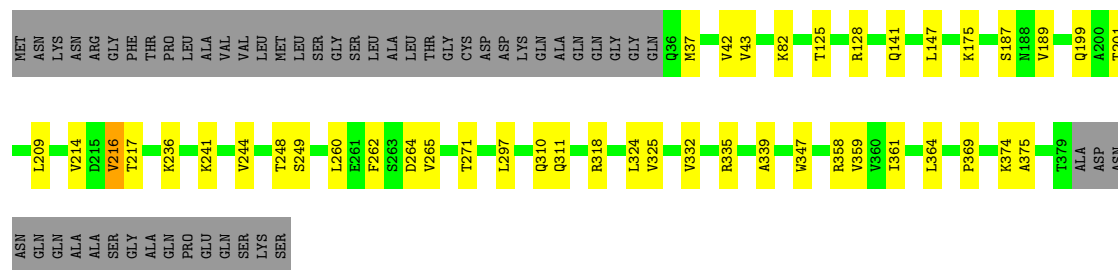
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A3: 76% 11% 13%



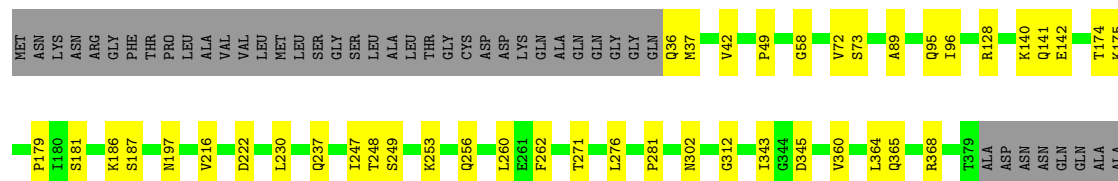
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain a2: 76% 11% 13%




• Molecule 3: Multidrug efflux pump subunit AcrA

Chain a1: 76% 11% 13%



SER
GLY
ALA
GLN
PRO
GLU
GLN
SER
LYS
SER


• Molecule 3: Multidrug efflux pump subunit AcrA

Chain a3:  78% 8% 13%

MET ASN LYS ASN ARG GLY PHE THR LEU ALA VAL VAL LEU MET LEU SER GLY SER LEU ALA THR THR CYS ASP ASP LYS GLN GLN GLN GLY GLN Q36 M37 P38 K46 I52 T53 K82 I87 E88 A89 R128 Q141 K175 S181 S187 N188

V189 L235 V244 T247 S249 F262 S263 D264 V265 T271 R294 A295 R296 L297 E298 Q310 R315 A339 W347 L353 K354 V373 T379 ALA ASP ASN GLN GLN ALA ALA SER GLY ALA GLN PRO GLU GLN SER LYS SER

• Molecule 4: Multidrug efflux pump subunit AcrB

Chain BL:  77% 21%

H1 I16 I17 I18 I19 I20 A26 I27 L28 K29 L30 P31 V43 T44 D53 Q58 T62 Q63 V64 Q67 I72 M76 V88 T91 E95 Q104 V107 Q108 L117 S128 V129 E130 K131 I143 T169 V172 L177 F178 G179 F380

I186 I187 M188 Q197 D202 Q213 L219 L220 V225 N231 T238 F246 S258 R259 L261 L270 Y275 A286 L291 T306 V340 L348 L349 L350 V351 M355 L359 Q360 N361 T365 L366 L367 P368 V374 L375 L376 L377 G378 T379 F380

A381 V382 F388 L393 T394 K395 V399 L400 A401 L405 T410 F414 N415 S434 R438 L444 L445 A446 L449 S462 L466 L472 S476 A477 N478 S481 A485 L488 T489 L492 C493 L497 F513 D517 N517 S530 T534 L535


R540 Y545 M552 A553 Y554 L555 R558 L559 P560 L564 P565 D566 G570 T583 Q584 K601 V612 Q622 L626 L631 R637 R643 M649 R653 A654 F655 L658 V663 G679 F682 F683 L684 T685 D686 Q687 L695 L702 L703

K704 E705 K708 M712 F718 F727 D732 D733 E734 K735 W754 W758 F759 M760 W772 V773 E776 K777 K778 W779 R780 M781 W788 W790 M791 R792 W798 S807 R808 W809 E810 Y811 Y819 L822 P823 D824 S824 S825 E826 L827 L828 G829

L843 Q846 S849 K850 A873 P874 S875 L879 V883 W884 F885 L886 A890 L891 E892 E893 Y901 N902 L903 Y904 P906 L907 G908 Y909 L910 L913 L914 T922 F927 Q928 Y929 G930 L931 L937 K940 I941 A942 L943 L944 L945 L960 R971 L974

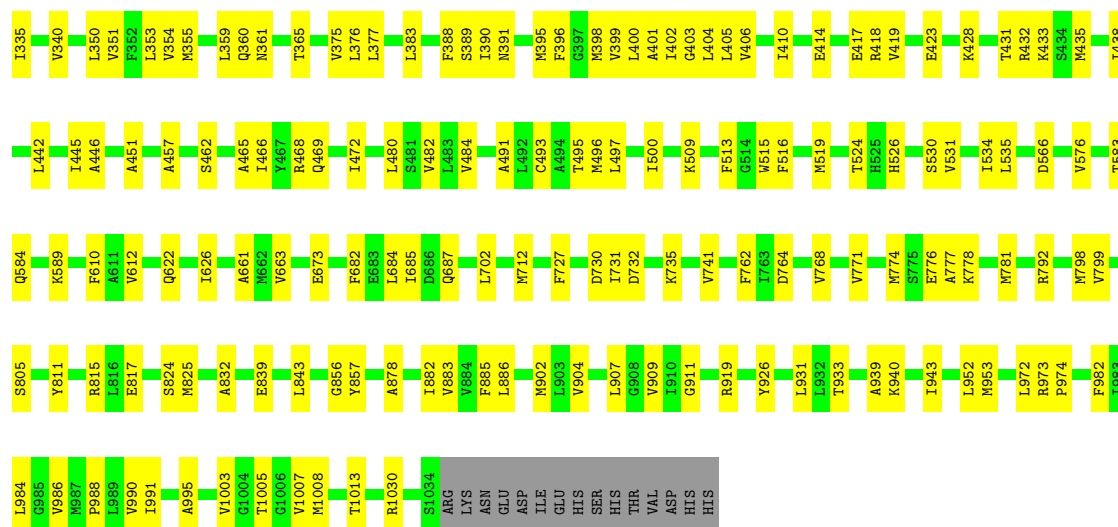
I975 L976 S979 I983 L984 L989 Q1000 M1008 M1011 A1014 T1015 V1016 L1017 F1020 Y1021 P1022 P1023 V1027 F1033 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS

• Molecule 4: Multidrug efflux pump subunit AcrB

Chain BT:  78% 21%

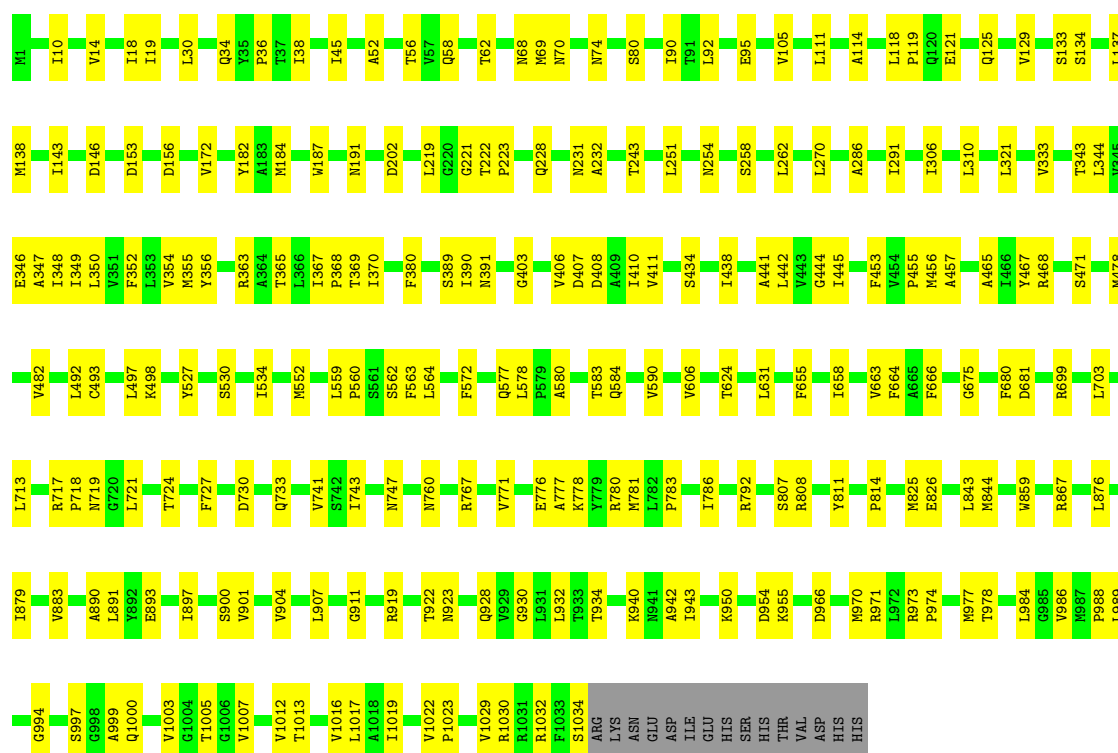
H1 P2 N3 I6 I10 W13 V14 M20 G23 L30 P31 P36 T37 T38 V43 T44 I45 Q58 T62 Q73 D73 R74 L75 V88 L92 V105 Q106 V107 Q108 N109 K110 L111 L112 L113 A114 M115 Q123 Q124 Q125 Q126 V127 S128 V129 E130 K131

L137 M138 N144 D153 S167 R168 T169 S170 D174 V175 Y182 A183 M184 W187 F196 Q197 D202 A212 Q213 V214 F223 F224 Q228 Q237 E244 E245 F246 Q247 K248 K252 S258 F281 L293 A303 R307 E314 G320 K131



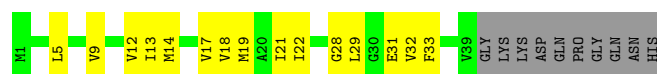
• Molecule 4: Multidrug efflux pump subunit AcrB

Chain BO: 77% 21% .

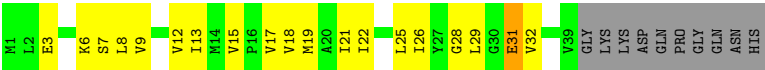


• Molecule 5: Multidrug efflux pump accessory protein AcrZ

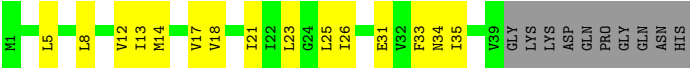
Chain ZL: 49% 31% 20%



• Molecule 5: Multidrug efflux pump accessory protein AcrZ



● Molecule 5: Multidrug efflux pump accessory protein AcrZ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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 >5	RMSZ	# Z >5
1	C1	0.12	0/3373	0.25	0/4584
1	C2	0.12	0/3373	0.25	0/4584
1	C3	0.12	0/3373	0.25	0/4584
2	P1	0.12	0/1204	0.35	0/1640
2	P2	0.14	0/1204	0.37	0/1640
2	P3	0.28	1/1204 (0.1%)	0.55	2/1640 (0.1%)
3	A1	0.10	0/2620	0.25	0/3564
3	A2	0.10	0/2620	0.24	0/3564
3	A3	0.10	0/2620	0.25	0/3564
3	a1	0.10	0/2620	0.24	0/3564
3	a2	0.10	0/2620	0.24	0/3564
3	a3	0.09	0/2620	0.22	0/3564
4	BL	0.11	0/7997	0.27	0/10861
4	BO	0.11	0/7987	0.29	0/10847
4	BT	0.12	0/7987	0.29	0/10847
5	ZL	0.22	0/298	0.53	0/403
5	ZO	0.24	0/298	0.68	0/403
5	ZT	0.16	0/298	0.56	0/403
All	All	0.12	1/54316 (0.0%)	0.29	2/73820 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P3	92	PRO	CG-CD	-6.17	1.29	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P3	92	PRO	CA-N-CD	-11.90	95.34	112.00
2	P3	92	PRO	N-CD-CG	-8.77	90.04	103.20

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	C1	3331	0	3278	57	0
1	C2	3331	0	3278	70	0
1	C3	3331	0	3278	54	0
2	P1	1182	0	1132	37	0
2	P2	1182	0	1132	37	0
2	P3	1182	0	1132	35	0
3	A1	2587	0	2648	33	0
3	A2	2587	0	2648	31	0
3	A3	2587	0	2648	33	0
3	a1	2587	0	2648	28	0
3	a2	2587	0	2648	32	0
3	a3	2587	0	2648	24	0
4	BL	7847	0	7975	164	0
4	BO	7837	0	7971	163	0
4	BT	7837	0	7971	150	0
5	ZL	294	0	330	13	0
5	ZO	294	0	330	10	0
5	ZT	294	0	330	15	0
All	All	53464	0	54025	883	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 8.

