



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 11:36 PM EST

PDB ID : 487D  
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 : 1CSV, 1CSW, 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

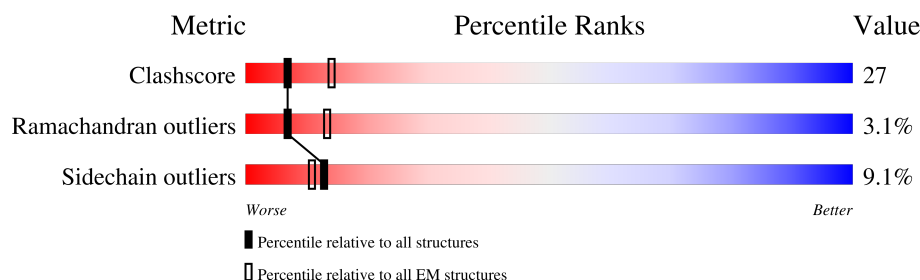
# 1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	89% 10% .
2	I	135	53% 36% 10%
3	J	164	77% 22% .
4	K	149	46% 44% 9% .
5	L	133	38% 44% 12% 5%
6	M	122	70% 27% .
7	N	94	81% 18% .

## 2 Entry composition [i](#)

There are 9 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 PROTEIN (50S L1 RIBOSOMAL PROTEIN).

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 PROTEIN (50S L2 RIBOSOMAL PROTEIN).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	113	MSE	MET	engineered mutation	UNP P04257
I	116	MSE	MET	engineered mutation	UNP P04257
I	182	MSE	MET	engineered mutation	UNP P04257

- Molecule 3 is a protein called PROTEIN (50S L6 RIBOSOMAL PROTEIN).

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 PROTEIN (50S L9 RIBOSOMAL PROTEIN).

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 PROTEIN (50S L11 RIBOSOMAL PROTEIN).

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

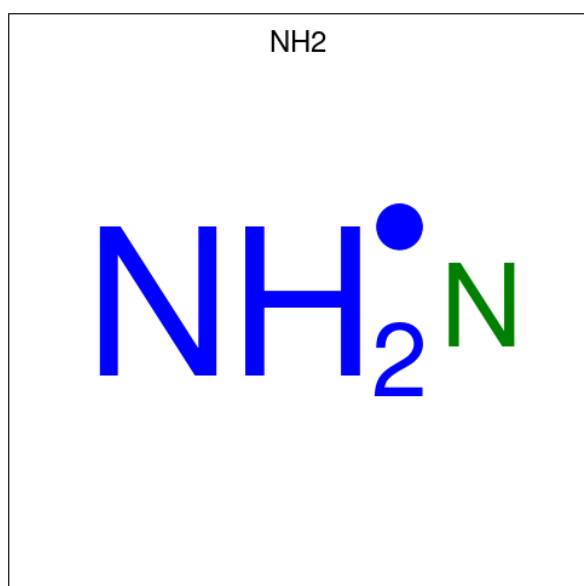
- Molecule 6 is a protein called PROTEIN (50S L14 RIBOSOMAL PROTEIN).

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 PROTEIN (50S L25 RIBOSOMAL PROTEIN).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	N	94	Total	C	H	N	O	S	0	0
			1415	478	666	136	132	3		

- Molecule 8 is AMINO GROUP (three-letter code: NH2) (formula: H<sub>2</sub>N).



Mol	Chain	Residues	Atoms		AltConf
8	N	1	Total	N	0
			1	1	

- Molecule 9 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
9	N	1	Total	C	O	0
			3	1	2	

### 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.

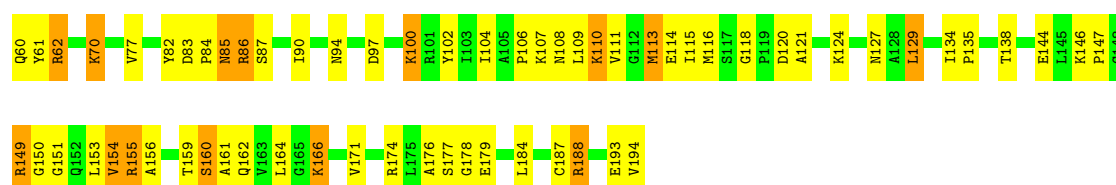
- Molecule 1: PROTEIN (50S L1 RIBOSOMAL PROTEIN)

