



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 12:25 AM JST

PDB ID : 9V55 / pdb_00009v55
EMDB ID : EMD-64787
Title : Structure of TolC, YbjP, and AcrA complex
Authors : Ge, X.F.; Gu, Z.W.; Wang, J.W.
Deposited on : 2025-05-25
Resolution : 3.26 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

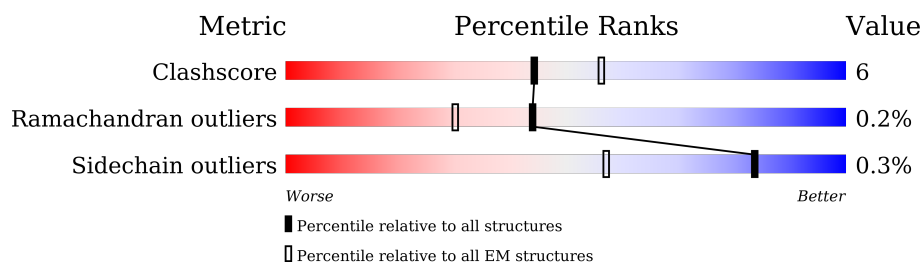
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	76% 12% 12%
1	C2	493	74% 14% 12%
1	C3	493	73% 14% 12%
2	P1	171	63% 26% 11%
2	P2	171	67% 22% 11%
2	P3	171	67% 21% 11%
3	A1	397	75% 12% 13%
3	A2	397	75% 12% 13%
3	A3	397	73% 14% 13%

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Mol	Chain	Length	Quality of chain
3	a1	397	 74% 12% 13%
3	a2	397	 76% 11% 13%
3	a3	397	 77% 10% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29061 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		

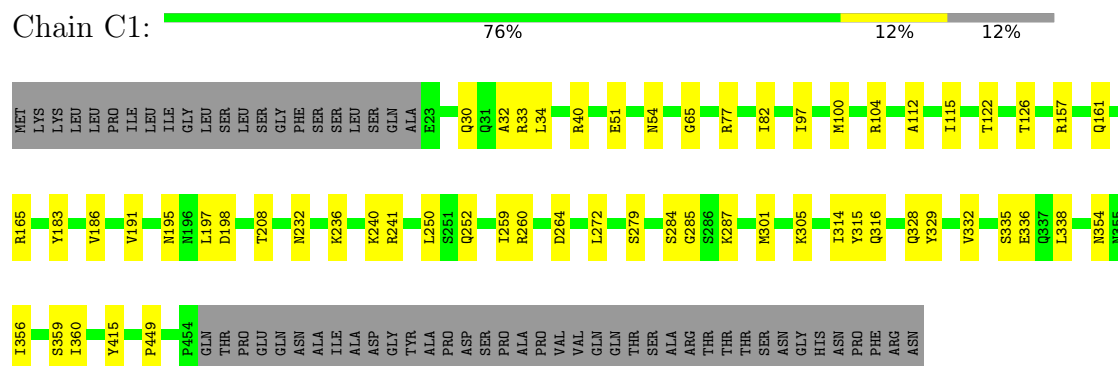
- Molecule 3 is a protein called Multidrug efflux pump subunit AcrA.

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		

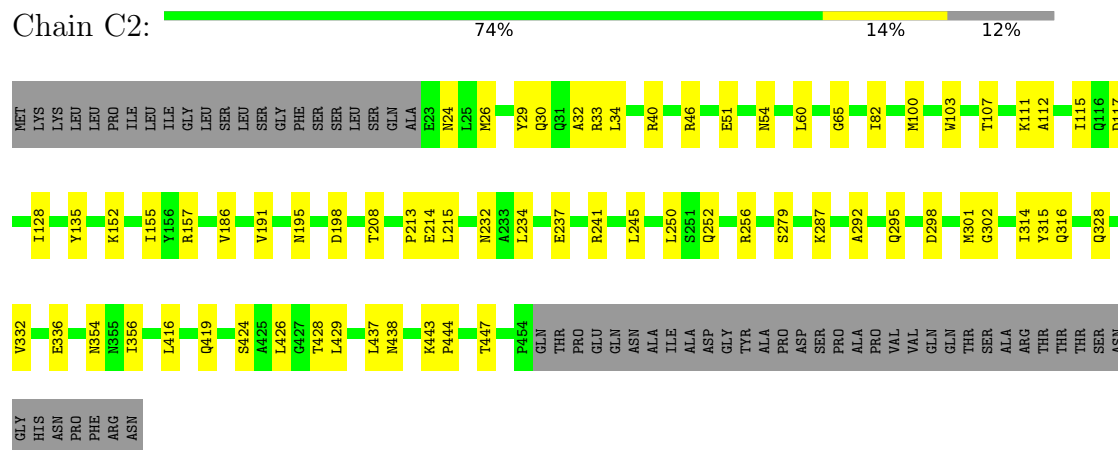
3 Residue-property plots

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.

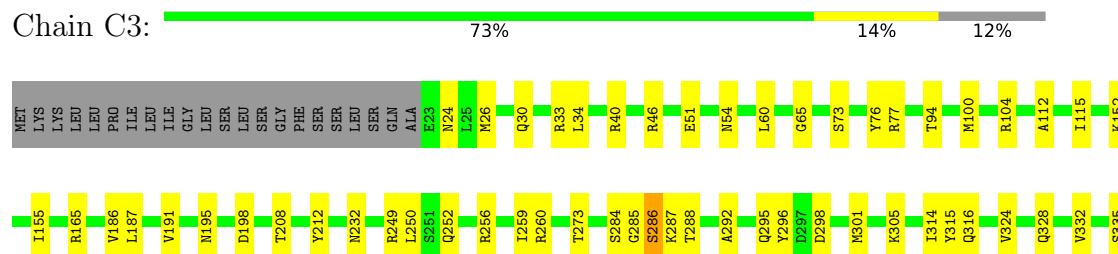
- Molecule 1: Outer membrane protein TolC

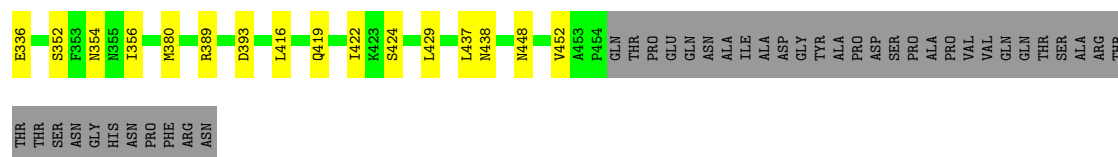


- Molecule 1: Outer membrane protein TolC



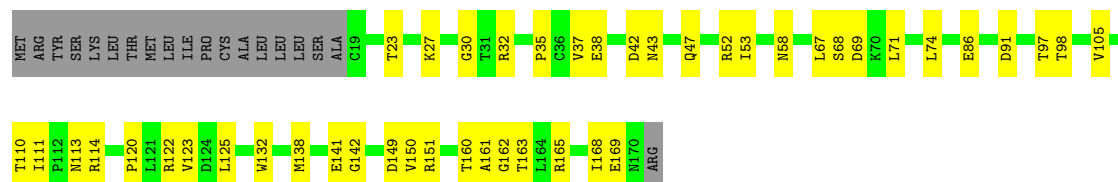
- Molecule 1: Outer membrane protein TolC