All (883) 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)
3:A2:36:GLN:HE21	3:A2:36:GLN:N	1.57	1.01
3:A3:36:GLN:HE21	3:A3:36:GLN:N	1.62	0.98
1:C2:259:ILE:HD11	1:C2:331:PHE:HB2	1.61	0.82
3:A2:36:GLN:N	3:A2:36:GLN:NE2	2.27	0.81
3:A3:36:GLN:N	3:A3:36:GLN:NE2	2.30	0.79
4:BL:449:LEU:HB2	4:BL:478:MET:HE1	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P3:41:PRO:HB3	2:P3:138:MET:HG3	1.66	0.75
2:P3:138:MET:HE1	2:P3:147:ILE:HD13	1.69	0.75
5:ZO:23:LEU:HA	5:ZO:26:ILE:HD12	1.70	0.73
4:BO:356:TYR:HA	4:BO:365:THR:HG21	1.71	0.73
3:A3:49:PRO:HB3	3:A3:303:PRO:HG3	1.69	0.72
4:BO:911:GLY:H	4:BO:1013:THR:HG21	1.55	0.72
4:BT:167:SER:O	4:BO:70:ASN:ND2	2.23	0.71
5:ZO:17:VAL:O	5:ZO:21:ILE:HD12	1.90	0.71
1:C1:40:ARG:HB2	1:C2:336:GLU:HG3	1.73	0.71
1:C3:236:LYS:HB2	2:P3:161:ALA:HB1	1.72	0.70
4:BO:876:LEU:HD21	4:BO:932:LEU:HD11	1.72	0.70
3:a2:43:VAL:HG22	3:a2:361:ILE:HD11	1.74	0.69
1:C1:40:ARG:HH22	2:P2:117:ARG:HG3	1.57	0.69
4:BL:415:ASN:OD1	4:BL:971:ARG:NH2	2.26	0.69
3:a1:271:THR:HG21	4:BL:258:SER:HB2	1.75	0.69
1:C1:253:ASP:OD1	2:P1:122:ARG:NH2	2.27	0.68
4:BL:552:MET:HE1	4:BL:910:ILE:HA	1.75	0.68
2:P2:86:GLU:N	2:P2:86:GLU:OE2	2.25	0.68
1:C2:424:SER:HB2	1:C2:429:LEU:HD22	1.77	0.67
1:C2:46:ARG:NH1	1:C2:117:ASP:OD2	2.28	0.67
3:A2:337:ILE:HG21	3:A2:353:LEU:HD23	1.77	0.67
1:C2:256:ARG:HA	1:C2:259:ILE:HD12	1.77	0.67
4:BT:10:ILE:HD11	4:BO:893:GLU:HA	1.76	0.67
4:BT:732:ASP:HB3	4:BT:735:LYS:HB2	1.77	0.67
2:P1:70:LYS:HE2	2:P1:165:ARG:HH12	1.59	0.66
1:C2:252:GLN:OE1	2:P2:122:ARG:NH1	2.28	0.66
4:BT:988:PRO:HA	4:BT:991:ILE:HG22	1.77	0.66
4:BO:989:LEU:HD22	4:BO:1000:GLN:HB3	1.77	0.66
2:P2:30:GLY:HA2	2:P2:142:GLY:HA2	1.78	0.66
4:BT:435:MET:HE3	4:BT:435:MET:HA	1.77	0.66
4:BT:446:ALA:HB2	4:BT:482:VAL:HG11	1.78	0.66
4:BL:67:GLN:OE1	4:BO:767:ARG:NH1	2.28	0.65
2:P3:39:GLY:O	2:P3:43:ASN:ND2	2.29	0.65
4:BT:878:ALA:O	4:BT:882:ILE:HG13	1.97	0.65
4:BT:919:ARG:HD3	4:BT:1005:THR:HG21	1.79	0.65
1:C1:314:ILE:HG22	1:C1:315:TYR:H	1.59	0.65
4:BL:446:ALA:HA	4:BL:478:MET:HE2	1.78	0.65
4:BO:1030:ARG:HH12	4:BO:1034:SER:HA	1.60	0.65
4:BT:314:GLU:N	4:BT:314:GLU:OE1	2.28	0.65
5:ZT:17:VAL:O	5:ZT:21:ILE:HD12	1.97	0.65
1:C2:314:ILE:HG22	1:C2:315:TYR:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:ZT:21:ILE:O	5:ZT:25:LEU:HD22	1.97	0.64
1:C2:149:GLN:HG3	1:C2:453:ALA:HB1	1.78	0.64
3:A2:337:ILE:HG22	3:A2:352:GLY:HA3	1.79	0.64
4:BL:622:GLN:OE1	4:BO:231:ASN:ND2	2.30	0.64
4:BO:897:ILE:HD11	4:BO:950:LYS:HG2	1.79	0.64
2:P1:147:ILE:HD12	2:P1:148:ASP:H	1.62	0.64
1:C2:232:ASN:HB3	2:P2:161:ALA:HB3	1.78	0.64
3:a1:256:GLN:HG2	3:a1:281:PRO:HG2	1.79	0.64
2:P3:119:ILE:HB	2:P3:138:MET:HB2	1.78	0.64
2:P1:27:LYS:HA	2:P1:114:ARG:HH21	1.63	0.63
1:C1:256:ARG:HH12	2:P1:122:ARG:HH21	1.45	0.63
4:BT:30:LEU:HD12	4:BT:31:PRO:HD2	1.81	0.63
2:P1:30:GLY:HA2	2:P1:142:GLY:HA2	1.79	0.63
5:ZT:8:LEU:O	5:ZT:12:VAL:HG23	1.99	0.63
1:C1:30:GLN:OE1	1:C1:33:ARG:NH2	2.32	0.63
5:ZL:17:VAL:O	5:ZL:21:ILE:HG23	1.99	0.63
4:BT:228:GLN:NE2	4:BO:781:MET:SD	2.71	0.63
3:A1:366:LYS:NZ	4:BL:658:ILE:O	2.32	0.63
4:BL:554:TYR:OH	4:BL:558:ARG:NH1	2.32	0.63
1:C1:51:GLU:OE2	1:C1:54:ASN:ND2	2.32	0.62
4:BL:960:LEU:HD21	4:BL:1027:VAL:HG13	1.80	0.62
4:BT:62:THR:HB	4:BT:88:VAL:HG21	1.81	0.62
5:ZT:9:VAL:O	5:ZT:13:ILE:HG12	1.98	0.62
1:C1:191:VAL:O	1:C1:195:ASN:ND2	2.31	0.62
1:C3:191:VAL:O	1:C3:195:ASN:ND2	2.31	0.62
1:C3:30:GLN:OE1	1:C3:33:ARG:NH2	2.32	0.62
2:P2:96:ARG:NH1	2:P2:155:GLY:O	2.32	0.62
3:a2:318:ARG:NH2	4:BT:153:ASP:OD1	2.33	0.62
4:BL:808:ARG:NH2	4:BL:810:GLU:OE2	2.32	0.62
4:BT:244:GLU:OE1	4:BT:248:LYS:NZ	2.33	0.62
2:P1:32:ARG:NH1	2:P1:68:SER:O	2.33	0.62
4:BL:20:MET:HE2	4:BL:374:VAL:HG22	1.80	0.62
4:BL:552:MET:HA	4:BL:552:MET:HE2	1.80	0.62
4:BO:444:GLY:HA2	4:BO:891:LEU:HD21	1.82	0.62
3:A3:301:LEU:HD12	3:A3:303:PRO:HD3	1.80	0.61
4:BT:445:ILE:HG12	4:BT:940:LYS:HD3	1.81	0.61
4:BO:478:MET:O	4:BO:482:VAL:HG23	2.00	0.61
4:BL:213:GLN:HE22	4:BL:238:THR:HG22	1.64	0.61
4:BT:340:VAL:HG21	4:BT:395:MET:HB3	1.83	0.61
1:C1:57:ARG:HA	1:C1:106:LEU:HD21	1.82	0.61
3:a2:325:VAL:HG21	3:a2:335:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:202:ASP:OD2	4:BL:792:ARG:NH2	2.34	0.61
4:BL:893:GLU:HA	4:BO:10:ILE:HD11	1.82	0.61
2:P3:139:ILE:HG13	2:P3:146:VAL:HB	1.82	0.61
3:A1:210:ASP:HB3	3:A1:211:PRO:HD3	1.83	0.60
4:BO:730:ASP:OD2	4:BO:808:ARG:NH1	2.27	0.60
1:C2:40:ARG:HH12	2:P3:117:ARG:HD3	1.65	0.60
4:BT:3:ASN:HA	4:BT:6:ILE:HD12	1.82	0.60
4:BT:184:MET:HB3	4:BT:771:VAL:HG12	1.84	0.60
1:C2:65:GLY:HA2	1:C3:314:ILE:HG12	1.83	0.60
1:C2:256:ARG:HH12	1:C2:260:ARG:HG3	1.66	0.60
1:C1:190:GLU:OE2	1:C1:194:ARG:NH2	2.35	0.60
3:A3:366:LYS:NZ	4:BO:658:ILE:O	2.30	0.60
1:C2:165:ARG:HG2	3:A2:132:LEU:HD21	1.83	0.60
4:BO:776:GLU:O	4:BO:778:LYS:N	2.35	0.60
4:BL:367:ILE:HG12	4:BL:492:LEU:HB3	1.84	0.60
4:BL:405:LEU:HD22	4:BL:481:SER:HB3	1.84	0.60
4:BL:545:TYR:OH	4:BL:903:LEU:O	2.18	0.60
4:BT:396:PHE:HE2	4:BT:1003:VAL:HG21	1.66	0.60
2:P3:42:ASP:N	2:P3:42:ASP:OD1	2.34	0.60
4:BL:18:ILE:HG13	4:BT:886:LEU:HD23	1.84	0.60
5:ZL:18:VAL:O	5:ZL:22:ILE:HG12	2.02	0.59
4:BO:1032:ARG:O	4:BO:1032:ARG:NH1	2.34	0.59
1:C1:39:LEU:HD11	1:C1:124:GLN:HG2	1.83	0.59
4:BT:712:MET:HE1	4:BT:839:GLU:HG2	1.85	0.59
4:BL:379:THR:HG22	4:BL:477:ALA:HA	1.84	0.59
4:BT:115:MET:O	4:BT:123:GLN:NE2	2.34	0.59
4:BO:445:ILE:HG23	4:BO:940:LYS:HG3	1.83	0.59
4:BO:577:GLN:HG2	4:BO:624:THR:HG22	1.84	0.59
4:BO:343:THR:HG23	4:BO:988:PRO:HB2	1.83	0.59
4:BO:919:ARG:HD3	4:BO:1005:THR:HG21	1.85	0.59
5:ZO:8:LEU:O	5:ZO:12:VAL:HG23	2.02	0.59
1:C2:32:ALA:HB2	1:C2:208:THR:HG22	1.83	0.59
3:a2:310:GLN:NE2	3:a2:311:GLN:OE1	2.35	0.59
4:BO:467:TYR:OH	4:BO:928:GLN:OE1	2.20	0.59
1:C2:205:ARG:NH2	2:P3:169:GLU:OE2	2.36	0.59
1:C3:253:ASP:OD1	2:P3:122:ARG:NH2	2.35	0.59
1:C2:155:ILE:HG13	1:C2:186:VAL:HG21	1.85	0.59
2:P2:136:VAL:HG23	2:P2:150:VAL:HG22	1.85	0.59
3:a2:324:LEU:HD12	3:a2:364:LEU:HD22	1.85	0.59
4:BL:62:THR:HB	4:BL:88:VAL:HG21	1.84	0.59
1:C2:152:LYS:HA	1:C2:186:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:32:ARG:NE	2:P1:36:CYS:SG	2.73	0.58
3:a3:244:VAL:HG22	3:a3:297:LEU:HD12	1.84	0.58
4:BL:979:SER:HA	4:BL:1011:MET:HE2	1.85	0.58
4:BT:197:GLN:HA	4:BT:798:MET:HE3	1.85	0.58
4:BL:291:ILE:HD13	4:BL:306:ILE:HD13	1.86	0.58
4:BT:414:GLU:HG2	4:BT:974:PRO:HG3	1.85	0.58
1:C2:51:GLU:HG2	1:C3:325:LYS:HB3	1.84	0.58
1:C2:191:VAL:O	1:C2:195:ASN:ND2	2.36	0.58
4:BL:30:LEU:HD12	4:BL:31:PRO:HD2	1.85	0.58
4:BL:104:GLN:OE1	4:BL:131:LYS:NZ	2.32	0.58
4:BO:153:ASP:OD1	4:BO:182:TYR:OH	2.19	0.58
4:BT:687:GLN:HE22	4:BT:856:GLY:HA3	1.68	0.58
3:A1:243:LYS:NZ	3:A1:257:ASP:OD2	2.37	0.58
1:C3:34:LEU:O	1:C3:40:ARG:NH1	2.36	0.58
3:A1:128:ARG:NH1	3:a1:141:GLN:OE1	2.34	0.58
4:BT:495:THR:HG23	4:BT:496:MET:HG3	1.86	0.58
2:P3:30:GLY:HA2	2:P3:142:GLY:HA2	1.84	0.57
1:C1:237:GLU:HG2	1:C1:426:LEU:HD21	1.86	0.57
2:P3:138:MET:HE2	2:P3:138:MET:HA	1.87	0.57
3:A1:42:VAL:HG11	3:A1:358:ARG:HB3	1.87	0.57
3:A1:212:ILE:HG21	3:A1:287:LEU:HD11	1.86	0.57
