



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 07:58 PM UTC

PDB ID : 487D / pdb_0000487d
Title : SEVEN RIBOSOMAL PROTEINS FITTED TO A CRYO-ELECTRON MICROSCOPIC MAP OF THE LARGE 50S SUBUNIT AT 7.5 ANGSTROMS RESOLUTION
Authors : Brimacombe, R.; Mueller, F.
Deposited on : 2000-02-23
Resolution : 7.50 Å (reported)
Based on initial models : 1CSW, 1CSV, 1CSX

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

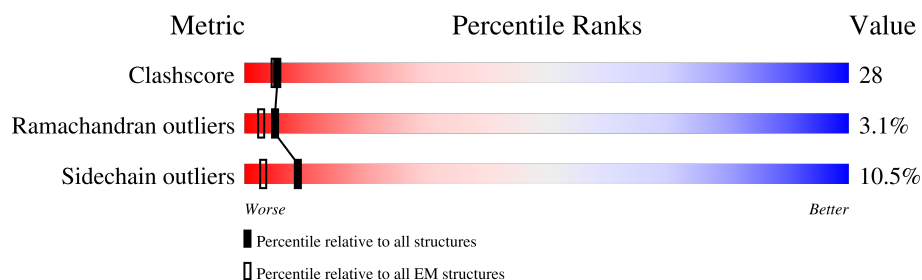
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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	H	224	84% 15% .
2	I	135	50% 35% 13% .
3	J	164	73% 26% .
4	K	149	46% 44% 9% .
5	L	133	38% 37% 17% 8%
6	M	122	68% 30% ..
7	N	94	74% 24% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8778 atoms, of which 953 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 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	224	Total	C	N	O	S	0	0
			1712	1083	311	314	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	179	CYS	SER	conflict	UNP P27150

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	135	Total	C	N	O	S	Se	0	0
			1024	645	187	188	1	3		

- Molecule 3 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	164	Total	C	N	O	S	0	0
			1251	787	225	237	2		

- Molecule 4 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
4	K	149	Total	C	H	N	O	S	0	0
			1435	729	287	206	212	1		

- Molecule 5 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	133	Total	C	N	O	S	0	0
			1000	642	169	183	6		

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	122	Total	C	N	O	S	0	0
			937	585	180	169	3		

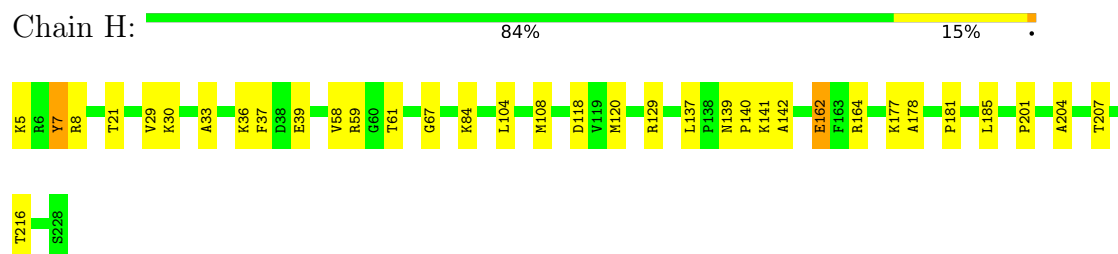
- Molecule 7 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	94	Total	C	H	N	O	S	0	0
			1419	479	666	137	134	3		

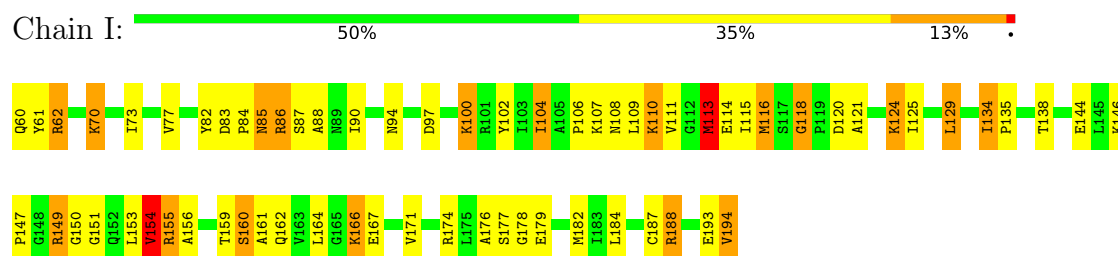
3 Residue-property plots [i](#)

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.

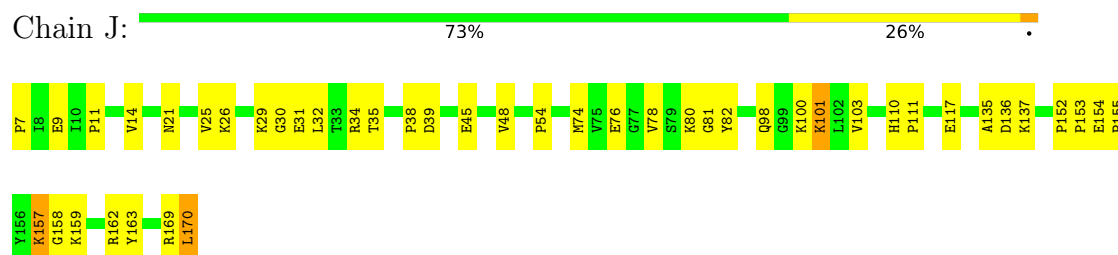
• Molecule 1: 50S ribosomal protein L1



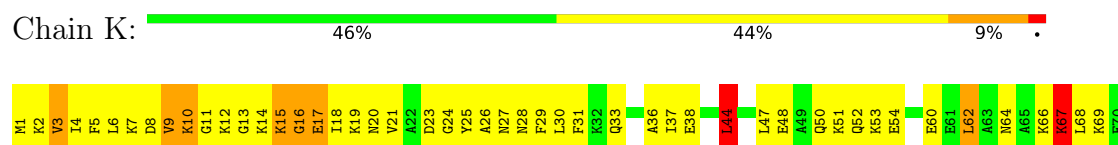
• Molecule 2: 50S ribosomal protein L2

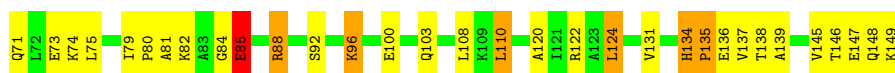


• Molecule 3: 50S ribosomal protein L6



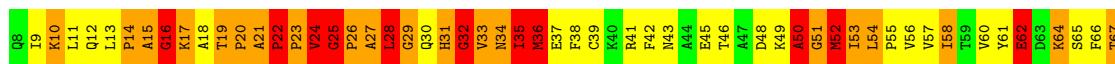
• Molecule 4: 50S ribosomal protein L9





• Molecule 5: 50S ribosomal protein L11

Chain L: 38% 37% 17% 8%



• Molecule 6: 50S ribosomal protein L14

Chain M: 68% 30% . .