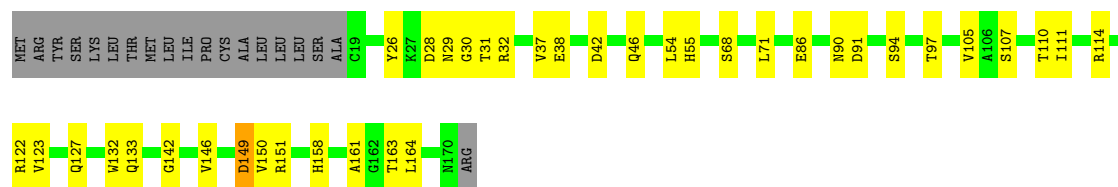
• Molecule 2: Uncharacterized lipoprotein YbjP

Chain P1: 63% 26% 11%



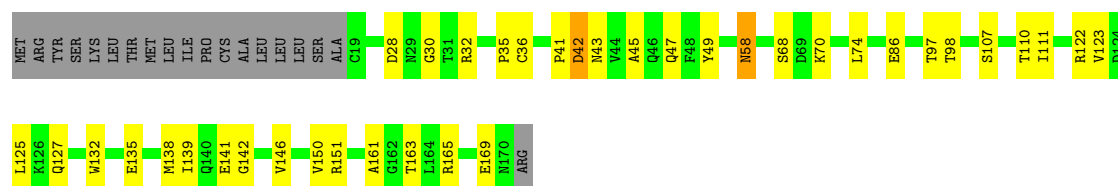
• Molecule 2: Uncharacterized lipoprotein YbjP

Chain P2: 67% 22% 11%



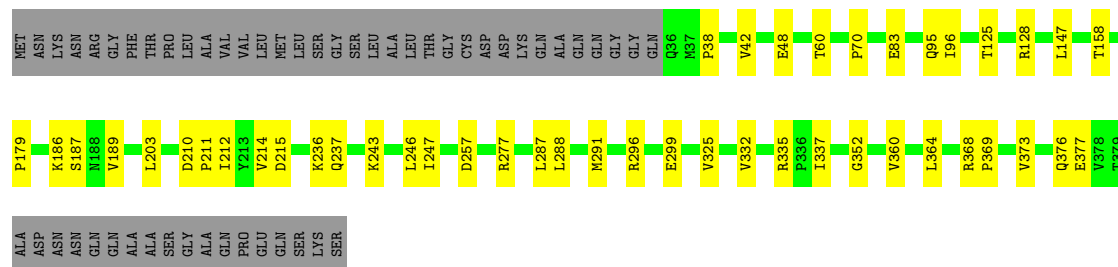
• Molecule 2: Uncharacterized lipoprotein YbjP

Chain P3: 67% 21% 11%



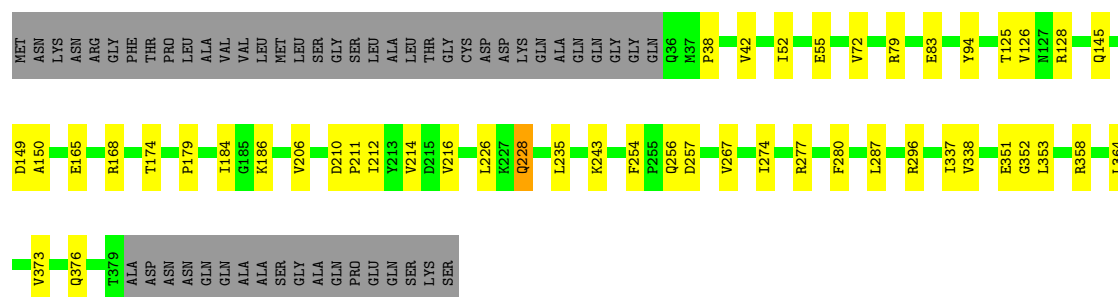
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A1: 75% 12% 13%



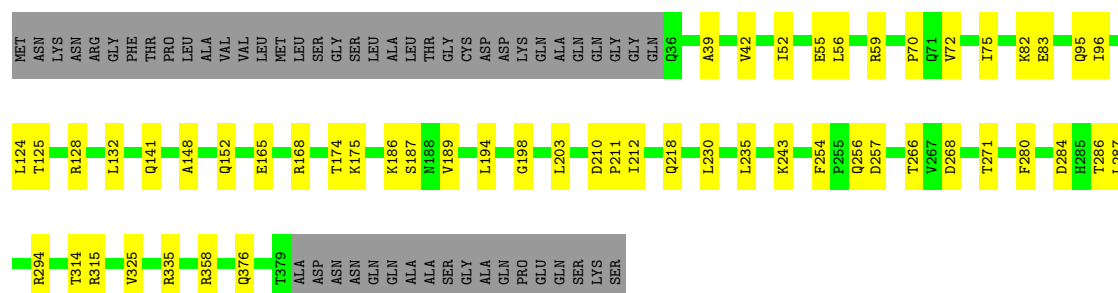
• Molecule 3: Multidrug efflux pump subunit AcrA

Chain A2:  75% 12% 13%



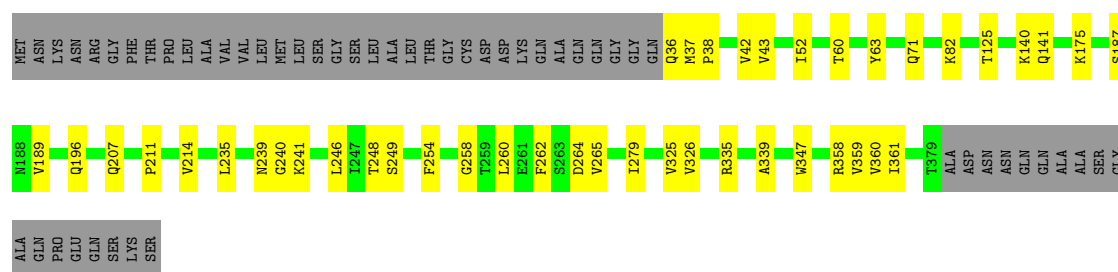
- Molecule 3: Multidrug efflux pump subunit AcrA