4:BL:43:VAL:HG11	4:BL:107:VAL:HG21	1.87	0.57
1:C3:26:MET:HA	1:C3:26:MET:HE3	1.85	0.57
3:A3:128:ARG:NH1	3:a3:141:GLN:OE1	2.38	0.57
5:ZL:5:LEU:O	5:ZL:9:VAL:HG12	2.04	0.57
2:P2:49:TYR:O	2:P2:53:ILE:HG12	2.04	0.57
4:BO:719:ASN:ND2	4:BO:826:GLU:OE1	2.36	0.57
1:C3:314:ILE:HG22	1:C3:315:TYR:H	1.69	0.57
4:BL:684:LEU:HD11	4:BL:702:LEU:HD23	1.87	0.57
4:BT:986:VAL:HG11	4:BT:1007:VAL:HG11	1.85	0.57
1:C1:77:ARG:NH2	1:C2:301:MET:O	2.37	0.57
2:P2:28:ASP:N	2:P2:28:ASP:OD1	2.37	0.57
4:BT:224:PRO:HA	4:BO:781:MET:HE1	1.86	0.57
4:BL:400:LEU:HD23	4:BL:929:VAL:HG12	1.87	0.56
1:C1:100:MET:HA	1:C1:103:TRP:HD1	1.69	0.56
4:BT:815:ARG:NH1	4:BT:817:GLU:OE2	2.38	0.56
1:C2:40:ARG:HB2	1:C3:336:GLU:HG3	1.87	0.56
2:P2:96:ARG:NH1	2:P2:156:SER:OG	2.38	0.56
1:C1:270:LEU:HD13	1:C1:310:PHE:HB2	1.88	0.56
4:BO:74:ASN:HB3	4:BO:95:GLU:HB3	1.88	0.56
4:BO:251:LEU:HD11	4:BO:262:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:340:VAL:HG11	4:BL:395:MET:HB3	1.88	0.56
4:BL:886:LEU:HD12	4:BO:18:ILE:HG13	1.88	0.56
3:a2:248:THR:HG22	3:a2:249:SER:H	1.70	0.56
4:BL:560:PRO:HG2	4:BL:922:THR:HG22	1.88	0.56
1:C1:57:ARG:HB2	1:C1:106:LEU:HD11	1.86	0.56
2:P1:105:VAL:HG12	2:P1:123:VAL:HG22	1.87	0.56
2:P3:105:VAL:HA	2:P3:123:VAL:HA	1.86	0.56
3:A2:218:GLN:HG2	3:A2:223:PHE:HB2	1.88	0.56
4:BL:350:LEU:HD11	4:BL:984:LEU:HD13	1.88	0.56
4:BL:58:GLN:HA	4:BL:62:THR:HG22	1.87	0.56
4:BT:137:LEU:HD23	4:BT:138:MET:HB3	1.88	0.56
4:BT:576:VAL:HG22	4:BT:663:VAL:HG22	1.88	0.56
4:BT:768:VAL:HG21	4:BO:119:PRO:HG3	1.88	0.56
1:C1:97:ILE:HD11	1:C1:272:LEU:HD23	1.87	0.55
4:BT:75:LEU:HD11	4:BT:92:LEU:HD23	1.88	0.55
1:C2:92:GLN:NE2	1:C2:274:ALA:O	2.39	0.55
3:a1:230:LEU:HD11	3:a1:237:GLN:HB2	1.87	0.55
4:BT:926:TYR:HB3	4:BT:1003:VAL:HG23	1.89	0.55
4:BO:655:PHE:HB3	4:BO:663:VAL:HG13	1.86	0.55
3:A3:83:GLU:HG2	3:A3:186:LYS:HA	1.86	0.55
4:BL:1016:VAL:HG12	4:BL:1017:LEU:HD23	1.88	0.55
4:BO:202:ASP:OD2	4:BO:792:ARG:NH2	2.39	0.55
4:BO:455:PRO:HG3	4:BO:883:VAL:HG11	1.89	0.55
3:A2:317:PRO:HA	4:BT:811:TYR:HB2	1.89	0.55
4:BO:1012:VAL:O	4:BO:1016:VAL:HG22	2.06	0.55
1:C2:34:LEU:O	1:C2:40:ARG:NH1	2.40	0.55
4:BT:531:VAL:HA	4:BT:534:ILE:HG12	1.89	0.55
4:BO:478:MET:HE3	4:BO:478:MET:HA	1.87	0.55
2:P3:71:LEU:HD11	2:P3:148:ASP:HA	1.89	0.55
4:BO:900:SER:HB3	4:BO:1029:VAL:HG11	1.88	0.55
4:BT:214:VAL:HG11	4:BO:747:ASN:HB3	1.89	0.55
1:C2:443:LYS:HD2	1:C2:444:PRO:HD2	1.88	0.54
4:BO:350:LEU:HD22	4:BO:984:LEU:HD12	1.88	0.54
4:BO:572:PHE:HE1	4:BO:631:LEU:HD21	1.72	0.54
1:C3:259:ILE:HD11	1:C3:328:GLN:HA	1.89	0.54
2:P2:52:ARG:HH21	2:P2:99:LEU:HD21	1.72	0.54
4:BT:990:VAL:HG21	4:BT:1008:MET:HG3	1.88	0.54
4:BL:908:GLY:HA2	4:BL:1014:ALA:HB2	1.88	0.54
1:C2:288:THR:HA	1:C2:296:TYR:HD2	1.72	0.54
1:C3:328:GLN:NE2	2:P3:109:SER:O	2.40	0.54
3:a2:332:VAL:HG23	3:a2:369:PRO:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:655:PHE:HB3	4:BL:663:VAL:HG13	1.89	0.54
4:BL:879:ILE:O	4:BL:883:VAL:HG22	2.08	0.54
4:BL:906:PRO:HA	4:BL:909:VAL:HG22	1.88	0.54
4:BT:350:LEU:HD11	4:BT:984:LEU:HB3	1.88	0.54
4:BO:121:GLU:OE2	4:BO:125:GLN:NE2	2.41	0.54
4:BO:407:ASP:OD1	4:BO:408:ASP:N	2.40	0.54
3:A2:83:GLU:HG2	3:A2:186:LYS:HA	1.88	0.54
4:BT:105:VAL:HG21	4:BO:105:VAL:HG13	1.88	0.54
3:A1:317:PRO:HA	4:BL:811:TYR:HB2	1.88	0.54
4:BO:562:SER:OG	4:BO:563:PHE:N	2.40	0.54
4:BT:359:LEU:HD22	4:BT:417:GLU:HG2	1.90	0.54
1:C1:236:LYS:HB2	2:P1:161:ALA:HB1	1.91	0.53
1:C3:70:TYR:HD1	1:C3:87:THR:HG22	1.73	0.53
4:BO:133:SER:OG	4:BO:134:SER:N	2.42	0.53
1:C2:202:GLU:OE1	1:C3:350:ARG:NH1	2.41	0.53
1:C3:284:SER:OG	1:C3:285:GLY:N	2.41	0.53
4:BL:231:ASN:ND2	4:BT:622:GLN:OE1	2.39	0.53
2:P3:113:ASN:HD21	2:P3:115:ASP:HB2	1.73	0.53
2:P3:28:ASP:OD1	2:P3:28:ASP:N	2.37	0.53
4:BL:177:LEU:HG	4:BL:179:GLY:H	1.73	0.53
4:BL:1034:SER:OG	4:BL:1035:ARG:N	2.42	0.53
4:BT:457:ALA:O	4:BT:468:ARG:NH1	2.41	0.53
1:C1:301:MET:HE2	1:C1:301:MET:HA	1.90	0.53
3:A1:230:LEU:HA	3:A1:235:LEU:HB2	1.90	0.53
3:A3:317:PRO:HA	4:BO:811:TYR:HB2	1.90	0.53
3:a3:247:ILE:HD11	3:a3:296:ARG:HH12	1.74	0.53
4:BL:776:GLU:HG3	4:BL:778:LYS:HG2	1.90	0.53
4:BT:395:MET:O	4:BT:399:VAL:HG13	2.09	0.53
1:C2:160:ASP:OD2	3:A2:137:TYR:OH	2.25	0.53
4:BT:153:ASP:OD1	4:BT:182:TYR:OH	2.25	0.53
4:BL:225:VAL:H	4:BT:781:MET:HE3	1.74	0.53
4:BT:38:ILE:HG22	4:BT:462:SER:HB3	1.91	0.53
4:BO:346:GLU:HA	4:BO:349:ILE:HG22	1.91	0.53
4:BL:776:GLU:HB3	4:BL:779:TYR:HD2	1.73	0.53
4:BT:530:SER:O	4:BT:534:ILE:HG23	2.09	0.53
3:A3:294:ARG:NH1	4:BO:191:ASN:OD1	2.42	0.52
4:BT:451:ALA:HB1	4:BT:883:VAL:HG12	1.91	0.52
4:BT:491:ALA:O	4:BT:495:THR:HG22	2.08	0.52
2:P1:42:ASP:OD1	2:P1:42:ASP:N	2.40	0.52
4:BO:527:TYR:OH	4:BO:1019:ILE:O	2.25	0.52
4:BO:971:ARG:HH22	4:BO:974:PRO:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:ZL:14:MET:O	5:ZL:18:VAL:HG23	2.09	0.52
3:A2:125:THR:OG1	3:a2:141:GLN:NE2	2.42	0.52
4:BL:545:TYR:HE1	4:BL:907:LEU:HD21	1.75	0.52
4:BT:72:ILE:HD11	4:BT:110:LYS:HG3	1.92	0.52
2:P2:160:THR:HG21	2:P2:167:SER:HB3	1.91	0.52
4:BL:275:TYR:HB2	4:BO:223:PRO:HD3	1.91	0.52
5:ZT:3:GLU:HA	5:ZT:6:LYS:HG2	1.92	0.52
1:C1:40:ARG:HH12	2:P2:117:ARG:HG3	1.75	0.52
3:A1:70:PRO:HD3	3:A1:203:LEU:HD13	1.91	0.52
3:A3:210:ASP:HB3	3:A3:211:PRO:HD3	1.92	0.52
4:BL:444:GLY:HA3	4:BL:891:LEU:HD22	1.91	0.52
4:BT:196:PHE:O	4:BT:252:LYS:NZ	2.42	0.52
4:BL:983:ILE:HG23	4:BL:1008:MET:SD	2.50	0.52
4:BO:713:LEU:HD13	4:BO:843:LEU:HD23	1.91	0.52
2:P2:90:ASN:HD22	2:P2:97:THR:HB	1.74	0.52
2:P3:127:GLN:HG3	2:P3:128:GLY:H	1.75	0.52
3:A3:187:SER:OG	3:A3:189:VAL:O	2.27	0.52
4:BT:20:MET:HG2	4:BT:377:LEU:HD12	1.92	0.52
2:P1:57:SER:O	2:P1:58:ASN:ND2	2.43	0.51
4:BL:395:MET:O	4:BL:399:VAL:HG13	2.09	0.51
2:P1:49:TYR:CE2	2:P1:123:VAL:HG11	2.45	0.51
4:BO:34:GLN:HB2	4:BO:333:VAL:HG22	1.92	0.51
1:C2:115:ILE:HG22	1:C2:250:LEU:HB3	1.92	0.51
3:a2:217:THR:HG21	4:BT:258:SER:HA	1.92	0.51
4:BL:355:MET:HG2	4:BL:365:THR:HA	1.92	0.51
4:BL:764:ASP:OD2	4:BL:769:LYS:NZ	2.31	0.51
4:BT:712:MET:HA	4:BT:832:ALA:HB2	1.92	0.51
4:BO:733:GLN:HG2	4:BO:743:ILE:HD12	1.93	0.51
1:C2:54:ASN:OD1	1:C2:57:ARG:NH2	2.43	0.51
2:P1:70:LYS:HE2	2:P1:165:ARG:HH22	1.74	0.51
3:a2:262:PHE:CG	3:a2:262:PHE:O	2.62	0.51
4:BL:72:ILE:HD13	4:BL:107:VAL:HG12	1.92	0.51
4:BT:115:MET:HE1	4:BT:127:VAL:HG22	1.93	0.51
4:BO:456:MET:HG2	4:BO:471:SER:HB2	1.92	0.51
1:C2:50:PHE:HB3	2:P3:22:VAL:HG12	1.93	0.51
3:A2:189:VAL:HG21	3:A2:203:LEU:HD22	1.93	0.51
3:A3:37:MET:HA	3:A3:37:MET:HE2	1.92	0.51
4:BT:223:PRO:HG2	4:BO:780:ARG:HH22	1.76	0.51
4:BL:703:LEU:HD11	4:BL:718:PRO:HG3	1.93	0.51
4:BT:187:TRP:HA	4:BT:774:MET:O	2.10	0.51
4:BT:401:ALA:O	4:BT:405:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:953:MET:HE1	4:BT:1030:ARG:HE	1.76	0.51
4:BL:44:THR:HG22	4:BL:91:THR:HG23	1.93	0.51
4:BL:76:MET:HE2	4:BL:95:GLU:HA	1.92	0.51
5:ZO:14:MET:O	5:ZO:18:VAL:HG23	2.10	0.51
2:P2:31:THR:HG22	2:P2:31:THR:O	2.11	0.51
4:BL:695:LEU:HG	4:BL:825:MET:HG3	1.91	0.51
5:ZL:29:LEU:HA	5:ZL:32:VAL:HG12	1.93	0.51
4:BT:335:ILE:HD13	4:BT:995:ALA:HB1	1.93	0.51
4:BT:465:ALA:O	4:BT:469:GLN:HG2	2.11	0.51