• Molecule 7: 50S ribosomal protein L25

Chain N: 74% 24% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 7.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-7.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8778	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	H	0.65	0/1743	1.07	6/2351 (0.3%)
2	I	0.64	3/1034 (0.3%)	1.00	7/1388 (0.5%)
3	J	0.84	0/1270	1.09	8/1715 (0.5%)
4	K	0.82	0/1160	1.11	5/1552 (0.3%)
5	L	0.83	2/1016 (0.2%)	1.34	19/1366 (1.4%)
6	M	1.33	2/946 (0.2%)	1.57	8/1269 (0.6%)
7	N	1.32	9/766 (1.2%)	1.43	5/1025 (0.5%)
All	All	0.91	16/7935 (0.2%)	1.21	58/10666 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	M	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	86	ILE	C-N	-28.35	0.95	1.33
6	M	87	ILE	C-N	24.25	1.67	1.33
2	I	113	MSE	SE-CE	-6.99	1.74	1.95
7	N	80	HIS	CE1-NE2	-6.71	1.25	1.32
7	N	44	HIS	CE1-NE2	-6.63	1.25	1.32
7	N	88	HIS	CE1-NE2	-6.49	1.26	1.32
2	I	116	MSE	SE-CE	-6.40	1.76	1.95
2	I	182	MSE	SE-CE	-6.22	1.76	1.95
5	L	24	VAL	CA-CB	6.07	1.62	1.54
7	N	88	HIS	CD2-NE2	5.93	1.44	1.37
7	N	88	HIS	CG-ND1	-5.93	1.31	1.38
7	N	44	HIS	CG-ND1	-5.93	1.31	1.38
5	L	22	PRO	CA-C	5.79	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	44	HIS	CD2-NE2	5.76	1.44	1.37
7	N	80	HIS	CD2-NE2	5.72	1.44	1.37
7	N	80	HIS	CG-ND1	-5.70	1.31	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	86	ILE	O-C-N	-19.77	97.85	122.57
6	M	87	ILE	CA-C-N	-19.16	84.95	121.54
6	M	87	ILE	C-N-CA	-19.16	84.95	121.54
6	M	86	ILE	CA-C-N	-18.70	88.31	121.97
6	M	86	ILE	C-N-CA	-18.70	88.31	121.97
6	M	87	ILE	O-C-N	12.74	138.50	122.57
5	L	22	PRO	N-CA-C	10.20	123.14	110.70
5	L	34	ASN	N-CA-C	-9.61	95.75	108.34
5	L	29	GLY	N-CA-C	-9.58	103.77	114.40
5	L	15	ALA	N-CA-C	8.99	121.85	110.61
1	H	142	ALA	N-CA-C	-8.97	102.04	113.16
4	K	11	GLY	N-CA-C	-8.13	104.19	111.67
5	L	67	THR	N-CA-C	-7.50	97.97	109.14
5	L	16	GLY	N-CA-C	-7.30	95.87	113.18
1	H	118	ASP	N-CA-C	7.22	121.68	113.01
5	L	32	GLY	N-CA-C	-7.07	96.44	113.18
5	L	50	ALA	N-CA-C	7.04	125.79	110.80
4	K	60	GLU	N-CA-C	-6.79	103.80	111.14
1	H	181	PRO	N-CA-C	-6.68	102.56	110.70
5	L	25	GLY	N-CA-C	6.67	125.95	112.34
1	H	21	THR	N-CA-C	-6.67	101.55	110.55
5	L	53	ILE	CB-CA-C	-6.66	102.90	110.96
3	J	154	GLU	CA-C-N	6.57	127.09	119.47
3	J	154	GLU	C-N-CA	6.57	127.09	119.47
1	H	67	GLY	N-CA-C	6.34	122.63	115.08
6	M	40	VAL	N-CA-C	-6.34	99.29	108.36
7	N	88	HIS	CG-CD2-NE2	-6.25	100.95	107.20
4	K	134	HIS	N-CA-CB	-6.22	105.42	111.27
7	N	44	HIS	CG-CD2-NE2	-6.11	101.09	107.20
7	N	80	HIS	CG-CD2-NE2	-6.07	101.13	107.20
5	L	31	HIS	N-CA-C	6.05	120.72	112.68
5	L	19	THR	CA-C-N	-6.02	110.52	120.88
5	L	19	THR	C-N-CA	-6.02	110.52	120.88
5	L	28	LEU	N-CA-C	-6.02	105.59	113.12
2	I	104	ILE	N-CA-C	-5.99	101.81	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	120	MET	N-CA-C	5.99	118.59	111.71
2	I	73	ILE	N-CA-C	5.84	112.88	107.56
3	J	155	PRO	N-CA-C	5.82	122.25	113.81
3	J	101	LYS	N-CA-C	5.48	118.86	110.20
2	I	134	ILE	N-CA-C	5.47	113.86	107.89
5	L	51	GLY	N-CA-C	-5.46	100.24	113.18
5	L	20	PRO	N-CA-C	-5.44	105.13	112.48
7	N	19	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	K	44	LEU	N-CA-C	-5.41	106.36	113.12
6	M	112	MET	N-CA-C	5.36	117.12	111.28
5	L	90	SER	N-CA-C	-5.34	106.72	113.18
3	J	100	LYS	N-CA-C	-5.24	106.84	113.18
5	L	52	MET	N-CA-C	5.24	115.30	108.07
3	J	74	MET	N-CA-C	-5.15	105.75	111.36
5	L	10	LYS	N-CA-C	-5.14	101.89	110.17
7	N	79	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	I	118	GLY	CA-C-N	5.10	124.89	119.28
2	I	118	GLY	C-N-CA	5.10	124.89	119.28
2	I	134	ILE	CA-C-N	5.10	125.34	119.83
2	I	134	ILE	C-N-CA	5.10	125.34	119.83
3	J	152	PRO	CA-C-N	5.08	125.32	119.83
3	J	152	PRO	C-N-CA	5.08	125.32	119.83
4	K	67	LYS	N-CA-C	-5.03	105.50	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	M	86	ILE	Mainchain

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	H	1712	0	1763	10	0
2	I	1024	0	1073	50	0
3	J	1251	0	1294	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	1148	287	1230	66	0
5	L	1000	0	1071	148	0
6	M	937	0	995	115	0
7	N	753	666	780	4	0
All	All	7825	953	8206	449	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 28.