Chain H: 




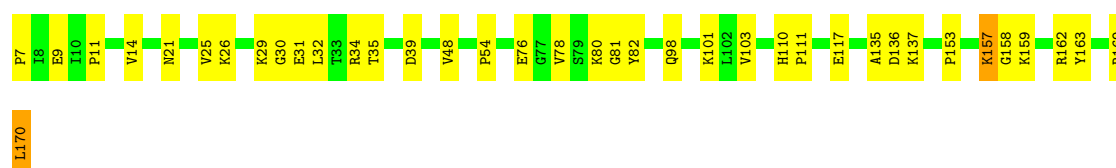
- Molecule 2: PROTEIN (50S L2 RIBOSOMAL PROTEIN)

Chain I: 



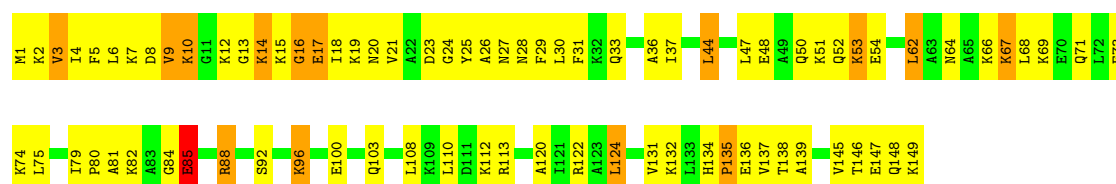
- Molecule 3: PROTEIN (50S L6 RIBOSOMAL PROTEIN)

Chain J: 

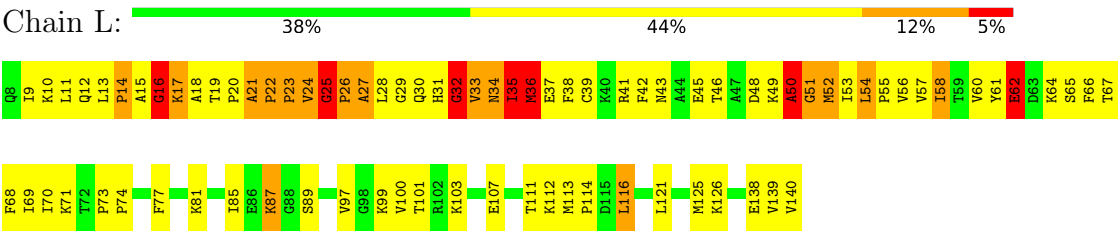


- Molecule 4: PROTEIN (50S L9 RIBOSOMAL PROTEIN)

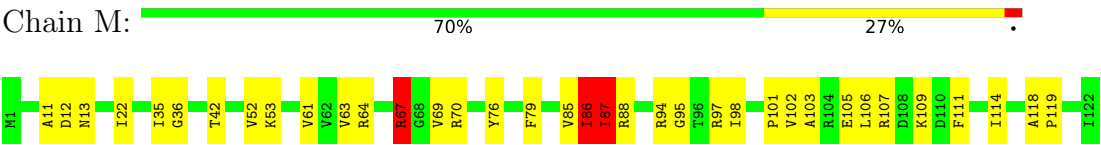
Chain K: 



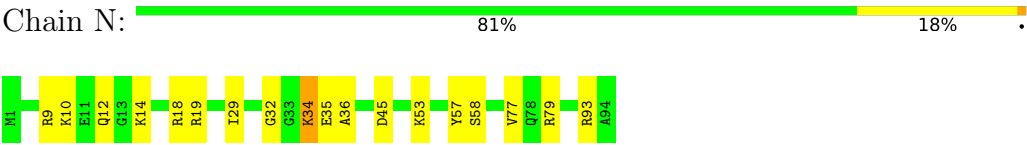
- Molecule 5: PROTEIN (50S L11 RIBOSOMAL PROTEIN)



• Molecule 6: PROTEIN (50S L14 RIBOSOMAL PROTEIN)



• Molecule 7: PROTEIN (50S L25 RIBOSOMAL PROTEIN)