4:BO:370:ILE:HD11	4:BO:492:LEU:HD11	1.92	0.51
1:C3:190:GLU:OE2	1:C3:194:ARG:NH2	2.41	0.50
4:BL:534:ILE:HD13	5:ZL:33:PHE:HE1	1.76	0.50
1:C2:236:LYS:HE2	2:P2:157:VAL:HG21	1.92	0.50
4:BL:559:LEU:HD12	4:BL:560:PRO:HD2	1.93	0.50
4:BT:137:LEU:HD12	4:BT:293:LEU:HB2	1.92	0.50
5:ZT:28:GLY:O	5:ZT:32:VAL:HG12	2.11	0.50
4:BO:583:THR:OG1	4:BO:584:GLN:N	2.45	0.50
1:C1:310:PHE:HD2	1:C3:68:ALA:HB3	1.76	0.50
1:C2:82:ILE:HD11	1:C2:287:LYS:HD3	1.92	0.50
3:a1:95:GLN:NE2	3:a1:96:ILE:O	2.44	0.50
4:BO:184:MET:HE1	4:BO:243:THR:HG22	1.92	0.50
1:C1:380:MET:HE3	1:C1:393:ASP:HB3	1.94	0.50
1:C3:301:MET:HE2	1:C3:301:MET:HA	1.92	0.50
4:BT:353:LEU:HD21	5:ZT:15:VAL:HG11	1.94	0.50
1:C3:228:PRO:HG3	1:C3:356:ILE:HG21	1.93	0.50
4:BO:441:ALA:O	4:BO:445:ILE:HD12	2.11	0.50
4:BO:681:ASP:OD1	4:BO:681:ASP:N	2.42	0.50
5:ZL:19:MET:HE2	5:ZL:19:MET:HA	1.93	0.50
4:BT:414:GLU:OE2	4:BT:973:ARG:NE	2.43	0.50
4:BO:363:ARG:HD2	4:BO:498:LYS:HZ2	1.77	0.50
3:A2:128:ARG:NH1	3:a2:141:GLN:OE1	2.44	0.50
3:a3:294:ARG:NH2	4:BL:734:GLU:OE2	2.35	0.50
5:ZO:21:ILE:O	5:ZO:25:LEU:HD22	2.12	0.50
2:P2:123:VAL:O	2:P2:133:GLN:HA	2.12	0.49
3:A3:335:ARG:HH21	3:A3:353:LEU:HA	1.76	0.49
3:a3:264:ASP:OD1	3:a3:265:VAL:N	2.44	0.49
4:BL:622:GLN:HE22	4:BO:221:GLY:HA2	1.77	0.49
1:C3:112:ALA:O	1:C3:115:ILE:HG12	2.13	0.49
4:BL:378:GLY:O	4:BL:382:VAL:HG12	2.12	0.49
4:BL:393:LEU:HD13	4:BL:466:ILE:HG23	1.95	0.49
4:BO:219:LEU:HD12	4:BO:232:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:148:ASP:OD1	2:P1:149:ASP:N	2.45	0.49
2:P3:88:LEU:HD12	2:P3:92:PRO:HG3	1.95	0.49
3:A2:95:GLN:NE2	3:A2:96:ILE:O	2.45	0.49
3:a1:89:ALA:N	3:a1:181:SER:OG	2.46	0.49
4:BL:63:GLN:O	4:BL:67:GLN:HG3	2.12	0.49
4:BT:375:VAL:HG13	4:BT:480:LEU:HB3	1.94	0.49
1:C1:332:VAL:O	1:C1:336:GLU:HG2	2.12	0.49
2:P1:163:THR:O	2:P1:167:SER:OG	2.26	0.49
3:a2:214:VAL:HG12	3:a2:216:VAL:HG23	1.94	0.49
4:BL:679:GLY:HA3	4:BL:829:GLY:O	2.13	0.49
4:BT:401:ALA:HA	4:BT:404:LEU:HG	1.94	0.49
4:BO:559:LEU:HD12	4:BO:560:PRO:HD2	1.94	0.49
1:C3:50:PHE:HB3	2:P1:22:VAL:HG12	1.94	0.49
4:BL:108:GLN:HG3	4:BL:129:VAL:HG11	1.95	0.49
4:BT:712:MET:SD	4:BT:843:LEU:HD13	2.53	0.49
4:BL:197:GLN:HA	4:BL:798:MET:HE2	1.94	0.49
1:C1:292:ALA:HB1	1:C1:295:GLN:HG3	1.95	0.49
1:C3:104:ARG:HH22	1:C3:260:ARG:HE	1.60	0.49
4:BL:682:PHE:HB3	4:BL:827:ILE:HG12	1.94	0.49
4:BL:754:TRP:HE1	4:BL:789:TRP:CD1	2.30	0.49
4:BL:904:VAL:HG11	4:BL:942:ALA:HB2	1.94	0.49
1:C1:57:ARG:HH22	2:P2:20:THR:HG23	1.77	0.49
1:C3:322:SER:O	1:C3:326:GLN:HG3	2.13	0.49
4:BT:281:PHE:HD1	4:BT:610:PHE:HD1	1.60	0.49
4:BO:156:ASP:HB2	4:BO:182:TYR:CD1	2.48	0.49
4:BO:457:ALA:HB1	4:BO:468:ARG:HG2	1.95	0.49
4:BO:727:PHE:CZ	4:BO:807:SER:HB2	2.48	0.49
3:a2:187:SER:OG	3:a2:189:VAL:O	2.25	0.48
4:BT:212:ALA:O	4:BT:237:GLN:NE2	2.46	0.48
1:C3:165:ARG:HG2	3:A3:132:LEU:HD21	1.95	0.48
4:BL:552:MET:SD	4:BL:909:VAL:HG23	2.53	0.48
4:BO:69:MET:HE1	4:BO:111:LEU:HA	1.94	0.48
4:BO:901:VAL:HG21	4:BO:943:ILE:HD13	1.95	0.48
5:ZO:31:GLU:O	5:ZO:35:ILE:HG22	2.12	0.48
1:C2:123:ASP:HA	1:C2:126:THR:HG22	1.95	0.48
2:P1:117:ARG:HH21	2:P1:139:ILE:HB	1.78	0.48
3:a2:82:LYS:HB2	3:a2:82:LYS:HE3	1.69	0.48
4:BL:781:MET:HE3	4:BO:228:GLN:HG3	1.95	0.48
4:BT:909:VAL:HG22	4:BT:931:LEU:HD11	1.95	0.48
3:A1:37:MET:HG3	3:A1:374:LYS:HD2	1.94	0.48
3:a2:264:ASP:OD1	3:a2:265:VAL:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:339:ALA:HB1	3:a3:347:TRP:HB3	1.94	0.48
4:BT:355:MET:HB3	4:BT:365:THR:HG22	1.95	0.48
4:BT:516:PHE:HA	4:BT:519:MET:HE3	1.95	0.48
4:BT:776:GLU:O	4:BT:778:LYS:N	2.46	0.48
5:ZO:5:LEU:H	5:ZO:5:LEU:HD12	1.76	0.48
4:BO:493:CYS:HB2	4:BO:497:LEU:HD12	1.94	0.48
4:BO:721:LEU:HD12	4:BO:814:PRO:HB2	1.95	0.48
1:C3:270:LEU:HD13	1:C3:310:PHE:HB2	1.94	0.48
3:a3:248:THR:HG22	3:a3:249:SER:H	1.79	0.48
4:BT:383:LEU:HG	4:BT:388:PHE:HB2	1.95	0.48
4:BT:682:PHE:CE1	4:BT:857:TYR:HB2	2.48	0.48
4:BO:187:TRP:HB3	4:BO:776:GLU:HB2	1.95	0.48
3:a2:199:GLN:NE2	3:a2:201:THR:O	2.45	0.48
4:BT:73:ASP:OD1	4:BT:73:ASP:N	2.47	0.48
4:BT:885:PHE:HB2	4:BT:902:MET:HE1	1.95	0.48
4:BO:389:SER:O	4:BO:391:ASN:ND2	2.43	0.48
3:A2:277:ARG:HH22	3:a1:186:LYS:HE2	1.79	0.48
3:A3:141:GLN:OE1	3:a2:128:ARG:NH1	2.41	0.48
4:BL:379:THR:CG2	4:BL:477:ALA:HA	2.43	0.48
4:BT:911:GLY:HA3	4:BT:1013:THR:OG1	2.14	0.48
3:A2:241:LYS:HE3	3:A2:261:GLU:HG2	1.95	0.48
3:a2:42:VAL:HG21	3:a2:358:ARG:HG2	1.96	0.48
4:BL:355:MET:HE1	4:BL:410:ILE:HG12	1.96	0.48
4:BT:400:LEU:HD11	4:BT:933:THR:HG21	1.96	0.48
1:C1:205:ARG:O	1:C1:209:GLY:N	2.46	0.48
3:a1:142:GLU:OE1	3:a1:142:GLU:N	2.45	0.48
4:BL:446:ALA:HA	4:BL:478:MET:CE	2.42	0.48
1:C1:338:LEU:HD23	2:P1:120:PRO:HG2	1.96	0.47
2:P2:105:VAL:HG12	2:P2:123:VAL:HB	1.96	0.47
4:BO:344:LEU:O	4:BO:348:ILE:HG23	2.15	0.47
3:A3:259:THR:HG22	3:A3:279:ILE:HG22	1.96	0.47
4:BO:930:GLY:O	4:BO:934:THR:HG23	2.14	0.47
2:P1:40:GLY:O	2:P1:44:VAL:N	2.34	0.47
2:P3:90:ASN:ND2	2:P3:97:THR:OG1	2.34	0.47
4:BL:259:ARG:HH21	4:BL:261:LEU:HD11	1.79	0.47
4:BL:434:SER:O	4:BL:438:ILE:HG12	2.14	0.47
4:BL:945:ILE:HD11	4:BL:975:ILE:HD11	1.95	0.47
4:BO:45:ILE:HG12	4:BO:129:VAL:HG22	1.95	0.47
4:BO:970:MET:HE3	4:BO:971:ARG:HD3	1.96	0.47
3:a2:271:THR:HG21	4:BT:258:SER:HB2	1.97	0.47
4:BL:128:SER:OG	4:BL:130:GLU:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:43:VAL:HG11	4:BT:107:VAL:HG21	1.96	0.47
4:BT:45:ILE:HG12	4:BT:129:VAL:HG12	1.96	0.47
1:C3:286:SER:OG	1:C3:287:LYS:N	2.48	0.47
3:A1:75:ILE:HD11	3:a1:179:PRO:HB3	1.97	0.47
4:BL:219:LEU:O	4:BL:231:ASN:HA	2.15	0.47
4:BL:348:ILE:O	4:BL:351:VAL:HG12	2.14	0.47
4:BT:14:VAL:HG11	4:BO:890:ALA:HB2	1.96	0.47
1:C2:39:LEU:HD22	1:C2:127:LEU:HD23	1.96	0.47
2:P2:67:LEU:HD13	2:P2:71:LEU:HB3	1.95	0.47
3:a3:82:LYS:HE3	3:a3:82:LYS:HB2	1.64	0.47
4:BL:414:GLU:CD	4:BL:974:PRO:HG3	2.39	0.47
4:BL:927:PHE:O	4:BL:931:LEU:HD23	2.15	0.47
1:C2:112:ALA:O	1:C2:115:ILE:HG12	2.15	0.47
2:P3:67:LEU:HB3	2:P3:71:LEU:HB2	1.97	0.47
2:P3:100:PRO:HG3	2:P3:125:LEU:HD23	1.95	0.47
3:A2:332:VAL:HG23	3:A2:369:PRO:HA	1.96	0.47
4:BO:354:VAL:HG13	4:BO:355:MET:CE	2.44	0.47
4:BO:534:ILE:HD11	5:ZO:33:PHE:HB3	1.97	0.47
4:BO:578:LEU:HD11	4:BO:590:VAL:HG21	1.97	0.47
3:a2:244:VAL:HG22	3:a2:297:LEU:HG	1.97	0.47
1:C1:220:VAL:HG12	1:C1:412:ARG:HH12	1.80	0.47
5:ZL:9:VAL:HA	5:ZL:12:VAL:HG22	1.97	0.47
4:BO:347:ALA:HB2	4:BO:988:PRO:HG2	1.97	0.47
3:a1:72:VAL:HG21	3:a1:174:THR:HG22	1.97	0.46
4:BO:68:ASN:CG	4:BO:114:ALA:HB2	2.39	0.46
4:BO:69:MET:HB3	4:BO:92:LEU:HD21	1.97	0.46
1:C2:356:ILE:HG13	1:C2:422:ILE:HD12	1.97	0.46
2:P1:127:GLN:HB2	2:P1:132:TRP:HH2	1.81	0.46
3:A2:42:VAL:HG11	3:A2:358:ARG:HB3	1.97	0.46
3:a3:38:PRO:HG2	3:a3:373:VAL:HG22	1.97	0.46
4:BL:219:LEU:HD11	4:BT:727:PHE:CD2	2.50	0.46
4:BL:513:PHE:O	4:BL:517:ASN:ND2	2.49	0.46
4:BO:403:GLY:HA2	4:BO:406:VAL:HG22	1.97	0.46
4:BL:367:ILE:HD13	4:BL:493:CYS:HB3	1.96	0.46
4:BL:686:ASP:HB3	4:BL:823:PRO:HG2	1.98	0.46
4:BT:361:ASN:O	4:BT:365:THR:HG23	2.15	0.46
4:BL:612:VAL:HB	4:BL:626:ILE:HG22	1.96	0.46
4:BT:731:ILE:HD13	4:BT:805:SER:HB2	1.98	0.46