Chain A3:  73% 14% 13%



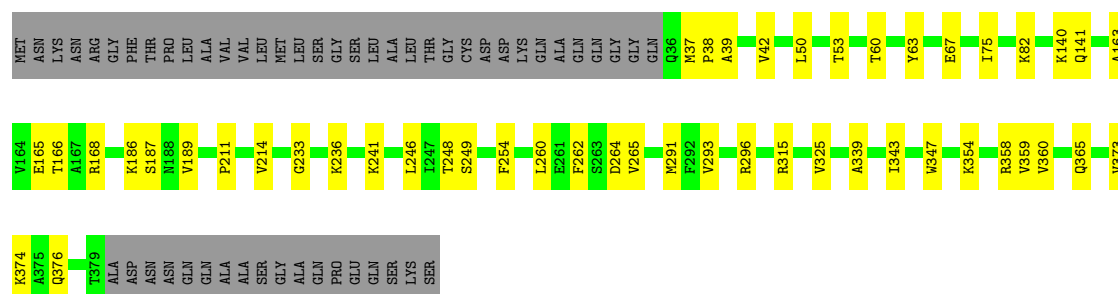
- Molecule 3: Multidrug efflux pump subunit AcrA

Chain a2:  76% 11% 13%

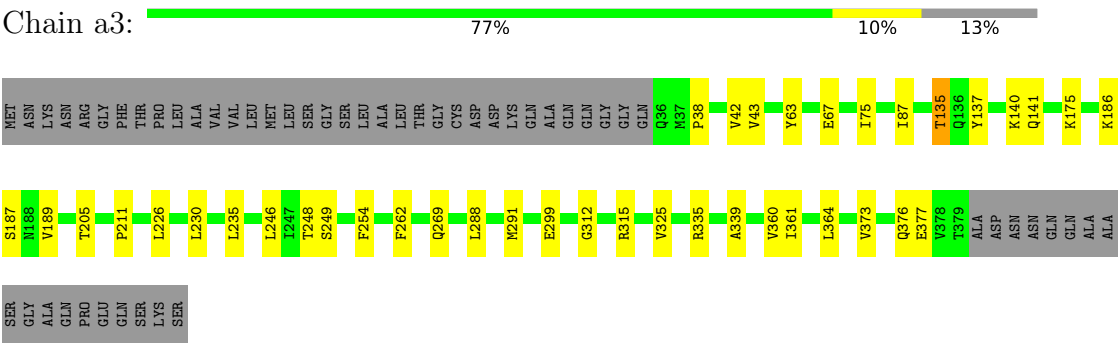


- Molecule 3: Multidrug efflux pump subunit AcrA

Chain a1:  74% 12% 13%



● Molecule 3: Multidrug efflux pump subunit AcrA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17043	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	0.26	0/4584
1	C2	0.13	0/3373	0.27	0/4584
1	C3	0.14	0/3373	0.28	0/4584
2	P1	0.13	0/1204	0.42	1/1640 (0.1%)
2	P2	0.14	0/1204	0.40	0/1640
2	P3	0.14	0/1204	0.44	0/1640
3	A1	0.12	0/2620	0.27	0/3564
3	A2	0.12	0/2620	0.26	0/3564
3	A3	0.11	0/2620	0.26	0/3564
3	a1	0.12	0/2620	0.30	0/3564
3	a2	0.12	0/2620	0.28	0/3564
3	a3	0.11	0/2620	0.27	0/3564
All	All	0.12	0/29451	0.29	1/40056 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P1	160	THR	CB-CA-C	-5.31	110.01	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by 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	40	0
1	C2	3331	0	3278	47	0
1	C3	3331	0	3278	51	0
2	P1	1182	0	1132	28	0
2	P2	1182	0	1132	27	0
2	P3	1182	0	1132	31	0
3	A1	2587	0	2648	30	0
3	A2	2587	0	2648	32	0
3	A3	2587	0	2648	36	0
3	a1	2587	0	2648	38	0
3	a2	2587	0	2648	31	0
3	a3	2587	0	2648	24	0
All	All	29061	0	29118	374	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 6.