All (449) 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)
6:M:79:PHE:CZ	6:M:103:ALA:HB2	1.33	1.64
6:M:79:PHE:CZ	6:M:103:ALA:CB	1.87	1.54
6:M:63:VAL:CB	6:M:106:LEU:HD21	1.34	1.52
6:M:87:ILE:C	6:M:88:ARG:N	1.67	1.49
6:M:63:VAL:HG12	6:M:106:LEU:CD2	1.38	1.48
3:J:29:LYS:CG	3:J:81:GLY:N	1.78	1.46
6:M:61:VAL:HG21	6:M:111:PHE:CE2	1.50	1.44
6:M:63:VAL:CG1	6:M:106:LEU:CD2	2.01	1.38
6:M:61:VAL:HG11	6:M:111:PHE:CE1	1.54	1.38
6:M:85:VAL:HG11	6:M:114:ILE:CD1	1.53	1.38
6:M:79:PHE:CE1	6:M:103:ALA:HB2	1.60	1.35
6:M:61:VAL:HG11	6:M:111:PHE:CZ	1.62	1.33
6:M:85:VAL:CG1	6:M:114:ILE:HD11	1.59	1.32
6:M:63:VAL:CG1	6:M:106:LEU:HD21	1.61	1.31
6:M:63:VAL:CA	6:M:106:LEU:HD21	1.58	1.30
3:J:32:LEU:CD2	3:J:136:ASP:HB2	1.64	1.27
3:J:29:LYS:HG3	3:J:81:GLY:CA	1.65	1.27
6:M:63:VAL:HB	6:M:106:LEU:CD1	1.65	1.27
6:M:64:ARG:NH1	6:M:102:VAL:HG12	1.51	1.25
6:M:63:VAL:CB	6:M:106:LEU:CD2	2.14	1.24
6:M:87:ILE:C	6:M:88:ARG:CA	2.11	1.22
6:M:35:ILE:HG21	6:M:105:GLU:HB3	1.19	1.17
5:L:24:VAL:HG23	5:L:25:GLY:H	1.05	1.16
6:M:35:ILE:HG21	6:M:105:GLU:CB	1.74	1.16
3:J:29:LYS:HG3	3:J:81:GLY:N	0.83	1.15
6:M:61:VAL:CG1	6:M:111:PHE:CZ	2.29	1.14
6:M:64:ARG:HH11	6:M:102:VAL:HA	1.10	1.12
6:M:79:PHE:CE1	6:M:103:ALA:CB	2.26	1.11
3:J:76:GLU:HB3	3:J:82:TYR:OH	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:23:PRO:O	5:L:24:VAL:HG22	1.51	1.09
6:M:87:ILE:CA	6:M:88:ARG:N	2.15	1.08
6:M:64:ARG:HH12	6:M:102:VAL:HG12	0.92	1.08
6:M:61:VAL:CG1	6:M:111:PHE:CE1	2.35	1.08
6:M:63:VAL:CG1	6:M:106:LEU:HD22	1.71	1.07
6:M:63:VAL:HB	6:M:106:LEU:HD11	1.08	1.07
6:M:36:GLY:CA	6:M:109:LYS:HG3	1.85	1.07
6:M:36:GLY:HA2	6:M:109:LYS:HG3	1.32	1.06
6:M:63:VAL:HA	6:M:106:LEU:HD21	1.38	1.06
5:L:49:LYS:CG	5:L:50:ALA:H	1.67	1.06
6:M:61:VAL:CB	6:M:111:PHE:CZ	2.39	1.05
6:M:85:VAL:CG2	6:M:114:ILE:HD13	1.85	1.05
5:L:49:LYS:HG3	5:L:50:ALA:N	1.66	1.05
3:J:32:LEU:HD21	3:J:136:ASP:HB2	1.29	1.04
6:M:64:ARG:HH12	6:M:102:VAL:CG1	1.71	1.04
3:J:32:LEU:CD2	3:J:136:ASP:CB	2.37	1.03
6:M:79:PHE:CZ	6:M:103:ALA:HB1	1.94	1.03
6:M:86:ILE:HG22	6:M:87:ILE:N	1.69	1.03
6:M:85:VAL:HG21	6:M:114:ILE:HD13	1.06	1.02
6:M:61:VAL:CG2	6:M:111:PHE:CE2	2.42	1.01
3:J:80:LYS:C	3:J:81:GLY:N	2.18	1.00
6:M:85:VAL:HG21	6:M:114:ILE:CD1	1.91	1.00
6:M:87:ILE:C	6:M:88:ARG:C	2.30	0.98
6:M:63:VAL:CB	6:M:106:LEU:HD11	1.93	0.98
6:M:63:VAL:HB	6:M:106:LEU:CG	1.94	0.98
5:L:24:VAL:HG23	5:L:25:GLY:N	1.78	0.97
6:M:61:VAL:HG21	6:M:111:PHE:CZ	1.98	0.97
3:J:32:LEU:HD21	3:J:136:ASP:CB	1.93	0.96
5:L:49:LYS:HG3	5:L:50:ALA:H	0.81	0.96
5:L:9:ILE:HD11	5:L:31:HIS:ND1	1.81	0.95
6:M:79:PHE:CZ	6:M:103:ALA:CA	2.48	0.95
6:M:63:VAL:HB	6:M:106:LEU:HD21	1.47	0.95
3:J:29:LYS:CG	3:J:81:GLY:CA	2.32	0.94
5:L:38:PHE:HD1	5:L:66:PHE:CE1	1.86	0.94
6:M:61:VAL:HG21	6:M:111:PHE:HE2	1.21	0.94
6:M:13:ASN:ND2	6:M:97:ARG:H	1.62	0.94
5:L:24:VAL:CG2	5:L:25:GLY:H	1.77	0.94
6:M:79:PHE:HZ	6:M:103:ALA:CB	1.65	0.93
6:M:35:ILE:CG2	6:M:105:GLU:HB3	1.97	0.92
5:L:18:ALA:HB1	5:L:39:CYS:SG	2.10	0.92
6:M:86:ILE:CG2	6:M:87:ILE:N	2.24	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:9:ILE:HD13	5:L:28:LEU:HD22	1.49	0.92
6:M:63:VAL:HG12	6:M:106:LEU:HD22	0.93	0.92
3:J:32:LEU:HD22	3:J:136:ASP:OD2	1.70	0.92
5:L:18:ALA:CB	5:L:39:CYS:HB3	2.00	0.92
6:M:64:ARG:NH1	6:M:102:VAL:CG1	2.30	0.92
3:J:32:LEU:HD22	3:J:136:ASP:HB2	1.53	0.91
5:L:32:GLY:CA	5:L:64:LYS:HD2	1.99	0.90
6:M:87:ILE:HA	6:M:88:ARG:N	1.85	0.89
6:M:61:VAL:CG2	6:M:111:PHE:CZ	2.56	0.89
5:L:9:ILE:HB	5:L:58:ILE:HG23	1.53	0.89
5:L:15:ALA:H	5:L:17:LYS:HE3	1.38	0.88
6:M:63:VAL:HA	6:M:106:LEU:CD2	2.04	0.88
5:L:14:PRO:HB2	5:L:17:LYS:HG3	1.55	0.88
6:M:63:VAL:CA	6:M:106:LEU:CD2	2.49	0.88
3:J:29:LYS:HB3	3:J:81:GLY:HA2	1.56	0.87
5:L:18:ALA:HB1	5:L:39:CYS:CB	2.05	0.86
5:L:18:ALA:HB1	5:L:39:CYS:HB3	1.56	0.86
3:J:32:LEU:HD22	3:J:136:ASP:CB	2.03	0.86
5:L:16:GLY:H	5:L:17:LYS:HG2	1.39	0.86
4:K:71:GLN:O	4:K:74:LYS:HG2	1.77	0.85
6:M:64:ARG:HH11	6:M:102:VAL:CA	1.90	0.85
6:M:64:ARG:NH1	6:M:102:VAL:HA	1.93	0.84
5:L:42:PHE:CE1	5:L:56:VAL:HG21	2.13	0.83
6:M:22:ILE:HD11	6:M:42:THR:HG23	1.59	0.82
6:M:85:VAL:CG1	6:M:114:ILE:CD1	2.36	0.82
5:L:46:THR:HG22	5:L:54:LEU:HD11	1.61	0.82
6:M:13:ASN:ND2	6:M:97:ARG:N	2.23	0.82
4:K:5:PHE:HE2	4:K:19:LYS:HB3	1.41	0.82
5:L:21:ALA:HB3	5:L:22:PRO:CD	2.10	0.82
5:L:46:THR:O	5:L:50:ALA:HB3	1.79	0.82
3:J:32:LEU:HD22	3:J:136:ASP:CG	2.04	0.81
6:M:35:ILE:HG21	6:M:105:GLU:HB2	1.63	0.81
6:M:63:VAL:HB	6:M:106:LEU:CD2	1.93	0.80
5:L:14:PRO:CB	5:L:17:LYS:HG3	2.11	0.80
5:L:15:ALA:CB	5:L:50:ALA:HB1	2.12	0.80
6:M:61:VAL:HB	6:M:111:PHE:CZ	2.17	0.80
5:L:15:ALA:N	5:L:17:LYS:HE3	1.97	0.79
5:L:65:SER:O	5:L:66:PHE:HB3	1.82	0.79
3:J:32:LEU:HD21	3:J:136:ASP:CA	2.12	0.79
6:M:61:VAL:HG11	6:M:111:PHE:CD1	2.16	0.79
5:L:32:GLY:HA2	5:L:64:LYS:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:135:PRO:O	2:I:138:THR:HG23	1.84	0.78
4:K:27:ASN:HA	4:K:31:PHE:HB2	1.64	0.77