1:C1:325:LYS:HB3	1:C3:51:GLU:HG2	1.98	0.46
1:C2:97:ILE:HD11	1:C2:272:LEU:HB3	1.98	0.46
1:C2:416:LEU:HD22	1:C2:437:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C3:115:ILE:HG22	1:C3:250:LEU:HB3	1.98	0.46
4:BT:423:GLU:HG3	4:BT:433:LYS:NZ	2.30	0.46
4:BT:684:LEU:HD21	4:BT:702:LEU:HD13	1.97	0.46
4:BT:762:PHE:CE2	4:BT:764:ASP:HB2	2.51	0.46
4:BO:52:ALA:HB1	4:BO:56:THR:OG1	2.15	0.46
4:BO:411:VAL:HG22	4:BO:974:PRO:HB3	1.97	0.46
4:BT:144:ASN:ND2	4:BT:320:GLY:O	2.45	0.46
1:C1:165:ARG:HG2	3:A1:132:LEU:HD21	1.98	0.46
1:C1:328:GLN:NE2	2:P1:109:SER:O	2.48	0.46
3:a2:37:MET:O	3:a2:374:LYS:NZ	2.48	0.46
4:BT:526:HIS:NE2	5:ZT:31:GLU:OE1	2.44	0.46
1:C1:158:GLN:HG2	1:C1:392:VAL:HG21	1.98	0.46
4:BT:23:GLY:HA3	4:BT:377:LEU:HB3	1.98	0.46
4:BO:137:LEU:HD23	4:BO:138:MET:HB3	1.98	0.46
3:A2:236:LYS:HB2	3:A2:301:LEU:HB2	1.97	0.46
3:a1:49:PRO:HA	3:a1:302:ASN:O	2.15	0.46
4:BT:509:LYS:HD2	4:BT:509:LYS:HA	1.78	0.46
4:BT:515:TRP:O	4:BT:519:MET:HE3	2.15	0.46
1:C1:40:ARG:NH2	2:P2:117:ARG:HG3	2.28	0.45
1:C2:161:GLN:HE21	1:C2:165:ARG:NH1	2.13	0.45
2:P2:96:ARG:HG3	2:P2:132:TRP:CE2	2.50	0.45
3:A1:221:ASN:OD1	3:A1:222:ASP:N	2.49	0.45
4:BL:355:MET:O	4:BL:359:LEU:HB2	2.16	0.45
4:BL:485:ALA:O	4:BL:489:THR:OG1	2.34	0.45
4:BL:601:LYS:HD3	4:BL:601:LYS:HA	1.71	0.45
4:BT:375:VAL:HG22	4:BT:484:VAL:HG21	1.99	0.45
4:BT:685:ILE:HG13	4:BT:824:SER:HB2	1.97	0.45
4:BT:687:GLN:OE1	4:BT:856:GLY:N	2.49	0.45
4:BO:352:PHE:HD1	4:BO:369:THR:HG21	1.81	0.45
4:BO:530:SER:O	4:BO:534:ILE:HG12	2.16	0.45
1:C1:284:SER:OG	1:C1:285:GLY:N	2.50	0.45
3:A3:141:GLN:NE2	3:a2:125:THR:OG1	2.49	0.45
4:BL:637:ARG:O	4:BL:643:LYS:NZ	2.49	0.45
4:BL:971:ARG:O	4:BL:974:PRO:HD2	2.17	0.45
4:BT:428:LYS:O	4:BT:432:ARG:HG3	2.15	0.45
4:BO:434:SER:O	4:BO:438:ILE:HG12	2.16	0.45
4:BO:943:ILE:HD12	4:BO:943:ILE:HA	1.82	0.45
2:P3:58:ASN:HD21	2:P3:99:LEU:HD22	1.82	0.45
3:A1:364:LEU:HD12	3:A1:364:LEU:H	1.80	0.45
3:A3:37:MET:HB3	3:A3:374:LYS:HD2	1.98	0.45
3:A3:282:ASN:HD21	3:A3:285:HIS:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:850:LYS:HA	4:BL:850:LYS:HD3	1.74	0.45
4:BO:1003:VAL:O	4:BO:1007:VAL:HG23	2.16	0.45
3:A1:284:ASP:HB2	3:A1:286:THR:HG23	1.99	0.45
4:BL:395:MET:HA	4:BL:395:MET:HE2	1.99	0.45
4:BT:566:ASP:OD1	4:BT:566:ASP:N	2.49	0.45
4:BO:954:ASP:OD2	4:BO:955:LYS:NZ	2.43	0.45
1:C2:205:ARG:O	1:C2:209:GLY:N	2.48	0.45
3:A2:210:ASP:HB3	3:A2:211:PRO:HD3	1.99	0.45
4:BL:497:LEU:HD23	4:BL:497:LEU:HA	1.78	0.45
4:BT:524:THR:HG23	4:BT:972:LEU:HD22	1.98	0.45
1:C3:111:LYS:O	1:C3:115:ILE:HG23	2.17	0.45
4:BL:732:ASP:HB3	4:BL:735:LYS:HB3	1.98	0.45
4:BL:108:GLN:NE2	4:BT:109:ASN:HB3	2.32	0.45
4:BT:169:THR:OG1	4:BT:170:SER:N	2.45	0.45
1:C1:256:ARG:HH12	2:P1:122:ARG:NH2	2.13	0.45
1:C2:111:LYS:O	1:C2:115:ILE:HG23	2.16	0.45
2:P2:19:CYS:O	2:P2:20:THR:OG1	2.35	0.45
3:A1:354:LYS:HD3	3:A1:355:ALA:N	2.32	0.45
4:BT:376:LEU:HD11	4:BT:402:ILE:HD11	1.98	0.45
1:C2:356:ILE:O	1:C2:360:ILE:HG12	2.17	0.45
1:C3:100:MET:HE3	1:C3:104:ARG:HD3	1.99	0.45
1:C3:272:LEU:HD12	1:C3:308:LEU:HD11	1.99	0.45
2:P1:136:VAL:HB	2:P1:147:ILE:HD11	1.99	0.45
3:A2:141:GLN:OE1	3:a1:128:ARG:NH1	2.41	0.45
4:BL:705:GLU:OE2	4:BL:708:LYS:NZ	2.40	0.45
4:BT:730:ASP:OD1	4:BT:730:ASP:N	2.39	0.45
3:A1:212:ILE:HG22	3:A1:280:PHE:HB2	1.99	0.45
3:a3:310:GLN:HA	3:a3:347:TRP:HD1	1.82	0.45
3:A2:82:LYS:HB2	3:A2:82:LYS:HE3	1.63	0.44
3:a3:315:ARG:NH2	3:a3:339:ALA:O	2.51	0.44
4:BL:462:SER:O	4:BL:466:ILE:HG13	2.16	0.44
4:BT:36:PRO:HD2	4:BT:38:ILE:HD11	1.99	0.44
1:C3:107:THR:O	1:C3:111:LYS:HG3	2.17	0.44
3:A3:265:VAL:HG11	3:a2:209:LEU:HD11	2.00	0.44
4:BL:570:GLY:O	4:BL:631:LEU:N	2.50	0.44
4:BT:825:MET:HE3	4:BT:825:MET:HB3	1.85	0.44
4:BO:182:TYR:HD2	4:BO:270:LEU:HD22	1.82	0.44
1:C1:194:ARG:NH1	1:C1:453:ALA:O	2.41	0.44
3:A2:366:LYS:NZ	4:BT:661:ALA:O	2.49	0.44
4:BL:30:LEU:HD12	4:BL:30:LEU:HA	1.85	0.44
1:C1:314:ILE:HD12	1:C3:65:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P1:49:TYR:O	2:P1:53:ILE:HG12	2.17	0.44
3:a2:339:ALA:HB1	3:a2:347:TRP:HB3	1.99	0.44
3:a1:247:ILE:HG23	3:a1:253:LYS:HD3	1.99	0.44
4:BO:703:LEU:HD11	4:BO:718:PRO:HG3	2.00	0.44
1:C1:100:MET:HA	1:C1:103:TRP:CD1	2.52	0.44
1:C2:104:ARG:NH1	1:C2:260:ARG:HD2	2.32	0.44
3:A3:212:ILE:HG22	3:A3:280:PHE:HB2	1.99	0.44
4:BT:174:ASP:OD2	4:BT:175:VAL:N	2.50	0.44
1:C3:319:MET:HB3	1:C3:320:VAL:H	1.67	0.44
2:P2:48:PHE:HE2	2:P2:63:LEU:HD13	1.82	0.44
3:A1:39:ALA:HB2	3:A1:374:LYS:HD3	2.00	0.44
4:BL:376:LEU:O	4:BL:379:THR:OG1	2.36	0.44
1:C2:332:VAL:O	1:C2:336:GLU:HG2	2.17	0.44
2:P1:37:VAL:HG12	2:P1:38:GLU:H	1.83	0.44
3:A3:148:ALA:O	3:A3:152:GLN:HG3	2.17	0.44
3:a2:147:LEU:HD12	3:a2:147:LEU:HA	1.88	0.44
3:a2:236:LYS:HD2	3:a2:236:LYS:HA	1.69	0.44
3:a1:58:GLY:HA3	3:a1:216:VAL:HG12	2.00	0.44
4:BO:58:GLN:HA	4:BO:62:THR:HG22	2.00	0.44
2:P1:70:LYS:HA	2:P1:73:THR:HG23	2.00	0.44
2:P2:156:SER:OG	2:P2:156:SER:O	2.27	0.44
3:A1:141:GLN:OE1	3:a3:128:ARG:NH1	2.42	0.44
3:a1:73:SER:OG	3:a1:197:ASN:N	2.51	0.44
3:a1:365:GLN:C	3:a1:368:ARG:HH22	2.26	0.44
4:BL:129:VAL:HG12	4:BT:113:LEU:HD11	2.00	0.44
4:BL:186:ILE:HD11	4:BL:246:PHE:HE2	1.83	0.44
4:BL:401:ALA:O	4:BL:405:LEU:HG	2.18	0.44
4:BL:727:PHE:CZ	4:BL:807:SER:HB2	2.53	0.44
4:BL:940:LYS:HE3	4:BL:940:LYS:HB3	1.85	0.44
4:BT:952:LEU:HD12	4:BT:952:LEU:HA	1.84	0.44
4:BO:172:VAL:HG11	4:BO:306:ILE:HD11	2.00	0.44
4:BL:361:ASN:O	4:BL:365:THR:HG23	2.18	0.44
1:C3:332:VAL:O	1:C3:336:GLU:HG2	2.18	0.43
3:A3:214:VAL:HG12	3:A3:216:VAL:HG23	1.99	0.43
4:BL:270:LEU:HD23	4:BL:270:LEU:HA	1.86	0.43
4:BL:685:ILE:HD11	4:BL:819:TYR:HD2	1.83	0.43
4:BL:712:MET:SD	4:BL:843:LEU:HD22	2.58	0.43
4:BO:699:ARG:HD3	4:BO:825:MET:HE2	2.00	0.43
1:C1:328:GLN:HE22	2:P1:109:SER:HB2	1.83	0.43
1:C3:157:ARG:HD2	1:C3:157:ARG:HA	1.60	0.43
2:P1:164:LEU:O	2:P1:168:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P2:36:CYS:HB3	2:P2:144:CYS:HB3	1.63	0.43
3:A2:70:PRO:HD3	3:A2:203:LEU:HG	2.00	0.43
4:BT:375:VAL:HG11	4:BT:405:LEU:HD22	2.00	0.43
4:BT:904:VAL:HG23	4:BT:907:LEU:HD12	2.00	0.43
4:BO:80:SER:HB2	4:BO:90:ILE:HG13	2.00	0.43
4:BO:456:MET:HE2	4:BO:932:LEU:HD13	2.00	0.43
1:C1:41:LYS:HE2	1:C2:337:GLN:HB2	1.99	0.43
1:C3:205:ARG:O	1:C3:209:GLY:N	2.41	0.43
1:C3:325:LYS:HB2	1:C3:325:LYS:HE2	1.87	0.43
4:BO:146:ASP:OD1	4:BO:146:ASP:N	2.51	0.43
4:BO:564:LEU:HD12	4:BO:564:LEU:HA	1.89	0.43
1:C1:236:LYS:HG3	2:P1:162:GLY:H	1.83	0.43
1:C1:324:VAL:O	1:C1:328:GLN:HG2	2.19	0.43
1:C2:41:LYS:HD2	1:C3:337:GLN:HG2	2.00	0.43
1:C2:56:ALA:O	1:C2:59:PRO:HD2	2.19	0.43
1:C2:157:ARG:HD2	1:C2:157:ARG:HA	1.61	0.43
1:C2:301:MET:SD	1:C2:301:MET:N	2.91	0.43
2:P2:90:ASN:HB2	2:P2:158:HIS:CE1	2.53	0.43
3:A3:302:ASN:N	3:A3:302:ASN:OD1	2.50	0.43
4:BL:940:LYS:NZ	4:BL:941:ASN:OD1	2.39	0.43
4:BL:1022:VAL:HG12	4:BL:1023:PRO:HD3	2.01	0.43
4:BO:971:ARG:NH2	4:BO:974:PRO:HG2	2.34	0.43
1:C1:35:SER:HB2	2:P2:117:ARG:NH2	2.33	0.43
2:P3:68:SER:HB3	2:P3:146:VAL:HG21	2.00	0.43
4:BL:960:LEU:HD11	4:BL:1027:VAL:HG22	1.99	0.43
4:BT:398:MET:O	4:BT:402:ILE:HG12	2.19	0.43