All (374) 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:a2:239:ASN:OD1	3:a2:240:GLY:N	2.17	0.76
2:P2:68:SER:HA	2:P2:146:VAL:HG11	1.69	0.74
3:A2:179:PRO:HB3	3:a1:75:ILE:HD11	1.72	0.72
2:P1:86:GLU:N	2:P1:86:GLU:OE1	2.22	0.71
2:P3:58:ASN:HD22	2:P3:58:ASN:C	1.99	0.71
2:P3:86:GLU:OE1	2:P3:86:GLU:N	2.23	0.70
3:a3:315:ARG:NH2	3:a3:339:ALA:O	2.26	0.69
1:C1:104:ARG:NH1	1:C1:264:ASP:OD2	2.26	0.68
2:P3:32:ARG:NH1	2:P3:68:SER:O	2.27	0.68
1:C2:424:SER:HB2	1:C2:429:LEU:HD22	1.77	0.67
2:P2:86:GLU:OE1	2:P2:86:GLU:N	2.24	0.67
1:C1:30:GLN:OE1	1:C1:33:ARG:NH2	2.28	0.66
1:C2:301:MET:HE3	1:C2:302:GLY:N	2.10	0.66
1:C3:380:MET:HE2	1:C3:393:ASP:HB3	1.75	0.66
3:A3:52:ILE:HD12	3:A3:235:LEU:HD21	1.77	0.66
1:C2:155:ILE:HG13	1:C2:186:VAL:HG21	1.77	0.66
3:A3:39:ALA:HB1	3:A3:376:GLN:HE22	1.61	0.66
1:C2:252:GLN:OE1	2:P2:122:ARG:NH2	2.25	0.66
1:C1:236:LYS:HG3	2:P1:162:GLY:H	1.62	0.65
1:C3:30:GLN:OE1	1:C3:33:ARG:NH2	2.26	0.65
1:C3:155:ILE:HG13	1:C3:186:VAL:HG21	1.78	0.65
3:a2:42:VAL:HG12	3:a2:358:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:246:LEU:HB3	3:a3:254:PHE:HB2	1.79	0.64
1:C3:424:SER:HB2	1:C3:429:LEU:HD22	1.80	0.64
1:C3:252:GLN:OE1	2:P3:122:ARG:NH2	2.29	0.63
2:P1:32:ARG:NH1	2:P1:68:SER:O	2.32	0.63
3:A1:364:LEU:HD23	3:A1:364:LEU:H	1.64	0.63
3:a1:325:VAL:HG23	3:a1:359:VAL:HG12	1.80	0.62
2:P1:67:LEU:HD12	2:P1:71:LEU:HB3	1.82	0.62
3:A3:128:ARG:NH1	3:a3:141:GLN:OE1	2.33	0.61
3:a3:376:GLN:NE2	3:a3:377:GLU:O	2.33	0.61
3:A1:237:GLN:NE2	3:A1:299:GLU:O	2.32	0.61
3:a3:43:VAL:HG22	3:a3:361:ILE:HD11	1.80	0.61
2:P1:58:ASN:ND2	2:P1:91:ASP:OD1	2.33	0.61
1:C3:191:VAL:O	1:C3:195:ASN:ND2	2.32	0.61
3:A3:325:VAL:HG11	3:A3:335:ARG:HE	1.66	0.60
1:C2:314:ILE:HG22	1:C2:315:TYR:H	1.67	0.60
3:A2:38:PRO:HG2	3:A2:373:VAL:HG12	1.83	0.60
1:C2:30:GLN:OE1	1:C2:33:ARG:NH2	2.25	0.60
1:C3:24:ASN:HB2	1:C3:438:ASN:HD21	1.66	0.60
1:C3:286:SER:OG	1:C3:287:LYS:N	2.33	0.60
3:A3:55:GLU:HG2	3:A3:294:ARG:HH21	1.67	0.60
3:A2:243:LYS:NZ	3:A2:257:ASP:OD2	2.35	0.60
3:a1:246:LEU:HB3	3:a1:254:PHE:HB2	1.83	0.59
1:C3:94:THR:HG22	1:C3:273:THR:HG23	1.82	0.59
2:P3:58:ASN:O	2:P3:58:ASN:ND2	2.26	0.59
1:C1:65:GLY:HA2	1:C2:314:ILE:HG13	1.82	0.59
2:P1:42:ASP:OD1	2:P1:42:ASP:N	2.35	0.59
3:a2:248:THR:HG22	3:a2:249:SER:H	1.67	0.59
1:C1:97:ILE:HD11	1:C1:272:LEU:HD23	1.84	0.59
3:A2:55:GLU:OE2	3:A2:296:ARG:NH2	2.35	0.59
3:a1:39:ALA:HB1	3:a1:376:GLN:HE22	1.67	0.59
1:C2:301:MET:HE3	1:C2:302:GLY:H	1.67	0.59
1:C1:314:ILE:HG22	1:C1:315:TYR:H	1.67	0.58
1:C3:314:ILE:HG22	1:C3:315:TYR:H	1.67	0.58
1:C1:252:GLN:OE1	2:P1:122:ARG:NH2	2.27	0.58
1:C1:34:LEU:O	1:C1:40:ARG:NH1	2.36	0.58
3:A2:128:ARG:NH1	3:a2:141:GLN:OE1	2.34	0.58
3:a1:37:MET:HE2	3:a1:374:LYS:HZ3	1.67	0.58
1:C3:259:ILE:HD11	1:C3:328:GLN:HA	1.86	0.58
3:a3:248:THR:HG22	3:a3:249:SER:H	1.69	0.58
3:A1:243:LYS:NZ	3:A1:257:ASP:OD2	2.37	0.57
3:a3:312:GLY:HA2	3:a3:364:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:236:LYS:O	3:A1:237:GLN:NE2	2.37	0.57
3:A3:376:GLN:N	3:A3:376:GLN:OE1	2.37	0.57
1:C2:443:LYS:HD3	1:C2:444:PRO:HD2	1.85	0.57
3:A2:186:LYS:HB3	3:a2:262:PHE:CE2	2.39	0.57
2:P2:32:ARG:NH1	2:P2:68:SER:O	2.36	0.57
2:P2:90:ASN:HB3	2:P2:97:THR:HB	1.86	0.57
3:A1:38:PRO:HG2	3:A1:373:VAL:HG12	1.86	0.57
3:a1:37:MET:HE3	3:a1:38:PRO:HD2	1.87	0.57
1:C1:51:GLU:OE2	1:C1:54:ASN:ND2	2.38	0.57
1:C1:279:SER:O	1:C3:77:ARG:NH2	2.38	0.57
3:A3:95:GLN:NE2	3:A3:96:ILE:O	2.37	0.57
3:A2:210:ASP:HB3	3:A2:211:PRO:HD3	1.86	0.57
3:A3:70:PRO:HD3	3:A3:203:LEU:HD13	1.87	0.57
3:a1:248:THR:HG22	3:a1:249:SER:H	1.70	0.56
3:A1:210:ASP:HB3	3:A1:211:PRO:HD3	1.87	0.56
1:C2:46:ARG:NH1	1:C2:117:ASP:OD2	2.37	0.56
1:C2:65:GLY:HA2	1:C3:314:ILE:HG13	1.87	0.56
3:A2:184:ILE:HB	3:A2:206:VAL:HG22	1.88	0.56
2:P1:27:LYS:HA	2:P1:114:ARG:HH21	1.70	0.56
2:P3:32:ARG:NH2	2:P3:35:PRO:O	2.40	0.55
2:P3:110:THR:O	2:P3:111:ILE:HD13	2.06	0.55
1:C1:301:MET:HE2	1:C1:301:MET:HA	1.86	0.55