5:L:28:LEU:O	5:L:33:VAL:HG23	1.84	0.77
5:L:42:PHE:HE1	5:L:56:VAL:HG21	1.46	0.77
5:L:27:ALA:HA	5:L:30:GLN:NE2	1.99	0.77
3:J:29:LYS:CB	3:J:81:GLY:HA2	2.14	0.77
5:L:73:PRO:O	5:L:112:LYS:HE2	1.85	0.76
5:L:15:ALA:H	5:L:17:LYS:CE	1.98	0.76
6:M:36:GLY:HA3	6:M:109:LYS:HG3	1.67	0.76
5:L:14:PRO:HB2	5:L:17:LYS:CG	2.16	0.75
5:L:20:PRO:O	5:L:22:PRO:HD2	1.86	0.75
5:L:32:GLY:HA3	5:L:64:LYS:HD2	1.67	0.75
5:L:46:THR:HB	5:L:50:ALA:CB	2.16	0.75
2:I:114:GLU:O	2:I:115:ILE:HD12	1.87	0.74
4:K:124:LEU:HD21	4:K:147:GLU:HB2	1.69	0.74
6:M:61:VAL:HB	6:M:111:PHE:HZ	1.51	0.74
4:K:64:ASN:O	4:K:67:LYS:HD3	1.88	0.74
6:M:79:PHE:CZ	6:M:103:ALA:HA	2.22	0.74
6:M:63:VAL:CB	6:M:106:LEU:CD1	2.55	0.74
2:I:166:LYS:NZ	2:I:166:LYS:HB3	2.01	0.73
5:L:9:ILE:HB	5:L:58:ILE:CG2	2.18	0.73
4:K:4:ILE:HB	4:K:37:ILE:HG22	1.71	0.73
4:K:2:LYS:HD3	4:K:20:ASN:HB2	1.70	0.73
6:M:86:ILE:O	6:M:87:ILE:CG2	2.27	0.73
6:M:13:ASN:CG	6:M:97:ARG:H	1.96	0.72
4:K:18:ILE:HD12	4:K:44:LEU:HD21	1.70	0.72
5:L:13:LEU:HB2	5:L:42:PHE:CZ	2.23	0.72
2:I:147:PRO:HD3	2:I:187:CYS:SG	2.29	0.72
6:M:64:ARG:NH1	6:M:101:PRO:O	2.22	0.72
5:L:23:PRO:O	5:L:24:VAL:CG2	2.36	0.72
4:K:12:LYS:HB3	4:K:14:LYS:HG3	1.72	0.71
6:M:87:ILE:C	6:M:88:ARG:O	2.33	0.71
3:J:29:LYS:O	3:J:135:ALA:HB2	1.90	0.71
2:I:61:TYR:CZ	2:I:85:ASN:HB2	2.26	0.71
5:L:42:PHE:HE1	5:L:56:VAL:CG2	2.03	0.71
3:J:30:GLY:HA3	3:J:135:ALA:CB	2.20	0.70
5:L:13:LEU:HD22	5:L:24:VAL:CG1	2.20	0.70
3:J:76:GLU:CB	3:J:82:TYR:OH	2.13	0.70
6:M:79:PHE:CE2	6:M:103:ALA:HB2	2.17	0.70
6:M:67:ARG:CG	6:M:67:ARG:HH11	2.04	0.70
6:M:67:ARG:HH11	6:M:67:ARG:HG3	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:52:MET:HB2	5:L:77:PHE:CZ	2.26	0.70
5:L:103:LYS:O	5:L:107:GLU:HG3	1.92	0.70
3:J:32:LEU:HD11	3:J:136:ASP:HA	1.74	0.69
5:L:28:LEU:C	5:L:30:GLN:N	2.48	0.69
6:M:36:GLY:HA3	6:M:109:LYS:CE	2.21	0.69
2:I:174:ARG:NE	2:I:178:GLY:HA2	2.06	0.69
6:M:36:GLY:HA3	6:M:109:LYS:HE2	1.74	0.69
6:M:79:PHE:CE1	6:M:103:ALA:HB1	2.18	0.69
6:M:85:VAL:CG2	6:M:114:ILE:CD1	2.63	0.69
5:L:14:PRO:HB2	5:L:17:LYS:CD	2.23	0.69
6:M:61:VAL:HG11	6:M:111:PHE:CE2	2.27	0.68
5:L:28:LEU:N	5:L:28:LEU:HD23	2.09	0.68
3:J:157:LYS:HE2	3:J:157:LYS:HA	1.76	0.68
5:L:36:MET:HG2	5:L:37:GLU:N	2.09	0.68
4:K:16:GLY:HA3	4:K:47:LEU:HD21	1.75	0.68
2:I:166:LYS:HD2	2:I:171:VAL:HG22	1.76	0.68
2:I:118:GLY:HA2	2:I:188:ARG:NH2	2.08	0.67
5:L:28:LEU:O	5:L:33:VAL:CG2	2.43	0.67
5:L:33:VAL:HG12	5:L:34:ASN:H	1.60	0.67
6:M:79:PHE:HZ	6:M:103:ALA:CA	2.00	0.67
5:L:28:LEU:C	5:L:30:GLN:H	2.00	0.67
1:H:61:THR:HG22	1:H:162:GLU:HG2	1.76	0.67
3:J:30:GLY:HA3	3:J:135:ALA:HB2	1.77	0.66
3:J:29:LYS:CE	3:J:81:GLY:N	2.58	0.66
3:J:29:LYS:CG	3:J:81:GLY:HA2	2.26	0.66
3:J:81:GLY:C	3:J:82:TYR:N	2.53	0.66
5:L:15:ALA:HB1	5:L:50:ALA:HB1	1.76	0.66
1:H:201:PRO:HG2	1:H:204:ALA:HB2	1.78	0.66
2:I:94:ASN:HD22	2:I:100:LYS:HG3	1.59	0.66
5:L:26:PRO:O	5:L:28:LEU:N	2.29	0.66
5:L:45:GLU:HA	5:L:45:GLU:OE1	1.95	0.65
5:L:69:ILE:HD11	5:L:71:LYS:HE3	1.78	0.65
6:M:52:VAL:HG22	6:M:94:ARG:NH1	2.10	0.65
3:J:29:LYS:CD	3:J:81:GLY:N	2.57	0.65
1:H:30:LYS:HE3	1:H:178:ALA:O	1.97	0.65
3:J:29:LYS:HE2	3:J:81:GLY:HA3	1.79	0.65
5:L:14:PRO:CG	5:L:17:LYS:HG3	2.28	0.64
4:K:80:PRO:HA	4:K:146:THR:O	1.97	0.64
1:H:141:LYS:HB2	1:H:164:ARG:HH21	1.62	0.64
5:L:101:THR:HA	5:L:140:VAL:OXT	1.97	0.64
5:L:121:LEU:O	5:L:125:MET:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:122:ARG:HH11	4:K:122:ARG:HB3	1.62	0.64
4:K:134:HIS:CD2	4:K:136:GLU:H	2.15	0.64
5:L:13:LEU:O	5:L:54:LEU:HD23	1.97	0.64
6:M:13:ASN:C	6:M:95:GLY:HA3	2.22	0.64
2:I:108:ASN:O	2:I:110:LYS:HE2	1.98	0.64
5:L:20:PRO:HD2	5:L:24:VAL:HG22	1.80	0.64
3:J:29:LYS:CD	3:J:81:GLY:CA	2.75	0.63
3:J:80:LYS:O	3:J:81:GLY:N	2.30	0.63
2:I:174:ARG:HE	2:I:178:GLY:HA2	1.61	0.63
5:L:21:ALA:CB	5:L:22:PRO:CD	2.77	0.63
2:I:159:THR:HB	2:I:176:ALA:CB	2.29	0.62
4:K:5:PHE:CE2	4:K:19:LYS:HB3	2.29	0.62
5:L:21:ALA:HB3	5:L:22:PRO:HD2	1.80	0.62
2:I:114:GLU:C	2:I:115:ILE:HD12	2.23	0.62
4:K:69:LYS:O	4:K:73:GLU:HG3	2.00	0.62
2:I:61:TYR:CE1	2:I:85:ASN:HB2	2.35	0.61
4:K:134:HIS:ND1	4:K:135:PRO:HD2	2.15	0.61
5:L:26:PRO:O	5:L:29:GLY:N	2.33	0.61
5:L:34:ASN:C	5:L:35:ILE:HG12	2.25	0.61
5:L:38:PHE:CD1	5:L:66:PHE:CE1	2.78	0.61
5:L:19:THR:HG23	5:L:39:CYS:SG	2.40	0.61
4:K:2:LYS:HA	4:K:20:ASN:HA	1.83	0.61
5:L:16:GLY:N	5:L:17:LYS:HE3	2.14	0.61
5:L:20:PRO:O	5:L:22:PRO:CD	2.48	0.61
5:L:39:CYS:O	5:L:43:ASN:ND2	2.34	0.61
4:K:50:GLN:HG3	4:K:51:LYS:N	2.16	0.60
6:M:52:VAL:CG2	6:M:94:ARG:NH1	2.64	0.60
5:L:14:PRO:O	5:L:42:PHE:CE2	2.55	0.60
4:K:4:ILE:HD11	4:K:44:LEU:HD22	1.83	0.60
5:L:46:THR:C	5:L:50:ALA:HB3	2.27	0.59
6:M:87:ILE:C	6:M:88:ARG:HA	2.24	0.59
5:L:21:ALA:HB3	5:L:22:PRO:HD3	1.84	0.59
3:J:21:ASN:ND2	3:J:35:THR:HG23	2.17	0.59
5:L:46:THR:HB	5:L:50:ALA:HB3	1.84	0.59
5:L:42:PHE:O	5:L:46:THR:HG23	2.03	0.59
3:J:29:LYS:CD	3:J:81:GLY:HA3	2.32	0.59
2:I:104:ILE:HG13	2:I:156:ALA:HB2	1.85	0.59