4:BO:38:ILE:HG22	4:BO:465:ALA:HB3	2.00	0.43
4:BO:291:ILE:HD13	4:BO:306:ILE:HD12	2.00	0.43
4:BO:492:LEU:HD23	4:BO:492:LEU:HA	1.86	0.43
2:P3:50:ASP:HA	2:P3:53:ILE:HG22	2.00	0.43
3:a1:140:LYS:HB2	3:a1:140:LYS:HE3	1.81	0.43
3:a3:89:ALA:N	3:a3:181:SER:OG	2.50	0.43
3:a3:187:SER:OG	3:a3:189:VAL:O	2.32	0.43
4:BL:989:LEU:HD22	4:BL:1000:GLN:HG2	2.01	0.43
4:BL:1033:PHE:O	4:BL:1035:ARG:N	2.52	0.43
5:ZL:9:VAL:O	5:ZL:13:ILE:HG12	2.18	0.43
4:BT:395:MET:N	4:BT:395:MET:SD	2.92	0.43
1:C2:270:LEU:HD13	1:C2:310:PHE:HB2	2.00	0.43
3:A1:214:VAL:HG12	3:A1:216:VAL:HG23	2.01	0.43
3:a3:52:ILE:HD11	3:a3:235:LEU:HD11	2.00	0.43
4:BL:583:THR:HG22	4:BL:584:GLN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:904:VAL:O	4:BL:907:LEU:HB2	2.18	0.43
4:BT:414:GLU:CD	4:BT:973:ARG:HE	2.27	0.43
4:BT:493:CYS:HA	4:BT:497:LEU:HD23	2.00	0.43
4:BO:254:ASN:ND2	4:BO:258:SER:OG	2.36	0.43
4:BO:310:LEU:HD23	4:BO:310:LEU:HA	1.85	0.43
4:BO:966:ASP:O	4:BO:970:MET:HG2	2.18	0.43
3:A1:83:GLU:HG2	3:A1:186:LYS:HA	2.01	0.43
3:A1:345:ASP:OD1	3:A1:345:ASP:N	2.47	0.43
4:BL:760:ASN:O	4:BL:771:VAL:HG12	2.18	0.43
4:BO:19:ILE:HD13	4:BO:19:ILE:HA	1.88	0.43
4:BO:219:LEU:O	4:BO:231:ASN:HA	2.19	0.43
4:BO:355:MET:SD	4:BO:410:ILE:HG21	2.58	0.43
4:BO:986:VAL:HG21	4:BO:1007:VAL:HB	2.01	0.43
1:C3:104:ARG:HH21	1:C3:257:GLU:CD	2.27	0.43
1:C3:314:ILE:O	1:C3:316:GLN:HG3	2.19	0.43
2:P3:32:ARG:NH2	2:P3:35:PRO:O	2.52	0.43
3:A3:332:VAL:HG23	3:A3:369:PRO:HA	1.99	0.43
3:a3:353:LEU:HD23	3:a3:353:LEU:HA	1.86	0.43
4:BL:885:PHE:HB2	4:BL:902:MET:HE1	2.01	0.43
4:BL:890:ALA:HB2	4:BO:14:VAL:HG11	1.99	0.43
5:ZT:6:LYS:HA	5:ZT:9:VAL:HG12	2.00	0.43
4:BO:407:ASP:HB2	4:BO:978:THR:HG22	2.00	0.43
2:P2:71:LEU:HD23	2:P2:71:LEU:HA	1.79	0.43
3:a1:222:ASP:OD1	3:a1:222:ASP:N	2.51	0.43
4:BT:403:GLY:HA3	4:BT:982:PHE:CE2	2.53	0.43
5:ZT:6:LYS:HG3	5:ZT:7:SER:N	2.34	0.43
4:BO:134:SER:OG	4:BO:675:GLY:O	2.37	0.43
4:BO:572:PHE:HB2	4:BO:666:PHE:O	2.18	0.43
4:BO:999:ALA:O	4:BO:1003:VAL:HG12	2.19	0.43
1:C3:123:ASP:HA	1:C3:126:THR:HG22	2.01	0.42
1:C3:164:GLN:O	1:C3:168:VAL:HG12	2.18	0.42
2:P2:125:LEU:HD11	2:P2:134:ASP:HB2	2.01	0.42
3:A2:49:PRO:HB3	3:A2:303:PRO:HA	1.99	0.42
3:A2:229:GLU:HG2	3:A2:235:LEU:HD23	2.01	0.42
4:BL:64:VAL:HG11	4:BL:117:LEU:HB3	2.01	0.42
4:BL:104:GLN:HA	4:BL:107:VAL:HG22	2.00	0.42
4:BL:367:ILE:HB	4:BL:368:PRO:HD3	2.01	0.42
4:BT:741:VAL:HG21	4:BT:799:VAL:HG11	2.00	0.42
3:A1:254:PHE:CE2	3:A1:256:GLN:HB2	2.54	0.42
3:A2:45:VAL:HG21	3:A2:353:LEU:HD12	2.01	0.42
4:BL:350:LEU:HD11	4:BL:984:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BL:355:MET:HE3	4:BL:368:PRO:HG2	2.01	0.42
4:BT:351:VAL:HA	4:BT:354:VAL:HG12	2.01	0.42
4:BT:500:ILE:HD12	4:BT:500:ILE:HA	1.91	0.42
4:BO:994:GLY:O	4:BO:997:SER:OG	2.34	0.42
1:C2:314:ILE:O	1:C2:316:GLN:HG3	2.19	0.42
3:a1:175:LYS:HE3	3:a1:175:LYS:HB2	1.90	0.42
4:BL:186:ILE:HD11	4:BL:246:PHE:CE2	2.54	0.42
4:BT:131:LYS:HB3	4:BT:131:LYS:HE2	1.65	0.42
3:A1:144:ASP:OD2	3:a3:128:ARG:NH2	2.37	0.42
3:a3:87:ILE:HD13	3:a3:87:ILE:HA	1.87	0.42
3:a3:175:LYS:HB2	3:a3:175:LYS:HE3	1.84	0.42
4:BL:143:ILE:HG22	4:BL:286:ALA:HB2	2.02	0.42
4:BL:937:LEU:HA	4:BL:937:LEU:HD23	1.71	0.42
4:BL:1020:PHE:CE2	5:ZL:29:LEU:HD22	2.53	0.42
4:BT:391:ASN:O	4:BT:395:MET:HG2	2.19	0.42
4:BO:143:ILE:HG22	4:BO:286:ALA:HB2	2.01	0.42
4:BO:680:PHE:HZ	4:BO:844:MET:HE3	1.85	0.42
1:C2:111:LYS:HB2	1:C2:254:LEU:HD13	2.00	0.42
2:P2:49:TYR:CE2	2:P2:123:VAL:HG21	2.55	0.42
3:A1:148:ALA:O	3:A1:152:GLN:HG3	2.19	0.42
3:a1:248:THR:HG22	3:a1:249:SER:H	1.85	0.42
4:BL:169:THR:O	4:BL:172:VAL:HG22	2.19	0.42
4:BT:360:GLN:HG2	4:BT:513:PHE:CD2	2.54	0.42
4:BT:939:ALA:O	4:BT:943:ILE:HG12	2.20	0.42
4:BO:530:SER:HA	5:ZO:34:ASN:HD21	1.83	0.42
1:C1:249:ARG:NH1	2:P1:135:GLU:OE1	2.53	0.42
1:C2:237:GLU:HG2	1:C2:426:LEU:HD21	2.02	0.42
1:C3:183:TYR:O	1:C3:186:VAL:HG12	2.19	0.42
3:a2:42:VAL:HG23	3:a2:359:VAL:O	2.20	0.42
3:a1:343:ILE:HD13	3:a1:343:ILE:HA	1.90	0.42
3:a3:53:THR:HG22	3:a3:298:GLU:HG2	2.01	0.42
4:BL:53:ASP:OD1	4:BL:53:ASP:N	2.40	0.42
4:BL:846:GLN:O	4:BL:849:SER:OG	2.29	0.42
4:BT:589:LYS:HB2	4:BT:589:LYS:HE3	1.78	0.42
4:BO:655:PHE:HB3	4:BO:663:VAL:CG1	2.49	0.42
2:P1:127:GLN:HB2	2:P1:132:TRP:CH2	2.55	0.42
2:P2:148:ASP:OD1	2:P2:149:ASP:N	2.51	0.42
3:A1:270:THR:O	3:A1:270:THR:OG1	2.38	0.42
3:A2:368:ARG:HG2	3:A2:369:PRO:HD2	2.00	0.42
4:BL:27:ILE:HD11	4:BL:380:PHE:CD2	2.55	0.42
4:BO:904:VAL:HG11	4:BO:942:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:256:ARG:NH1	1:C2:260:ARG:HG3	2.33	0.42
2:P3:128:GLY:O	2:P3:130:GLN:HG3	2.19	0.42
4:BL:355:MET:HE2	4:BL:355:MET:HB2	1.81	0.42
4:BT:10:ILE:HA	4:BT:13:TRP:HB2	2.02	0.42
4:BT:612:VAL:HB	4:BT:626:ILE:HG22	2.02	0.42
4:BO:118:LEU:HG	4:BO:119:PRO:HD2	2.02	0.42
4:BO:348:ILE:HG13	4:BO:349:ILE:N	2.34	0.42
4:BO:922:THR:OG1	4:BO:923:ASN:N	2.53	0.42
1:C1:70:TYR:HD1	1:C1:87:THR:HG22	1.84	0.42
1:C1:363:ILE:HD13	1:C1:363:ILE:HA	1.93	0.42
1:C2:103:TRP:CD1	1:C2:103:TRP:H	2.37	0.42
1:C2:256:ARG:HA	1:C2:256:ARG:HD2	1.78	0.42
2:P1:70:LYS:HE2	2:P1:165:ARG:NH1	2.30	0.42
2:P2:32:ARG:NH1	2:P2:68:SER:HA	2.35	0.42
3:A3:227:LYS:HE2	3:A3:227:LYS:HB2	1.92	0.42
3:a2:42:VAL:HG11	3:a2:375:ALA:HB1	2.02	0.42
4:BL:29:LYS:HA	4:BL:29:LYS:HD3	1.94	0.42
4:BL:649:MET:SD	4:BL:653:ARG:NH2	2.93	0.42
4:BL:901:VAL:HG11	4:BL:943:ILE:HG13	2.02	0.42
4:BO:350:LEU:O	4:BO:354:VAL:HG12	2.20	0.42
4:BO:606:VAL:HA	4:BO:631:LEU:HA	2.02	0.42
1:C2:347:GLN:HE21	1:C2:347:GLN:C	2.28	0.42
2:P2:37:VAL:HG12	2:P2:38:GLU:H	1.85	0.42
2:P2:122:ARG:H	2:P2:122:ARG:HG2	1.72	0.42
3:A1:65:ILE:HG13	3:A1:207:GLN:HG3	2.02	0.42
3:a2:42:VAL:HG23	3:a2:359:VAL:C	2.44	0.42
3:a1:186:LYS:NZ	3:a1:187:SER:O	2.53	0.42
4:BL:875:SER:O	4:BL:879:ILE:HG23	2.20	0.42
4:BL:1020:PHE:CD2	5:ZL:29:LEU:HD22	2.55	0.42
4:BT:438:ILE:HG13	4:BT:442:LEU:HD23	2.02	0.42
4:BO:354:VAL:HG13	4:BO:355:MET:HE3	2.02	0.42
4:BO:365:THR:O	4:BO:368:PRO:HD2	2.20	0.42
4:BO:367:ILE:HB	4:BO:368:PRO:HD3	2.01	0.42
4:BO:380:PHE:HE2	4:BO:390:ILE:HG12	1.84	0.42
1:C1:183:TYR:O	1:C1:186:VAL:HG12	2.20	0.41
1:C2:104:ARG:HD2	1:C2:261:GLN:HA	2.00	0.41
1:C2:423:LYS:HB3	1:C2:429:LEU:HD13	2.02	0.41
1:C3:367:LYS:O	1:C3:370:VAL:HG12	2.19	0.41
3:A3:261:GLU:O	3:A3:261:GLU:HG3	2.19	0.41
5:ZL:28:GLY:O	5:ZL:31:GLU:HG2	2.19	0.41
4:BT:376:LEU:HD23	4:BT:376:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:245:LEU:HD12	1:C1:245:LEU:HA	1.80	0.41
2:P3:165:ARG:HE	2:P3:165:ARG:HB3	1.68	0.41
3:A1:45:VAL:HG11	3:A1:353:LEU:HD22	2.01	0.41
3:a1:36:GLN:HB3	3:a1:37:MET:H	1.57	0.41
3:a1:42:VAL:HG22	3:a1:360:VAL:HG22	2.02	0.41
4:BT:534:ILE:HG13	4:BT:535:LEU:N	2.33	0.41
4:BT:583:THR:OG1	4:BT:584:GLN:N	2.50	0.41
4:BO:346:GLU:O	4:BO:350:LEU:HD12	2.19	0.41
4:BL:564:LEU:HD12	4:BL:564:LEU:HA	1.92	0.41
4:BL:685:ILE:HG22	4:BL:687:GLN:HG2	2.02	0.41
4:BL:790:TYR:HB3	4:BL:798:MET:HB3	2.02	0.41
4:BO:445:ILE:CG2	4:BO:940:LYS:HG3	2.50	0.41
4:BO:453:PHE:N	4:BO:453:PHE:CD1	2.88	0.41
4:BO:664:PHE:CD2	4:BO:717:ARG:HD2	2.55	0.41
4:BO:727:PHE:CZ	4:BO:783:PRO:HB3	2.55	0.41