2:P1:105:VAL:HG22	2:P1:123:VAL:HG22	1.86	0.55
1:C3:256:ARG:NH2	2:P3:107:SER:OG	2.35	0.55
2:P2:42:ASP:OD1	2:P2:42:ASP:N	2.39	0.55
3:A1:83:GLU:HG2	3:A1:186:LYS:HA	1.88	0.55
3:A2:125:THR:OG1	3:a2:141:GLN:NE2	2.39	0.55
2:P1:30:GLY:HA2	2:P1:142:GLY:HA2	1.88	0.55
1:C1:314:ILE:HG13	1:C3:65:GLY:HA2	1.88	0.55
1:C3:332:VAL:O	1:C3:336:GLU:HG2	2.06	0.55
3:A2:337:ILE:HG21	3:A2:353:LEU:HG	1.89	0.55
3:A3:210:ASP:HB3	3:A3:211:PRO:HD3	1.90	0.54
1:C2:198:ASP:OD2	1:C3:354:ASN:ND2	2.41	0.54
1:C1:191:VAL:O	1:C1:195:ASN:ND2	2.41	0.54
1:C1:198:ASP:OD2	1:C2:354:ASN:ND2	2.37	0.54
3:A1:70:PRO:HD3	3:A1:203:LEU:HD13	1.90	0.54
3:A1:212:ILE:HG21	3:A1:287:LEU:HD11	1.90	0.54
3:a2:187:SER:OG	3:a2:189:VAL:O	2.20	0.54
3:A3:83:GLU:HG2	3:A3:186:LYS:HA	1.89	0.54
3:A3:284:ASP:HB3	3:A3:286:THR:HG23	1.90	0.54
2:P2:91:ASP:OD1	2:P2:94:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a2:339:ALA:HB1	3:a2:347:TRP:HB3	1.89	0.53
1:C2:152:LYS:HA	1:C2:186:VAL:HG11	1.89	0.53
1:C2:256:ARG:NH2	2:P2:107:SER:OG	2.42	0.53
2:P2:30:GLY:HA2	2:P2:142:GLY:HA2	1.91	0.53
2:P2:151:ARG:HA	2:P2:163:THR:HA	1.91	0.53
2:P3:139:ILE:HG13	2:P3:146:VAL:HG23	1.90	0.53
3:A1:187:SER:OG	3:A1:189:VAL:O	2.27	0.53
3:A3:125:THR:OG1	3:a3:141:GLN:NE2	2.39	0.53
3:a1:315:ARG:NH2	3:a1:339:ALA:O	2.32	0.53
2:P3:135:GLU:OE1	2:P3:151:ARG:NH1	2.38	0.53
3:A2:376:GLN:N	3:A2:376:GLN:OE1	2.41	0.53
1:C1:332:VAL:O	1:C1:336:GLU:HG2	2.09	0.52
3:A1:325:VAL:HG11	3:A1:335:ARG:HG3	1.91	0.52
1:C2:298:ASP:OD1	1:C2:298:ASP:N	2.40	0.52
1:C1:122:THR:O	1:C1:126:THR:HG23	2.09	0.52
1:C3:208:THR:HG21	1:C3:212:TYR:HE1	1.73	0.52
2:P1:138:MET:HE3	2:P1:138:MET:HA	1.92	0.52
3:A2:364:LEU:HD12	3:A2:364:LEU:H	1.72	0.52
2:P3:42:ASP:N	2:P3:42:ASP:OD1	2.40	0.52
2:P3:58:ASN:C	2:P3:58:ASN:ND2	2.68	0.52
2:P1:43:ASN:O	2:P1:47:GLN:HG3	2.09	0.52
3:A3:243:LYS:NZ	3:A3:257:ASP:OD2	2.42	0.52
2:P2:28:ASP:OD1	2:P2:28:ASP:N	2.41	0.52
3:A2:72:VAL:HG21	3:A2:174:THR:HG22	1.92	0.52
1:C3:380:MET:HE3	1:C3:380:MET:HA	1.92	0.51
1:C1:32:ALA:HB2	1:C1:208:THR:HG22	1.92	0.51
1:C2:328:GLN:NE2	2:P2:110:THR:OG1	2.43	0.51
1:C3:51:GLU:OE1	1:C3:54:ASN:ND2	2.43	0.51
2:P3:45:ALA:HB2	2:P3:138:MET:HE3	1.93	0.51
3:a3:288:LEU:H	3:a3:291:MET:HE3	1.75	0.51
1:C2:356:ILE:HD11	1:C2:419:GLN:HG2	1.92	0.51
1:C3:284:SER:OG	1:C3:285:GLY:N	2.43	0.51
1:C3:416:LEU:HD22	1:C3:437:LEU:HD22	1.93	0.51
3:A2:277:ARG:HH22	3:a1:186:LYS:HE2	1.75	0.51
3:a2:241:LYS:HB3	3:a2:260:LEU:O	2.10	0.51
1:C2:191:VAL:O	1:C2:195:ASN:ND2	2.43	0.51
1:C2:292:ALA:HB1	1:C2:295:GLN:HG3	1.92	0.51
3:A3:55:GLU:OE2	3:A3:294:ARG:NE	2.43	0.51
1:C2:82:ILE:HD11	1:C2:287:LYS:HE3	1.92	0.51
3:A2:212:ILE:HG22	3:A2:280:PHE:HB2	1.93	0.51
3:a2:42:VAL:HG11	3:a2:358:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C3:301:MET:HE2	1:C3:301:MET:HA	1.92	0.51
2:P1:37:VAL:HG12	2:P1:38:GLU:H	1.76	0.51
2:P1:74:LEU:HB3	2:P1:168:ILE:HD11	1.91	0.51
3:A2:83:GLU:HG2	3:A2:186:LYS:HA	1.92	0.50
3:a1:37:MET:HE2	3:a1:374:LYS:NZ	2.25	0.50
1:C1:284:SER:OG	1:C1:285:GLY:N	2.44	0.50
1:C2:234:LEU:HD22	1:C2:426:LEU:HD11	1.92	0.50
2:P1:110:THR:O	2:P1:111:ILE:HD13	2.12	0.50
1:C3:115:ILE:HG22	1:C3:250:LEU:HB3	1.93	0.50
2:P2:37:VAL:HG12	2:P2:38:GLU:H	1.77	0.50
3:A3:56:LEU:HD13	3:A3:218:GLN:HB2	1.93	0.50
1:C1:77:ARG:NH2	1:C2:279:SER:O	2.45	0.50
3:a1:246:LEU:HD11	3:a1:293:VAL:HB	1.93	0.50
1:C3:165:ARG:HG2	3:A3:132:LEU:HD21	1.92	0.49
1:C3:152:LYS:HA	1:C3:186:VAL:HG11	1.94	0.49
3:A1:186:LYS:HB3	3:a1:262:PHE:CE2	2.47	0.49
3:A2:257:ASP:OD1	3:A2:257:ASP:N	2.44	0.49
3:A3:212:ILE:HG21	3:A3:287:LEU:HD11	1.92	0.49
1:C1:305:LYS:HD3	1:C3:73:SER:HB2	1.94	0.49
1:C3:288:THR:HA	1:C3:296:TYR:HD2	1.77	0.49
3:a2:360:VAL:C	3:a2:361:ILE:HD13	2.38	0.49
1:C3:104:ARG:HE	1:C3:260:ARG:HB3	1.78	0.49
3:A1:337:ILE:HG22	3:A1:352:GLY:HA3	1.95	0.49
3:a1:187:SER:OG	3:a1:189:VAL:O	2.30	0.49
1:C2:332:VAL:O	1:C2:336:GLU:HG2	2.13	0.49
2:P2:90:ASN:HB2	2:P2:158:HIS:CE1	2.47	0.49