2:I:164:LEU:HD13	2:I:174:ARG:HB2	1.85	0.59
3:J:39:ASP:O	3:J:54:PRO:HD3	2.03	0.59
5:L:19:THR:CG2	5:L:39:CYS:SG	2.90	0.59
5:L:100:VAL:HG23	5:L:139:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:13:LEU:CD2	5:L:24:VAL:HG12	2.33	0.58
3:J:29:LYS:CB	3:J:81:GLY:CA	2.77	0.58
5:L:19:THR:HG22	5:L:35:ILE:HG22	1.86	0.58
5:L:15:ALA:HB1	5:L:46:THR:HB	1.86	0.58
4:K:3:VAL:HB	4:K:21:VAL:HG22	1.85	0.58
4:K:9:VAL:HG12	4:K:10:LYS:H	1.67	0.58
5:L:89:SER:HB2	5:L:97:VAL:HG13	1.86	0.58
5:L:52:MET:HB2	5:L:77:PHE:CE2	2.38	0.57
2:I:90:ILE:HD12	2:I:102:TYR:CD2	2.39	0.57
4:K:110:LEU:HD21	4:K:131:VAL:HG11	1.86	0.57
5:L:53:ILE:O	5:L:73:PRO:HB3	2.03	0.57
5:L:19:THR:O	5:L:21:ALA:N	2.32	0.57
6:M:11:ALA:O	6:M:98:ILE:HG23	2.05	0.57
2:I:77:VAL:HG23	2:I:115:ILE:HD13	1.87	0.57
5:L:27:ALA:HA	5:L:30:GLN:CD	2.30	0.57
2:I:107:LYS:HG2	2:I:108:ASN:ND2	2.21	0.56
6:M:85:VAL:CB	6:M:114:ILE:CD1	2.82	0.56
3:J:29:LYS:HE2	3:J:81:GLY:CA	2.34	0.56
3:J:158:GLY:HA3	3:J:170:LEU:HD11	1.88	0.56
5:L:19:THR:C	5:L:21:ALA:H	2.13	0.56
4:K:9:VAL:HG21	4:K:13:GLY:HA3	1.86	0.56
2:I:153:LEU:C	2:I:154:VAL:HG23	2.30	0.55
2:I:118:GLY:HA2	2:I:188:ARG:HH22	1.70	0.55
5:L:27:ALA:O	5:L:30:GLN:HB2	2.06	0.55
2:I:154:VAL:HG12	2:I:194:VAL:HG11	1.88	0.55
5:L:14:PRO:O	5:L:42:PHE:HE2	1.90	0.55
3:J:29:LYS:HE2	3:J:81:GLY:N	2.22	0.55
4:K:26:ALA:C	4:K:31:PHE:HD2	2.15	0.55
5:L:35:ILE:O	5:L:36:MET:C	2.50	0.55
5:L:19:THR:C	5:L:21:ALA:N	2.65	0.54
5:L:100:VAL:O	5:L:139:VAL:HA	2.07	0.54
6:M:12:ASP:HA	6:M:98:ILE:HD13	1.89	0.54
4:K:9:VAL:HG11	4:K:17:GLU:HG3	1.90	0.54
5:L:54:LEU:HD23	5:L:54:LEU:H	1.71	0.54
5:L:89:SER:HA	5:L:97:VAL:HG11	1.89	0.54
2:I:174:ARG:CZ	2:I:178:GLY:HA2	2.39	0.53
5:L:61:TYR:O	5:L:64:LYS:N	2.41	0.53
3:J:32:LEU:HD21	3:J:136:ASP:N	2.22	0.53
3:J:76:GLU:HG3	3:J:80:LYS:HD2	1.90	0.53
5:L:27:ALA:C	5:L:28:LEU:HD23	2.34	0.53
3:J:32:LEU:CD1	3:J:136:ASP:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:82:TYR:OH	2:I:87:SER:HA	2.08	0.53
5:L:15:ALA:HB2	5:L:50:ALA:HB1	1.87	0.53
2:I:160:SER:OG	2:I:193:GLU:HA	2.08	0.53
4:K:6:LEU:O	4:K:14:LYS:HB3	2.08	0.53
5:L:22:PRO:HG2	5:L:23:PRO:HD2	1.91	0.53
4:K:69:LYS:HG3	4:K:139:ALA:HB2	1.90	0.52
5:L:13:LEU:HD22	5:L:24:VAL:HG12	1.89	0.52
2:I:164:LEU:CD1	2:I:174:ARG:HB2	2.40	0.52
5:L:24:VAL:CG2	5:L:25:GLY:N	2.49	0.52
5:L:34:ASN:O	5:L:35:ILE:HG12	2.10	0.52
6:M:70:ARG:HG3	6:M:76:TYR:CE2	2.45	0.52
5:L:37:GLU:HG2	5:L:41:ARG:HE	1.75	0.52
3:J:11:PRO:HG2	3:J:14:VAL:HG21	1.90	0.51
4:K:62:LEU:O	4:K:66:LYS:HG3	2.10	0.51
6:M:64:ARG:HD3	6:M:102:VAL:HA	1.92	0.51
6:M:85:VAL:HG11	6:M:114:ILE:HD11	0.68	0.51
5:L:18:ALA:C	5:L:20:PRO:HD3	2.35	0.51
5:L:85:ILE:HD12	5:L:87:LYS:O	2.11	0.51
3:J:29:LYS:CE	3:J:81:GLY:HA3	2.40	0.51
4:K:27:ASN:HA	4:K:31:PHE:CD2	2.46	0.51
5:L:21:ALA:CB	5:L:22:PRO:HD3	2.40	0.51
4:K:79:ILE:O	4:K:145:VAL:HA	2.11	0.50
5:L:55:PRO:HD3	5:L:73:PRO:HA	1.92	0.50
2:I:144:GLU:O	2:I:187:CYS:HB3	2.11	0.50
5:L:14:PRO:HG2	5:L:17:LYS:HG3	1.93	0.50
4:K:4:ILE:HD11	4:K:44:LEU:CD2	2.41	0.50
4:K:75:LEU:HD23	4:K:75:LEU:N	2.26	0.50
5:L:20:PRO:O	5:L:22:PRO:N	2.45	0.50
6:M:64:ARG:NH1	6:M:102:VAL:CA	2.63	0.50
3:J:25:VAL:HG12	3:J:78:VAL:HG21	1.93	0.50
2:I:121:ALA:HB3	2:I:129:LEU:HG	1.94	0.49
4:K:50:GLN:O	4:K:53:LYS:HG3	2.12	0.49
4:K:131:VAL:O	4:K:138:THR:HA	2.12	0.49
6:M:36:GLY:HA3	6:M:109:LYS:HZ3	1.76	0.49
2:I:110:LYS:H	2:I:113:MSE:SE	2.45	0.49
4:K:16:GLY:CA	4:K:47:LEU:HD21	2.42	0.49
5:L:9:ILE:CD1	5:L:28:LEU:HD22	2.33	0.49
5:L:27:ALA:HA	5:L:30:GLN:HE21	1.76	0.49
3:J:162:ARG:HG3	3:J:163:TYR:O	2.12	0.49
5:L:10:LYS:O	5:L:11:LEU:HG	2.13	0.49
5:L:15:ALA:C	5:L:17:LYS:HE3	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:9:ILE:HG22	5:L:11:LEU:HG	1.95	0.49
5:L:65:SER:O	5:L:66:PHE:CB	2.57	0.49
5:L:42:PHE:CD1	5:L:56:VAL:HG21	2.46	0.49
2:I:162:GLN:O	2:I:164:LEU:HD12	2.12	0.48
5:L:9:ILE:HD11	5:L:31:HIS:CE1	2.45	0.48
5:L:61:TYR:O	5:L:62:GLU:C	2.56	0.48
6:M:63:VAL:CG2	6:M:106:LEU:HD11	2.44	0.48
1:H:39:GLU:HG2	1:H:216:THR:HB	1.95	0.48
5:L:61:TYR:HB2	5:L:65:SER:HB3	1.96	0.48
5:L:13:LEU:HD12	5:L:42:PHE:CE1	2.48	0.48
5:L:55:PRO:HD3	5:L:74:PRO:HD3	1.94	0.48
4:K:82:LYS:NZ	4:K:149:LYS:NZ	2.62	0.48
4:K:122:ARG:HB3	4:K:122:ARG:NH1	2.29	0.48
5:L:15:ALA:CA	5:L:17:LYS:HE3	2.43	0.47
4:K:7:LYS:HG2	4:K:12:LYS:HE2	1.96	0.47
3:J:110:HIS:HB3	3:J:111:PRO:HD2	1.96	0.47
6:M:79:PHE:CE2	6:M:103:ALA:HA	2.49	0.47
4:K:81:ALA:O	4:K:147:GLU:HA	2.15	0.47
2:I:151:GLY:O	2:I:155:ARG:NH1	2.44	0.47
2:I:174:ARG:NH2	2:I:178:GLY:HA2	2.29	0.47
3:J:98:GLN:HG3	3:J:103:VAL:HG21	1.96	0.47
6:M:69:VAL:CG2	6:M:105:GLU:OE2	2.63	0.47
4:K:30:LEU:HD23	4:K:36:ALA:HB2	1.96	0.47
5:L:54:LEU:H	5:L:54:LEU:CD2	2.27	0.47
5:L:113:MET:HA	5:L:116:LEU:HB2	1.96	0.47
6:M:36:GLY:HA3	6:M:109:LYS:NZ	2.30	0.47
6:M:79:PHE:CE2	6:M:103:ALA:CA	2.95	0.46
3:J:101:LYS:HE3	3:J:101:LYS:HB2	1.75	0.46
4:K:148:GLN:HG3	4:K:149:LYS:HG2	1.98	0.46