4:BO:859:TRP:CD1	4:BO:867:ARG:HE	2.38	0.41
1:C1:325:LYS:HB2	1:C1:325:LYS:HE2	1.87	0.41
1:C2:107:THR:O	1:C2:111:LYS:HG3	2.20	0.41
2:P3:68:SER:HB3	2:P3:146:VAL:HG11	2.02	0.41
2:P3:137:LEU:HB3	2:P3:148:ASP:HB3	2.02	0.41
3:A1:63:TYR:CD2	3:A1:211:PRO:HG2	2.55	0.41
3:A1:246:LEU:HA	3:A1:246:LEU:HD23	1.78	0.41
3:a2:241:LYS:HB3	3:a2:260:LEU:O	2.21	0.41
4:BL:16:ALA:HB2	4:BL:488:LEU:HD22	2.01	0.41
4:BT:673:GLU:H	4:BT:673:GLU:HG2	1.70	0.41
4:BO:30:LEU:HD12	4:BO:30:LEU:HA	1.84	0.41
4:BO:970:MET:HG3	4:BO:971:ARG:HG2	2.01	0.41
1:C2:268:PRO:HB3	1:C2:312:LEU:HD13	2.01	0.41
1:C3:104:ARG:HH22	1:C3:260:ARG:NE	2.18	0.41
1:C3:224:LYS:HD2	1:C3:224:LYS:HA	1.84	0.41
1:C3:328:GLN:HE21	1:C3:328:GLN:HB3	1.69	0.41
3:a1:312:GLY:HA2	3:a1:364:LEU:HD11	2.03	0.41
4:BL:259:ARG:HE	4:BL:261:LEU:HD21	1.85	0.41
4:BL:758:TYR:CE1	4:BL:770:LYS:HB3	2.55	0.41
4:BT:187:TRP:HB3	4:BT:776:GLU:HB2	2.02	0.41
4:BT:462:SER:O	4:BT:466:ILE:HG13	2.20	0.41
4:BO:321:LEU:HD12	4:BO:321:LEU:HA	1.85	0.41
1:C1:232:ASN:HB3	2:P1:161:ALA:HB3	2.02	0.41
2:P1:160:THR:HG22	2:P1:161:ALA:N	2.36	0.41
3:A1:72:VAL:HG21	3:A1:174:THR:HG22	2.02	0.41
3:A1:326:VAL:HG12	3:A1:358:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:271:THR:HG21	4:BO:258:SER:HB2	2.03	0.41
4:BL:388:PHE:HE2	4:BL:472:ILE:HG21	1.85	0.41
4:BL:472:ILE:O	4:BL:476:SER:OG	2.31	0.41
4:BL:885:PHE:HD1	4:BL:902:MET:HE1	1.85	0.41
4:BL:903:LEU:HD23	4:BL:903:LEU:HA	1.88	0.41
4:BO:859:TRP:HD1	4:BO:867:ARG:HE	1.68	0.41
2:P1:67:LEU:HD13	2:P1:147:ILE:HG23	2.03	0.41
2:P2:85:ARG:H	2:P2:85:ARG:HG3	1.64	0.41
2:P3:32:ARG:NE	2:P3:36:CYS:SG	2.87	0.41
3:A3:82:LYS:HB2	3:A3:82:LYS:HE3	1.71	0.41
3:A3:84:GLY:HA3	3:a3:262:PHE:HD1	1.86	0.41
4:BT:31:PRO:HG2	4:BT:389:SER:HB3	2.02	0.41
4:BT:184:MET:HE3	4:BT:246:PHE:CD2	2.55	0.41
4:BT:390:ILE:HG23	4:BT:395:MET:SD	2.60	0.41
4:BT:735:LYS:HE2	4:BT:735:LYS:HB3	1.85	0.41
5:ZT:18:VAL:HA	5:ZT:21:ILE:HD12	2.03	0.41
4:BO:955:LYS:HA	4:BO:955:LYS:HD3	1.78	0.41
1:C1:417:ILE:HD13	1:C1:417:ILE:HA	1.96	0.41
1:C1:420:LEU:HD23	1:C1:420:LEU:HA	1.84	0.41
4:BL:540:ARG:HA	4:BL:540:ARG:HD3	1.74	0.41
4:BL:566:ASP:OD1	4:BL:566:ASP:N	2.53	0.41
4:BT:58:GLN:HA	4:BT:62:THR:HG22	2.02	0.41
4:BT:406:VAL:O	4:BT:410:ILE:HG12	2.20	0.41
4:BO:901:VAL:O	4:BO:904:VAL:HG12	2.21	0.41
1:C2:147:TYR:CE1	1:C2:403:ASN:HB2	2.56	0.41
1:C2:240:LYS:HB3	1:C2:240:LYS:HE3	1.88	0.41
1:C2:322:SER:O	1:C2:326:GLN:HG3	2.20	0.41
1:C3:103:TRP:CD1	1:C3:103:TRP:H	2.38	0.41
2:P3:102:SER:OG	2:P3:126:LYS:HB3	2.21	0.41
3:A2:132:LEU:HD12	3:A2:132:LEU:HA	1.85	0.41
3:A2:246:LEU:HD23	3:A2:246:LEU:HA	1.85	0.41
3:A3:119:ALA:HA	3:A3:153:ALA:HB1	2.02	0.41
3:A3:212:ILE:HD12	3:A3:212:ILE:HA	1.95	0.41
3:A3:311:GLN:HG2	3:A3:361:ILE:HD11	2.03	0.41
3:a2:175:LYS:HE3	3:a2:175:LYS:HB2	1.90	0.41
3:a2:311:GLN:HB3	3:a2:361:ILE:HG22	2.03	0.41
4:BL:26:ALA:O	4:BL:30:LEU:HB2	2.21	0.41
4:BL:188:MET:SD	4:BL:773:VAL:HG13	2.61	0.41
4:BL:530:SER:O	4:BL:534:ILE:HG22	2.21	0.41
4:BL:535:LEU:HD21	4:BL:1027:VAL:HG21	2.03	0.41
4:BL:555:LEU:HD23	4:BL:913:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BT:202:ASP:OD2	4:BT:792:ARG:NH2	2.54	0.41
4:BT:423:GLU:HG3	4:BT:433:LYS:HZ2	1.85	0.41
5:ZT:22:ILE:HD12	5:ZT:25:LEU:HD23	2.03	0.41
4:BO:36:PRO:HG2	4:BO:38:ILE:HG23	2.02	0.41
5:ZO:13:ILE:O	5:ZO:17:VAL:HG22	2.21	0.41
1:C1:111:LYS:HE3	1:C1:253:ASP:HB3	2.02	0.41
1:C1:112:ALA:O	1:C1:115:ILE:HG12	2.21	0.41
1:C1:423:LYS:HB3	1:C1:429:LEU:HD13	2.03	0.41
1:C2:40:ARG:HH22	2:P3:117:ARG:HG3	1.86	0.41
1:C2:197:LEU:HD22	1:C2:449:PRO:HG3	2.03	0.41
1:C3:51:GLU:OE2	1:C3:54:ASN:ND2	2.54	0.41
1:C3:226:ASP:OD1	1:C3:226:ASP:N	2.53	0.41
3:A3:212:ILE:HG21	3:A3:287:LEU:HD11	2.02	0.41
3:a1:345:ASP:OD2	3:a1:345:ASP:C	2.64	0.41
4:BT:472:ILE:HD13	4:BT:472:ILE:HA	1.90	0.41
2:P3:37:VAL:HG12	2:P3:38:GLU:H	1.85	0.40
4:BT:418:ARG:HG3	4:BT:419:VAL:N	2.35	0.40
5:ZT:19:MET:O	5:ZT:22:ILE:HG22	2.22	0.40
4:BO:438:ILE:O	4:BO:442:LEU:HG	2.20	0.40
4:BO:727:PHE:CE1	4:BO:807:SER:HB2	2.55	0.40
4:BO:786:ILE:HD12	4:BO:786:ILE:HA	1.92	0.40
1:C1:76:TYR:N	1:C2:302:GLY:O	2.53	0.40
1:C2:26:MET:HE1	1:C2:434:LEU:C	2.47	0.40
1:C2:70:TYR:HD1	1:C2:87:THR:HG22	1.86	0.40
4:BT:45:ILE:HD13	4:BT:111:LEU:HD22	2.02	0.40
4:BT:303:ALA:O	4:BT:307:ARG:HG2	2.21	0.40
1:C1:391:ILE:O	1:C1:394:VAL:HG22	2.21	0.40
1:C3:100:MET:HE2	1:C3:100:MET:HB3	1.85	0.40
2:P1:139:ILE:HG13	2:P1:146:VAL:HG23	2.02	0.40
3:A2:270:THR:O	3:A2:270:THR:OG1	2.37	0.40
3:A2:310:GLN:HG2	3:A2:347:TRP:CD1	2.56	0.40
3:a1:260:LEU:HD11	3:a1:276:LEU:HB3	2.02	0.40
3:a3:354:LYS:HE2	3:a3:354:LYS:HB2	1.90	0.40
4:BL:781:MET:HB3	4:BO:228:GLN:HE21	1.86	0.40
5:ZT:22:ILE:O	5:ZT:26:ILE:HG12	2.21	0.40
5:ZT:25:LEU:O	5:ZT:29:LEU:HD23	2.22	0.40
4:BO:137:LEU:N	4:BO:291:ILE:O	2.51	0.40
4:BO:760:ASN:O	4:BO:771:VAL:HG12	2.22	0.40
4:BO:1022:VAL:N	4:BO:1023:PRO:HD2	2.37	0.40
1:C3:147:TYR:CE1	1:C3:403:ASN:HB2	2.56	0.40
1:C3:268:PRO:HB3	1:C3:312:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P2:149:ASP:O	2:P2:164:LEU:HB3	2.22	0.40
3:A1:125:THR:OG1	3:a1:141:GLN:NE2	2.49	0.40
3:a3:46:LYS:HE2	3:a3:46:LYS:HB2	1.95	0.40
4:BL:976:LEU:HD12	5:ZL:22:ILE:HD12	2.03	0.40
4:BT:14:VAL:HG21	4:BO:890:ALA:HB2	2.04	0.40
4:BT:30:LEU:HD12	4:BT:30:LEU:HA	1.80	0.40
4:BO:907:LEU:HD12	4:BO:1017:LEU:HB3	2.03	0.40
1:C2:245:LEU:HD23	1:C2:245:LEU:HA	1.87	0.40
4:BL:275:TYR:CG	4:BO:223:PRO:HG3	2.56	0.40
4:BL:472:ILE:HD13	4:BL:472:ILE:HA	1.91	0.40
4:BL:873:ALA:N	4:BL:874:PRO:HD2	2.36	0.40
4:BT:431:THR:O	4:BT:435:MET:HG2	2.22	0.40
4:BO:182:TYR:CD2	4:BO:270:LEU:HD22	2.57	0.40
4:BO:580:ALA:HB1	4:BO:724:THR:HG22	2.02	0.40
4:BO:879:ILE:HD13	4:BO:879:ILE:HA	1.96	0.40
4:BO:973:ARG:O	4:BO:977:MET:HG2	2.21	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 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	C1	430/493 (87%)	420 (98%)	10 (2%)	0	100	100
1	C2	430/493 (87%)	421 (98%)	9 (2%)	0	100	100
1	C3	430/493 (87%)	420 (98%)	9 (2%)	1 (0%)	43	71
2	P1	150/171 (88%)	122 (81%)	27 (18%)	1 (1%)	18	47
2	P2	150/171 (88%)	125 (83%)	24 (16%)	1 (1%)	18	47
2	P3	150/171 (88%)	127 (85%)	22 (15%)	1 (1%)	18	47
3	A1	342/397 (86%)	335 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A2	342/397 (86%)	333 (97%)	9 (3%)	0	100	100
3	A3	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a1	342/397 (86%)	333 (97%)	8 (2%)	1 (0%)	36	65
3	a2	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a3	342/397 (86%)	333 (97%)	8 (2%)	1 (0%)	36	65
4	BL	1034/1049 (99%)	1008 (98%)	25 (2%)	1 (0%)	48	78
4	BO	1032/1049 (98%)	995 (96%)	35 (3%)	2 (0%)	43	71
4	BT	1032/1049 (98%)	1006 (98%)	25 (2%)	1 (0%)	48	78
5	ZL	37/49 (76%)	36 (97%)	1 (3%)	0	100	100
5	ZO	37/49 (76%)	37 (100%)	0	0	100	100
5	ZT	37/49 (76%)	37 (100%)	0	0	100	100
All	All	7001/7668 (91%)	6752 (96%)	239 (3%)	10 (0%)	49	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C3	286	SER
4	BT	777	ALA
4	BO	777	ALA
4	BL	1034	SER
4	BO	222	THR
3	a3	262	PHE
2	P1	150	VAL
2	P2	150	VAL
2	P3	150	VAL
3	a1	262	PHE