3:a1:42:VAL:HG12	3:a1:358:ARG:HG2	1.95	0.49
1:C3:356:ILE:HD11	1:C3:419:GLN:HG2	1.94	0.49
3:A2:337:ILE:HG22	3:A2:352:GLY:HA3	1.94	0.49
3:A1:179:PRO:HB3	3:a3:75:ILE:HD11	1.95	0.48
3:A1:376:GLN:OE1	3:A1:376:GLN:N	2.46	0.48
3:A3:187:SER:OG	3:A3:189:VAL:O	2.30	0.48
1:C2:416:LEU:HD22	1:C2:437:LEU:HD22	1.94	0.48
3:a2:60:THR:HG22	3:a2:214:VAL:HG22	1.95	0.48
2:P3:32:ARG:HB2	2:P3:141:GLU:O	2.14	0.48
1:C3:34:LEU:O	1:C3:40:ARG:NH1	2.46	0.48
1:C3:298:ASP:OD1	1:C3:298:ASP:N	2.42	0.48
1:C2:112:ALA:O	1:C2:115:ILE:HG12	2.14	0.48
1:C3:252:GLN:NE2	1:C3:335:SER:OG	2.42	0.48
3:a2:264:ASP:OD1	3:a2:265:VAL:N	2.41	0.48
1:C2:237:GLU:O	1:C2:241:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a3:187:SER:OG	3:a3:189:VAL:O	2.30	0.48
2:P2:158:HIS:C	2:P2:158:HIS:CD2	2.92	0.48
2:P3:125:LEU:HB2	2:P3:132:TRP:CE3	2.49	0.48
3:A1:125:THR:OG1	3:a1:141:GLN:NE2	2.47	0.47
1:C3:292:ALA:HB1	1:C3:295:GLN:HG2	1.96	0.47
1:C3:112:ALA:O	1:C3:115:ILE:HG12	2.14	0.47
1:C3:152:LYS:HD2	1:C3:187:LEU:HD23	1.95	0.47
1:C1:112:ALA:O	1:C1:115:ILE:HG12	2.14	0.47
3:A2:165:GLU:OE2	3:A2:168:ARG:NH2	2.47	0.47
1:C2:34:LEU:O	1:C2:40:ARG:NH1	2.46	0.47
3:A1:42:VAL:O	3:A1:377:GLU:HA	2.14	0.47
2:P2:46:GLN:HG2	2:P2:105:VAL:HB	1.96	0.47
3:a1:60:THR:HG22	3:a1:214:VAL:HG22	1.97	0.47
3:a1:241:LYS:HB3	3:a1:260:LEU:O	2.14	0.47
1:C3:314:ILE:O	1:C3:316:GLN:HG3	2.15	0.47
3:A2:212:ILE:HG21	3:A2:287:LEU:HD11	1.95	0.47
3:a2:326:VAL:N	3:a2:358:ARG:O	2.33	0.47
3:a1:38:PRO:HG2	3:a1:373:VAL:HG13	1.97	0.47
3:A3:59:ARG:HD3	3:a3:269:GLN:HG2	1.97	0.47
3:a2:140:LYS:HE3	3:a2:140:LYS:HB2	1.74	0.47
1:C1:338:LEU:HD23	2:P1:120:PRO:HG2	1.97	0.46
3:A2:42:VAL:HG11	3:A2:358:ARG:HB3	1.97	0.46
3:a3:63:TYR:HB2	3:a3:211:PRO:O	2.16	0.46
1:C3:76:TYR:HD1	1:C3:77:ARG:H	1.63	0.46
1:C2:314:ILE:O	1:C2:316:GLN:HG3	2.16	0.46
3:a2:262:PHE:O	3:a2:262:PHE:CG	2.68	0.46
2:P3:151:ARG:HG3	2:P3:163:THR:HG22	1.98	0.46
1:C3:305:LYS:HB2	1:C3:305:LYS:HE2	1.62	0.46
2:P3:135:GLU:HB3	2:P3:151:ARG:HB2	1.98	0.46
1:C1:314:ILE:O	1:C1:316:GLN:HG3	2.15	0.46
1:C1:354:ASN:ND2	1:C3:198:ASP:OD2	2.47	0.46
1:C3:352:SER:HB3	1:C3:422:ILE:HG13	1.97	0.46
3:A1:42:VAL:HG22	3:A1:360:VAL:HA	1.98	0.46
1:C1:115:ILE:HG22	1:C1:250:LEU:HB3	1.98	0.46
1:C2:32:ALA:HB2	1:C2:208:THR:HG22	1.98	0.46
2:P1:151:ARG:HA	2:P1:163:THR:HA	1.98	0.46
3:A1:48:GLU:N	3:A1:48:GLU:OE1	2.49	0.46
2:P1:32:ARG:HB2	2:P1:141:GLU:O	2.15	0.46
2:P3:32:ARG:HH21	2:P3:36:CYS:HB3	1.80	0.46
2:P3:97:THR:HG23	2:P3:98:THR:HG23	1.97	0.46
3:A2:126:VAL:HG21	3:A2:150:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a1:37:MET:HE3	3:a1:37:MET:HA	1.96	0.46
3:a1:140:LYS:HB2	3:a1:140:LYS:HE3	1.76	0.46
3:A2:52:ILE:HD12	3:A2:235:LEU:HD21	1.98	0.46
1:C1:161:GLN:O	1:C1:165:ARG:HG3	2.15	0.45
2:P1:97:THR:HG23	2:P1:98:THR:HG23	1.97	0.45
3:A3:72:VAL:HG21	3:A3:174:THR:HG22	1.97	0.45
3:a1:233:GLY:O	3:a1:236:LYS:NZ	2.31	0.45
1:C2:51:GLU:OE2	1:C2:54:ASN:ND2	2.50	0.45
2:P3:70:LYS:HD3	2:P3:70:LYS:N	2.31	0.45
3:a3:226:LEU:HD13	3:a3:299:GLU:HG2	1.99	0.45
2:P2:54:LEU:HD23	2:P2:55:HIS:CE1	2.52	0.45
3:a3:135:THR:HG23	3:a3:137:TYR:CD2	2.52	0.45
3:a2:36:GLN:HB3	3:a2:37:MET:H	1.49	0.45
3:a1:50:LEU:HD11	3:a1:343:ILE:HG13	1.97	0.45
3:a1:67:GLU:OE1	3:a1:67:GLU:N	2.49	0.45
1:C1:34:LEU:HD11	2:P2:29:ASN:HA	1.99	0.45
1:C2:157:ARG:HD2	1:C2:157:ARG:HA	1.60	0.45
3:A2:338:VAL:HG12	3:A2:351:GLU:HG2	1.98	0.45
3:a2:63:TYR:HB2	3:a2:211:PRO:O	2.17	0.45
1:C1:240:LYS:HG3	1:C1:241:ARG:HG2	1.99	0.44
3:a2:325:VAL:HA	3:a2:359:VAL:HA	1.99	0.44
1:C2:426:LEU:HB2	1:C2:428:THR:HG22	1.99	0.44
3:A3:42:VAL:HG11	3:A3:358:ARG:HB3	1.98	0.44
3:A3:254:PHE:CE2	3:A3:256:GLN:HB2	2.52	0.44
1:C1:157:ARG:HA	1:C1:157:ARG:HD2	1.62	0.44
3:a1:165:GLU:OE2	3:a1:168:ARG:NE	2.42	0.44
1:C1:100:MET:HE3	1:C1:100:MET:HB3	1.85	0.44
2:P3:30:GLY:HA2	2:P3:142:GLY:HA2	1.98	0.44
3:A1:60:THR:HG22	3:A1:214:VAL:HG22	2.00	0.44
3:a2:43:VAL:HG22	3:a2:361:ILE:HG13	1.99	0.44
3:a2:82:LYS:HB2	3:a2:82:LYS:HE3	1.62	0.44