## 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	34.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, NH2

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	0.48	0/1743	0.74	0/2351
2	I	0.48	0/1034	0.65	0/1388
3	J	0.63	0/1270	0.76	0/1715
4	K	0.63	0/1160	0.79	0/1552
5	L	0.64	0/1016	0.89	6/1366 (0.4%)
6	M	0.86	2/946 (0.2%)	1.18	7/1269 (0.6%)
7	N	0.91	0/762	1.14	4/1020 (0.4%)
All	All	0.65	2/7931 (0.0%)	0.87	17/10661 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	86	ILE	C-N	-16.94	0.95	1.34
6	M	87	ILE	C-N	14.61	1.67	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	86	ILE	O-C-N	-15.53	97.85	122.70
6	M	87	ILE	CA-C-N	-14.87	84.49	117.20
6	M	87	ILE	C-N-CA	-14.70	84.95	121.70
6	M	86	ILE	C-N-CA	-13.35	88.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	87	ILE	O-C-N	9.88	138.50	122.70
6	M	86	ILE	CA-C-N	-9.13	97.12	117.20
7	N	19	ARG	NE-CZ-NH2	7.55	124.08	120.30
7	N	79	ARG	NE-CZ-NH2	7.01	123.81	120.30
5	L	16	GLY	N-CA-C	-6.89	95.87	113.10
5	L	32	GLY	N-CA-C	-6.67	96.44	113.10
5	L	34	ASN	N-CA-C	-5.65	95.75	111.00
5	L	50	ALA	N-CA-C	5.48	125.79	111.00
6	M	67	ARG	NE-CZ-NH1	5.28	122.94	120.30
7	N	93	ARG	NE-CZ-NH2	5.17	122.89	120.30
5	L	51	GLY	N-CA-C	-5.15	100.24	113.10
5	L	25	GLY	N-CA-C	5.14	125.95	113.10
7	N	9	ARG	NE-CZ-NH2	5.14	122.87	120.30

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	46	0
3	J	1251	0	1294	56	0
4	K	1148	287	1230	66	0
5	L	1000	0	1071	142	0
6	M	937	0	995	114	0
7	N	749	666	775	2	0
8	N	1	0	0	0	0
9	N	3	0	0	0	0
All	All	7825	953	8201	436	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 27.

All (436) 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: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:87:ILE:C	6:M:88:ARG:N	1.67	1.45
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	1.18
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:M:85:VAL:HG21	6:M:114:ILE:CD1	1.91	1.00
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
3:J:80:LYS:C	3:J:81:GLY:N	2.18	0.95
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
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
6:M:87:ILE:C	6:M:88:ARG:C	2.30	0.89
5:L:15:ALA:H	5:L:17:LYS:HE3	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:M:86:ILE:O	6:M:87:ILE:CG2	2.27	0.78
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
3:J:32:LEU:HD22	3:J:136:ASP:CG	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:16:GLY:HA3	4:K:47:LEU:HD21	1.75	0.68
6:M:13:ASN:CG	6:M:97:ARG:H	1.96	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
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
6:M:87:ILE:C	6:M:88:ARG:O	2.33	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
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:28:LEU:C	5:L:30:GLN:N	2.48	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
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
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
5:L:28:LEU:C	5:L:30:GLN:H	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:69:LYS:O	4:K:73:GLU:HG3	2.00	0.62
3:J:81:GLY:C	3:J:82:TYR:N	2.53	0.61
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: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: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
6:M:13:ASN:C	6:M:95:GLY:HA3	2.22	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
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:114:GLU:C	2:I:115:ILE:HD12	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:107:LYS:HG2	2:I:108:ASN:ND2	2.21	0.56
5:L:34:ASN:C	5:L:35:ILE:HG12	2.25	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
4:K:9:VAL:HG21	4:K:13:GLY:HA3	1.86	0.56
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
5:L:46:THR:C	5:L:50:ALA:HB3	2.27	0.55
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
4:K:112:LYS:HZ3	4:K:113:ARG:HH12	1.54	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
3:J:32:LEU:CD1	3:J:136:ASP:HA	2.39	0.53
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:27:ALA:HA	5:L:30:GLN:CD	2.30	0.52
2:I:153:LEU:C	2:I:154:VAL:HG23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:K:26:ALA:C	4:K:31:PHE:HD2	2.15	0.50
5:L:14:PRO:HG2	5:L:17:LYS:HG3	1.93	0.50
5:L:19:THR:C	5:L:21:ALA:H	2.13	0.50
5:L:35:ILE:O	5:L:36:MET:C	2.50	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
5:L:19:THR:C	5:L:21:ALA:N	2.65	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
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: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
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
5:L:27:ALA:C	5:L:28:LEU:HD23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:ALA:C	5:L:20:PRO:HD3	2.35	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
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
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
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
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
7:N:34:LYS:NZ	7:N:35:GLU:OE1	2.49	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:ALA:C	5:L:17:LYS:HE3	2.38	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
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
4:K:82:LYS:HZ2	4:K:149:LYS:NZ	2.14	0.43
5:L:61:TYR:O	5:L:62:GLU:C	2.56	0.43
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
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
6:M:87:ILE:C	6:M:88:ARG:HA	2.24	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
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
3:J:34:ARG:HG2	3:J:34:ARG:HH11	1.84	0.42
4:K:25:TYR:CD1	4:K:29:PHE:HD2	2.37	0.42
5:L:60:VAL:HG12	5:L:65:SER:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:146:LYS:O	2:I:147:PRO:C	2.59	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
4:K:27:ASN:N	4:K:31:PHE:HD2	2.19	0.41
5:L:32:GLY:H	5:L:33:VAL:HG23	1.85	0.41
5:L:62:GLU:C	5:L:64:LYS:H	2.24	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
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
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
6:M:36:GLY:HA3	6:M:109:LYS:HZ3	1.86	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:148:GLN:O	4:K:149:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	222/224 (99%)	211 (95%)	9 (4%)	2 (1%)	17	57
2	I	133/135 (98%)	124 (93%)	7 (5%)	2 (2%)	10	46
3	J	159/164 (97%)	156 (98%)	3 (2%)	0	100	100
4	K	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	26
5	L	131/133 (98%)	101 (77%)	14 (11%)	16 (12%)	0	5
6	M	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9	42
7	N	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	22
All	All	1004/1021 (98%)	910 (91%)	63 (6%)	31 (3%)	7	27