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	C1	361/412 (88%)	361 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C2	361/412 (88%)	360 (100%)	1 (0%)	86	84
1	C3	361/412 (88%)	361 (100%)	0	100	100
2	P1	131/148 (88%)	131 (100%)	0	100	100
2	P2	131/148 (88%)	129 (98%)	2 (2%)	57	69
2	P3	131/148 (88%)	130 (99%)	1 (1%)	73	77
3	A1	278/318 (87%)	278 (100%)	0	100	100
3	A2	278/318 (87%)	277 (100%)	1 (0%)	84	83
3	A3	278/318 (87%)	277 (100%)	1 (0%)	84	83
3	a1	278/318 (87%)	278 (100%)	0	100	100
3	a2	278/318 (87%)	277 (100%)	1 (0%)	84	83
3	a3	278/318 (87%)	278 (100%)	0	100	100
4	BL	834/855 (98%)	831 (100%)	3 (0%)	84	83
4	BO	834/855 (98%)	832 (100%)	2 (0%)	87	85
4	BT	834/855 (98%)	833 (100%)	1 (0%)	88	89
5	ZL	33/41 (80%)	33 (100%)	0	100	100
5	ZO	33/41 (80%)	33 (100%)	0	100	100
5	ZT	33/41 (80%)	32 (97%)	1 (3%)	36	59
All	All	5745/6276 (92%)	5731 (100%)	14 (0%)	85	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C2	347	GLN
2	P2	136	VAL
2	P2	144	CYS
2	P3	46	GLN
3	A2	36	GLN
3	A3	36	GLN
3	a2	216	VAL
4	BL	492	LEU
4	BL	822	LEU
4	BL	914	LEU
4	BT	125	GLN
5	ZT	31	GLU
4	BO	552	MET
4	BO	741	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	74	ASN
1	C1	206	GLN
1	C1	300	ASN
1	C1	321	ASN
1	C1	328	GLN
1	C1	330	ASN
1	C1	414	ASN
1	C1	419	GLN
1	C1	451	ASN
1	C2	63	GLN
1	C2	74	ASN
1	C2	83	ASN
1	C2	140	ASN
1	C2	161	GLN
1	C2	199	ASN
1	C2	321	ASN
1	C2	403	ASN
1	C2	410	ASN
1	C2	418	ASN
1	C3	36	ASN
1	C3	316	GLN
1	C3	323	GLN
1	C3	414	ASN
1	C3	451	ASN
2	P1	55	HIS
2	P1	84	HIS
2	P2	83	ASN
2	P2	127	GLN
2	P2	133	GLN
2	P2	158	HIS
3	A2	102	GLN
3	A2	196	GLN
3	A2	237	GLN
3	A2	376	GLN
3	A3	218	GLN
3	a2	102	GLN
3	a2	310	GLN
3	a2	341	GLN
3	a1	102	GLN
3	a1	152	GLN
3	a1	196	GLN

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Mol	Chain	Res	Type
3	a3	136	GLN
3	a3	237	GLN
4	BL	3	ASN
4	BL	70	ASN
4	BL	108	GLN
4	BL	109	ASN
4	BL	112	GLN
4	BL	120	GLN
4	BL	124	GLN
4	BL	189	ASN
4	BL	284	GLN
4	BL	360	GLN
4	BL	439	GLN
4	BL	517	ASN
4	BL	584	GLN
4	BL	797	GLN
4	BT	106	GLN
4	BT	228	GLN
4	BT	284	GLN
4	BT	697	GLN
4	BT	737	GLN
4	BO	3	ASN
4	BO	70	ASN
4	BO	104	GLN
4	BO	517	ASN
4	BO	526	HIS
4	BO	657	GLN
4	BO	737	GLN
5	ZO	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.