5:L:19:THR:HG22	5:L:39:CYS:SG	2.55	0.46
5:L:46:THR:CA	5:L:50:ALA:HB3	2.46	0.46
1:H:33:ALA:HB2	1:H:216:THR:HG21	1.97	0.46
6:M:87:ILE:HB	6:M:88:ARG:O	2.15	0.46
2:I:146:LYS:O	2:I:147:PRO:C	2.59	0.46
4:K:96:LYS:O	4:K:100:GLU:HG3	2.15	0.46
5:L:27:ALA:HA	5:L:30:GLN:CG	2.46	0.46
5:L:52:MET:HB2	5:L:77:PHE:HZ	1.76	0.46
1:H:58:VAL:O	1:H:164:ARG:HA	2.16	0.46
4:K:88:ARG:HD3	4:K:122:ARG:O	2.15	0.46
6:M:36:GLY:CA	6:M:109:LYS:HE2	2.45	0.46
3:J:11:PRO:HG2	3:J:14:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:61:TYR:CE2	2:I:85:ASN:HB2	2.51	0.46
5:L:35:ILE:O	5:L:38:PHE:N	2.49	0.46
5:L:62:GLU:C	5:L:64:LYS:H	2.24	0.45
6:M:67:ARG:HG3	6:M:67:ARG:NH1	2.28	0.45
2:I:70:LYS:NZ	2:I:97:ASP:OD2	2.48	0.45
7:N:34:LYS:NZ	7:N:35:GLU:OE1	2.49	0.45
2:I:144:GLU:OE2	2:I:147:PRO:HA	2.16	0.45
2:I:177:SER:OG	2:I:179:GLU:HB2	2.16	0.45
5:L:15:ALA:H	5:L:17:LYS:NZ	2.14	0.45
5:L:14:PRO:HB2	5:L:17:LYS:CE	2.47	0.45
2:I:82:TYR:CE2	2:I:84:PRO:HA	2.52	0.45
2:I:166:LYS:HB3	2:I:166:LYS:HZ1	1.77	0.45
5:L:18:ALA:O	5:L:19:THR:C	2.59	0.45
6:M:64:ARG:CZ	6:M:101:PRO:O	2.64	0.45
4:K:9:VAL:HG12	4:K:10:LYS:HD2	1.99	0.45
5:L:37:GLU:CD	5:L:41:ARG:HH21	2.25	0.45
6:M:35:ILE:HD13	6:M:105:GLU:HB2	1.99	0.45
4:K:68:LEU:O	4:K:68:LEU:HD12	2.16	0.44
4:K:103:GLN:HA	4:K:108:LEU:O	2.17	0.44
5:L:54:LEU:CD2	5:L:54:LEU:N	2.80	0.44
3:J:153:PRO:HA	3:J:159:LYS:O	2.17	0.44
4:K:27:ASN:HA	4:K:31:PHE:CB	2.41	0.44
5:L:23:PRO:C	5:L:24:VAL:HG22	2.34	0.44
5:L:15:ALA:H	5:L:17:LYS:HZ1	1.66	0.44
3:J:29:LYS:CE	3:J:81:GLY:CA	2.94	0.44
3:J:26:LYS:HG2	3:J:31:GLU:HG3	2.00	0.44
4:K:62:LEU:HD23	4:K:134:HIS:CD2	2.52	0.44
5:L:12:GLN:HA	5:L:55:PRO:HA	1.99	0.44
5:L:60:VAL:HG12	5:L:66:PHE:HB3	1.99	0.44
6:M:86:ILE:O	6:M:87:ILE:HG22	2.14	0.44
7:N:65:VAL:O	7:N:66:ASP:C	2.59	0.44
2:I:134:ILE:HA	2:I:135:PRO:HD3	1.81	0.44
4:K:9:VAL:CG2	4:K:13:GLY:HA3	2.48	0.44
5:L:58:ILE:HA	5:L:68:PHE:HA	2.00	0.44
1:H:185:LEU:HA	1:H:185:LEU:HD23	1.77	0.44
6:M:36:GLY:HA3	6:M:109:LYS:CG	2.40	0.44
6:M:79:PHE:HZ	6:M:103:ALA:HA	1.67	0.44
6:M:118:ALA:HA	6:M:119:PRO:HD3	1.85	0.43
4:K:85:GLU:O	4:K:88:ARG:HB2	2.18	0.43
6:M:22:ILE:HD11	6:M:42:THR:CG2	2.41	0.43
6:M:87:ILE:HA	6:M:88:ARG:H	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:3:VAL:HG22	4:K:36:ALA:HB1	2.00	0.43
4:K:14:LYS:HD2	4:K:15:LYS:N	2.34	0.43
2:I:83:ASP:OD2	2:I:86:ARG:HD2	2.18	0.43
6:M:79:PHE:HZ	6:M:103:ALA:HB1	1.47	0.43
3:J:21:ASN:ND2	3:J:35:THR:CG2	2.81	0.43
3:J:7:PRO:HB2	3:J:48:VAL:HB	2.00	0.43
1:H:139:ASN:HA	1:H:140:PRO:HD2	1.88	0.43
4:K:81:ALA:N	4:K:146:THR:O	2.48	0.43
2:I:86:ARG:C	2:I:88:ALA:N	2.77	0.43
6:M:107:ARG:HG3	6:M:107:ARG:HH11	1.84	0.43
5:L:111:THR:O	5:L:114:PRO:HD2	2.19	0.42
2:I:106:PRO:HD2	2:I:109:LEU:HD22	2.02	0.42
4:K:134:HIS:CG	4:K:135:PRO:HD2	2.54	0.42
6:M:71:ARG:HH21	6:M:105:GLU:CD	2.28	0.42
3:J:34:ARG:HG2	3:J:34:ARG:HH11	1.84	0.42
2:I:177:SER:C	2:I:179:GLU:H	2.27	0.42
4:K:25:TYR:CD1	4:K:29:PHE:HD2	2.37	0.42
5:L:22:PRO:O	5:L:23:PRO:C	2.62	0.42
5:L:60:VAL:HG12	5:L:65:SER:O	2.20	0.42
2:I:124:LYS:O	2:I:125:ILE:C	2.62	0.42
2:I:144:GLU:HG3	2:I:150:GLY:O	2.19	0.42
7:N:57:TYR:CD2	7:N:58:SER:N	2.88	0.42
3:J:32:LEU:CD2	3:J:136:ASP:CA	2.87	0.41
4:K:92:SER:HB3	4:K:122:ARG:HG2	2.01	0.41
5:L:99:LYS:HA	5:L:138:GLU:O	2.20	0.41
4:K:62:LEU:HD23	4:K:134:HIS:NE2	2.35	0.41
2:I:146:LYS:O	2:I:149:ARG:HB2	2.20	0.41
4:K:1:MET:O	4:K:21:VAL:N	2.54	0.41
2:I:62:ARG:CD	2:I:62:ARG:H	2.34	0.41
4:K:92:SER:HB2	4:K:120:ALA:HB1	2.02	0.41
3:J:82:TYR:HB3	3:J:137:LYS:HD3	2.02	0.41
5:L:60:VAL:HA	5:L:65:SER:O	2.21	0.41
2:I:85:ASN:O	2:I:85:ASN:CG	2.64	0.41
4:K:27:ASN:N	4:K:31:PHE:HD2	2.19	0.41
5:L:16:GLY:C	5:L:17:LYS:CG	2.93	0.41
5:L:32:GLY:H	5:L:33:VAL:HG23	1.85	0.41
7:N:16:ALA:O	7:N:17:SER:C	2.64	0.41
4:K:134:HIS:HB3	4:K:137:VAL:HB	2.03	0.41
5:L:18:ALA:CB	5:L:39:CYS:CB	2.75	0.41
6:M:85:VAL:O	6:M:87:ILE:HG23	2.21	0.41
6:M:64:ARG:NH1	6:M:102:VAL:CB	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:50:GLN:O	4:K:54:GLU:HG3	2.22	0.40
5:L:53:ILE:O	5:L:73:PRO:CB	2.68	0.40
1:H:84:LYS:HA	1:H:84:LYS:HD3	1.95	0.40
4:K:31:PHE:CE1	4:K:38:GLU:CD	3.00	0.40
5:L:22:PRO:HG2	5:L:23:PRO:CD	2.51	0.40
5:L:57:VAL:O	5:L:68:PHE:HA	2.22	0.40
2:I:129:LEU:HD12	2:I:129:LEU:N	2.36	0.40
4:K:24:GLY:HA2	4:K:27:ASN:HD21	1.85	0.40
4:K:82:LYS:HZ1	4:K:149:LYS:NZ	2.19	0.40
4:K:148:GLN:O	4:K:149:LYS:HB2	2.22	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	H	222/224 (99%)	211 (95%)	9 (4%)	2 (1%)	14	51
2	I	133/135 (98%)	124 (93%)	7 (5%)	2 (2%)	8	40
3	J	159/164 (97%)	156 (98%)	3 (2%)	0	100	100
4	K	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	21
5	L	131/133 (98%)	101 (77%)	14 (11%)	16 (12%)	0	4
6	M	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	7	36
7	N	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	17
All	All	1004/1021 (98%)	910 (91%)	63 (6%)	31 (3%)	5	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	8	ASP