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	8	ASP
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

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Mol	Chain	Res	Type
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%)	169 (96%)	8 (4%)	27	52
2	I	107/104 (103%)	87 (81%)	20 (19%)	1	9
3	J	137/137 (100%)	132 (96%)	5 (4%)	35	59
4	K	119/119 (100%)	100 (84%)	19 (16%)	2	13
5	L	108/108 (100%)	94 (87%)	14 (13%)	4	18
6	M	101/101 (100%)	99 (98%)	2 (2%)	55	74
7	N	77/78 (99%)	70 (91%)	7 (9%)	9	29
All	All	826/824 (100%)	751 (91%)	75 (9%)	13	29

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	LYS
1	H	7	TYR
1	H	29	VAL
1	H	59	ARG
1	H	104	LEU
1	H	108	MET
1	H	129	ARG
1	H	162	GLU
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

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Mol	Chain	Res	Type
2	I	111	VAL
2	I	113	MSE
2	I	116	MSE
2	I	120	ASP
2	I	124	LYS
2	I	127	ASN
2	I	129	LEU
2	I	149	ARG
2	I	155	ARG
2	I	160	SER
2	I	166	LYS
2	I	184	LEU
2	I	188	ARG
3	J	9	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	14	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	53	LYS
4	K	62	LEU
4	K	67	LYS
4	K	85	GLU
4	K	88	ARG
4	K	96	LYS
4	K	124	LEU
4	K	132	LYS
4	K	135	PRO
5	L	17	LYS
5	L	33	VAL
5	L	35	ILE
5	L	36	MET
5	L	52	MET

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Mol	Chain	Res	Type
5	L	54	LEU
5	L	58	ILE
5	L	62	GLU
5	L	67	THR
5	L	70	ILE
5	L	81	LYS
5	L	87	LYS
5	L	116	LEU
5	L	126	LYS
6	M	53	LYS
6	M	67	ARG
7	N	10	LYS
7	N	14	LYS
7	N	18	ARG
7	N	29	ILE
7	N	34	LYS
7	N	45	ASP
7	N	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	85	ASN
2	I	94	ASN
2	I	108	ASN
2	I	127	ASN
3	J	146	ASN
4	K	33	GLN
4	K	43	ASN
4	K	148	GLN
5	L	30	GLN
6	M	56	GLN
7	N	51	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is modelled with single atom - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	FMT	N	96	7	2,2,2	0.83	0	1,1,1	0.69	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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