2:P1:32:ARG:NH2	2:P1:35:PRO:O	2.51	0.44
2:P3:41:PRO:HB3	2:P3:138:MET:HG3	2.00	0.44
3:A1:247:ILE:HD11	3:A1:296:ARG:HD3	1.99	0.44
3:A2:145:GLN:NE2	3:A2:149:ASP:OD1	2.50	0.44
2:P2:127:GLN:HB2	2:P2:132:TRP:CZ2	2.53	0.44
1:C1:359:SER:HG	1:C1:415:TYR:HB2	1.83	0.44
2:P1:125:LEU:HD12	2:P1:132:TRP:NE1	2.32	0.44
3:A2:79:ARG:HG3	3:A2:94:TYR:HE1	1.82	0.44
3:A2:228:GLN:O	3:A2:228:GLN:NE2	2.43	0.44
3:A2:267:VAL:HG22	3:A2:274:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:100:MET:HA	1:C2:103:TRP:HD1	1.82	0.44
1:C3:249:ARG:HD2	2:P3:122:ARG:HD3	2.00	0.44
2:P3:43:ASN:O	2:P3:47:GLN:HG3	2.18	0.44
3:a2:37:MET:HE3	3:a2:38:PRO:HD2	2.00	0.44
3:A3:75:ILE:HD11	3:A3:194:LEU:HD12	2.01	0.43
1:C1:197:LEU:HD22	1:C1:449:PRO:HG3	1.99	0.43
1:C2:232:ASN:HB3	2:P2:161:ALA:HB2	2.00	0.43
1:C3:100:MET:HE3	1:C3:100:MET:HB3	1.94	0.43
1:C3:208:THR:HG21	1:C3:212:TYR:CE1	2.53	0.43
2:P3:127:GLN:HB2	2:P3:132:TRP:CH2	2.54	0.43
1:C2:214:GLU:OE2	1:C2:444:PRO:HB2	2.18	0.43
2:P3:49:TYR:CE2	2:P3:123:VAL:HG21	2.54	0.43
3:a3:325:VAL:HG11	3:a3:335:ARG:HD2	1.99	0.43
3:a2:258:GLY:HA3	3:a2:279:ILE:O	2.18	0.43
3:a1:42:VAL:HG13	3:a1:359:VAL:C	2.43	0.43
1:C2:213:PRO:HA	1:C2:447:THR:HG22	2.01	0.43
2:P2:71:LEU:HA	2:P2:71:LEU:HD23	1.79	0.43
3:A1:368:ARG:HG3	3:A1:369:PRO:HD2	1.99	0.43
3:A3:175:LYS:HE3	3:A3:175:LYS:HB2	1.84	0.43
1:C1:329:TYR:OH	2:P1:113:ASN:ND2	2.52	0.43
1:C1:356:ILE:O	1:C1:360:ILE:HG12	2.19	0.43
3:A3:198:GLY:HA3	3:a2:196:GLN:NE2	2.34	0.43
1:C2:60:LEU:HD23	1:C2:60:LEU:HA	1.91	0.42
2:P2:105:VAL:HG22	2:P2:123:VAL:HG12	2.00	0.42
1:C2:24:ASN:ND2	1:C2:438:ASN:HD21	2.17	0.42
3:a2:52:ILE:HD12	3:a2:235:LEU:HD21	2.01	0.42
3:a1:264:ASP:OD1	3:a1:265:VAL:N	2.48	0.42
2:P2:127:GLN:HB2	2:P2:132:TRP:HZ2	1.84	0.42
3:A3:165:GLU:OE2	3:A3:168:ARG:NH2	2.39	0.42
3:a3:67:GLU:HG2	3:a3:205:THR:HG22	2.00	0.42
1:C1:183:TYR:O	1:C1:186:VAL:HG12	2.19	0.42
1:C1:232:ASN:HB3	2:P1:161:ALA:HB2	2.00	0.42
3:A3:141:GLN:NE2	3:a2:125:THR:OG1	2.50	0.42
3:A3:314:THR:OG1	3:A3:315:ARG:N	2.52	0.42
3:a1:82:LYS:HB2	3:a1:82:LYS:HE3	1.59	0.42
3:a1:365:GLN:CD	3:a1:365:GLN:H	2.28	0.42
1:C3:380:MET:HE1	1:C3:389:ARG:HE	1.84	0.42
3:a1:291:MET:H	3:a1:291:MET:HG2	1.69	0.42
1:C1:259:ILE:HD11	1:C1:328:GLN:HA	2.00	0.42
3:A1:147:LEU:HD12	3:A1:147:LEU:HA	1.92	0.42
3:a1:339:ALA:HB1	3:a1:347:TRP:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:245:LEU:HD23	1:C2:245:LEU:HA	1.80	0.42
3:A1:277:ARG:NH2	3:a3:186:LYS:HD2	2.35	0.42
2:P1:52:ARG:NH2	2:P1:91:ASP:OD2	2.53	0.42
3:a2:325:VAL:HG11	3:a2:335:ARG:NH2	2.34	0.42
3:A1:332:VAL:HG23	3:A1:369:PRO:HA	2.02	0.42
3:A3:268:ASP:HB3	3:A3:271:THR:HG22	2.02	0.42
2:P3:165:ARG:O	2:P3:169:GLU:HB2	2.20	0.42
3:A1:128:ARG:NH1	3:a1:141:GLN:OE1	2.48	0.42
3:A3:124:LEU:HD23	3:A3:124:LEU:HA	1.87	0.42
3:A3:266:THR:HB	3:a2:207:GLN:HE22	1.85	0.42
3:a1:42:VAL:HG22	3:a1:360:VAL:HA	2.02	0.42
1:C2:287:LYS:HB2	1:C2:287:LYS:HE2	1.88	0.41
2:P2:26:TYR:O	2:P2:114:ARG:NH2	2.49	0.41
2:P3:68:SER:HB2	2:P3:141:GLU:OE1	2.20	0.41
1:C2:115:ILE:HG22	1:C2:250:LEU:HB3	2.01	0.41
1:C3:324:VAL:O	1:C3:328:GLN:HG3	2.20	0.41
3:A1:215:ASP:CG	3:A1:277:ARG:HH21	2.27	0.41
3:A2:226:LEU:HD12	3:A2:226:LEU:HA	1.92	0.41
3:A2:214:VAL:HG12	3:A2:216:VAL:HG23	2.02	0.41
3:a1:42:VAL:CG1	3:a1:358:ARG:HG2	2.50	0.41
3:a3:175:LYS:HE3	3:a3:175:LYS:HB2	1.94	0.41
3:a2:246:LEU:HB3	3:a2:254:PHE:HB2	2.02	0.41
3:a1:163:ALA:O	3:a1:166:THR:HG22	2.20	0.41
3:a3:42:VAL:HG22	3:a3:360:VAL:HA	2.02	0.41
1:C1:104:ARG:NH1	1:C1:260:ARG:HB3	2.36	0.41
1:C3:60:LEU:HD23	1:C3:60:LEU:HA	1.88	0.41
3:A1:288:LEU:O	3:A1:291:MET:HG2	2.21	0.41
1:C3:26:MET:O	1:C3:30:GLN:HG2	2.20	0.41
3:A2:254:PHE:CE2	3:A2:256:GLN:HB2	2.56	0.41
3:A3:230:LEU:HA	3:A3:235:LEU:HB2	2.02	0.41
3:a2:175:LYS:HE3	3:a2:175:LYS:HB2	1.98	0.41
1:C1:82:ILE:HD11	1:C1:287:LYS:HE3	2.02	0.41
1:C2:26:MET:O	1:C2:30:GLN:HG2	2.20	0.41
2:P2:123:VAL:O	2:P2:133:GLN:HA	2.21	0.41