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Mol	Chain	Res	Type
4	K	85	GLU
5	L	21	ALA
5	L	24	VAL
5	L	25	GLY
5	L	27	ALA
5	L	36	MET
5	L	50	ALA
6	M	87	ILE
1	H	37	PHE
4	K	9	VAL
5	L	22	PRO
5	L	35	ILE
6	M	86	ILE
5	L	23	PRO
5	L	32	GLY
5	L	51	GLY
5	L	62	GLU
7	N	12	GLN
1	H	7	TYR
2	I	161	ALA
5	L	14	PRO
5	L	26	PRO
5	L	16	GLY
5	L	48	ASP
7	N	36	ALA
4	K	16	GLY
2	I	154	VAL
4	K	84	GLY
7	N	32	GLY
7	N	77	VAL

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	H	177/177 (100%)	164 (93%)	13 (7%)	13 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	107/104 (103%)	85 (79%)	22 (21%)	1	6
3	J	137/137 (100%)	130 (95%)	7 (5%)	21	42
4	K	119/119 (100%)	101 (85%)	18 (15%)	3	12
5	L	108/108 (100%)	91 (84%)	17 (16%)	2	12
6	M	101/101 (100%)	99 (98%)	2 (2%)	48	66
7	N	78/78 (100%)	70 (90%)	8 (10%)	7	23
All	All	827/824 (100%)	740 (90%)	87 (10%)	9	21

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	LYS
1	H	7	TYR
1	H	8	ARG
1	H	29	VAL
1	H	36	LYS
1	H	59	ARG
1	H	104	LEU
1	H	108	MET
1	H	129	ARG
1	H	137	LEU
1	H	162	GLU
1	H	177	LYS
1	H	207	THR
2	I	60	GLN
2	I	62	ARG
2	I	70	LYS
2	I	85	ASN
2	I	86	ARG
2	I	100	LYS
2	I	110	LYS
2	I	111	VAL
2	I	113	MSE
2	I	116	MSE
2	I	120	ASP
2	I	124	LYS
2	I	129	LEU
2	I	149	ARG
2	I	154	VAL
2	I	155	ARG

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Mol	Chain	Res	Type
2	I	160	SER
2	I	166	LYS
2	I	167	GLU
2	I	184	LEU
2	I	188	ARG
2	I	194	VAL
3	J	9	GLU
3	J	38	PRO
3	J	45	GLU
3	J	117	GLU
3	J	157	LYS
3	J	169	ARG
3	J	170	LEU
4	K	3	VAL
4	K	10	LYS
4	K	15	LYS
4	K	17	GLU
4	K	23	ASP
4	K	28	ASN
4	K	33	GLN
4	K	44	LEU
4	K	48	GLU
4	K	52	GLN
4	K	62	LEU
4	K	67	LYS
4	K	85	GLU
4	K	88	ARG
4	K	96	LYS
4	K	110	LEU
4	K	124	LEU
4	K	135	PRO
5	L	17	LYS
5	L	28	LEU
5	L	33	VAL
5	L	35	ILE
5	L	36	MET
5	L	52	MET
5	L	54	LEU
5	L	58	ILE
5	L	62	GLU
5	L	64	LYS
5	L	67	THR

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Mol	Chain	Res	Type
5	L	70	ILE
5	L	81	LYS
5	L	87	LYS
5	L	112	LYS
5	L	116	LEU
5	L	126	LYS
6	M	53	LYS
6	M	67	ARG
7	N	14	LYS
7	N	18	ARG
7	N	29	ILE
7	N	34	LYS
7	N	40	ILE
7	N	53	LYS
7	N	70	ILE
7	N	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	94	ASN
2	I	108	ASN
2	I	127	ASN
2	I	152	GLN
3	J	146	ASN
4	K	33	GLN
4	K	43	ASN
4	K	71	GLN
4	K	148	GLN
5	L	8	GLN
5	L	30	GLN
5	L	43	ASN
6	M	3	GLN
6	M	56	GLN
7	N	51	GLN
7	N	80	HIS
7	N	87	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	J	2
6	M	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	81:GLY	C	82:TYR	N	2.53
1	J	80:LYS	C	81:GLY	N	2.18
1	M	87:ILE	C	88:ARG	N	1.67
1	M	86:ILE	C	87:ILE	N	0.95