1:C2:107:THR:O	1:C2:111:LYS:HG3	2.21	0.41
2:P1:71:LEU:HD12	2:P1:71:LEU:HA	1.80	0.41
3:a1:53:THR:HB	3:a1:296:ARG:HG3	2.01	0.41
3:a1:63:TYR:HB2	3:a1:211:PRO:O	2.20	0.41
3:a1:354:LYS:HA	3:a1:354:LYS:HD2	1.90	0.41
1:C2:429:LEU:HD12	1:C2:429:LEU:HA	1.93	0.41
2:P1:165:ARG:O	2:P1:169:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:132:LEU:HD12	3:A3:132:LEU:HA	1.91	0.41
3:A3:212:ILE:HG22	3:A3:280:PHE:HB2	2.02	0.41
1:C1:252:GLN:NE2	1:C1:335:SER:OG	2.45	0.40
1:C3:448:ASN:O	1:C3:452:VAL:HG22	2.22	0.40
2:P3:28:ASP:OD2	2:P3:28:ASP:N	2.54	0.40
1:C3:46:ARG:NH2	2:P1:23:THR:O	2.55	0.40
2:P3:70:LYS:O	2:P3:74:LEU:HB2	2.20	0.40
3:A1:246:LEU:HD12	3:A1:246:LEU:HA	1.89	0.40
3:a3:87:ILE:HD13	3:a3:87:ILE:HA	1.84	0.40
1:C2:29:TYR:CE1	1:C2:128:ILE:HG12	2.57	0.40
3:A2:228:GLN:HE21	3:A2:228:GLN:C	2.25	0.40
3:a3:38:PRO:HG2	3:a3:373:VAL:HG13	2.03	0.40
3:a3:230:LEU:HD23	3:a3:235:LEU:HB2	2.03	0.40
2:P2:111:ILE:HD13	2:P2:111:ILE:HA	1.97	0.40
3:A3:82:LYS:HB2	3:A3:82:LYS:HE3	1.76	0.40
3:a2:239:ASN:CG	3:a2:240:GLY:N	2.80	0.40
3:a3:140:LYS:HE3	3:a3:140:LYS:HB2	1.74	0.40
1:C2:135:TYR:HE1	1:C2:215:LEU:HD22	1.87	0.40
1:C3:232:ASN:HB3	2:P3:161:ALA:HB2	2.02	0.40
2:P1:68:SER:OG	2:P1:69:ASP:N	2.54	0.40
2:P2:149:ASP:O	2:P2:164:LEU:HB3	2.22	0.40
3:A1:95:GLN:NE2	3:A1:96:ILE:O	2.54	0.40
3:A3:148:ALA:O	3:A3:152:GLN:HG3	2.22	0.40
3:a1:262:PHE:O	3:a1:262:PHE:CG	2.74	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%)	419 (97%)	11 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C2	430/493 (87%)	422 (98%)	8 (2%)	0	100	100
1	C3	430/493 (87%)	419 (97%)	10 (2%)	1 (0%)	43	70
2	P1	150/171 (88%)	123 (82%)	25 (17%)	2 (1%)	9	34
2	P2	150/171 (88%)	126 (84%)	22 (15%)	2 (1%)	9	34
2	P3	150/171 (88%)	123 (82%)	26 (17%)	1 (1%)	18	48
3	A1	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	A2	342/397 (86%)	330 (96%)	12 (4%)	0	100	100
3	A3	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a1	342/397 (86%)	335 (98%)	7 (2%)	0	100	100
3	a2	342/397 (86%)	332 (97%)	10 (3%)	0	100	100
3	a3	342/397 (86%)	333 (97%)	8 (2%)	1 (0%)	36	66
All	All	3792/4374 (87%)	3626 (96%)	159 (4%)	7 (0%)	44	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C3	286	SER
2	P2	150	VAL
2	P1	149	ASP
2	P1	150	VAL
2	P2	149	ASP
2	P3	150	VAL
3	a3	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
1	C2	361/412 (88%)	361 (100%)	0	100	100
1	C3	361/412 (88%)	361 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P1	131/148 (88%)	130 (99%)	1 (1%)	73	78
2	P2	131/148 (88%)	130 (99%)	1 (1%)	73	78
2	P3	131/148 (88%)	129 (98%)	2 (2%)	57	71
3	A1	278/318 (87%)	277 (100%)	1 (0%)	84	84
3	A2	278/318 (87%)	277 (100%)	1 (0%)	84	84
3	A3	278/318 (87%)	278 (100%)	0	100	100
3	a1	278/318 (87%)	278 (100%)	0	100	100
3	a2	278/318 (87%)	277 (100%)	1 (0%)	84	84
3	a3	278/318 (87%)	277 (100%)	1 (0%)	84	84
All	All	3144/3588 (88%)	3136 (100%)	8 (0%)	84	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P1	53	ILE
2	P2	31	THR
2	P3	42	ASP
2	P3	58	ASN
3	A1	158	THR
3	A2	228	GLN
3	a2	71	GLN
3	a3	135	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C1	74	ASN
1	C1	178	ASN
1	C1	206	GLN
1	C1	247	GLN
1	C1	300	ASN
1	C1	403	ASN
1	C1	438	ASN
1	C2	74	ASN
1	C2	83	ASN
1	C2	300	ASN
1	C2	328	GLN
1	C2	403	ASN

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Mol	Chain	Res	Type
1	C2	430	ASN
1	C2	438	ASN
1	C3	92	GLN
1	C3	178	ASN
1	C3	206	GLN
1	C3	222	ASN
1	C3	247	GLN
2	P1	29	ASN
2	P1	90	ASN
2	P1	127	GLN
2	P1	158	HIS
2	P2	43	ASN
2	P2	47	GLN
2	P2	55	HIS
2	P2	90	ASN
2	P2	118	ASN
2	P2	127	GLN
2	P2	158	HIS
2	P3	55	HIS
2	P3	58	ASN
2	P3	118	ASN
3	A1	95	GLN
3	A1	145	GLN
3	A1	228	GLN
3	A2	341	GLN
3	A3	145	GLN
3	A3	228	GLN
3	a2	102	GLN
3	a2	365	GLN
3	a1	102	GLN
3	a1	196	GLN
3	a1	256	GLN
3	a3	102	GLN
3	a3	376	GLN

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 [i](#)

There are no oligosaccharides 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.