Full wwPDB EM Validation Report ⓘ

May 19, 2024 – 12:08 AM JST

PDB ID	:	8IP0
EMDB ID	:	EMD-35629
Title	:	Cryo-EM structure of type I-B Cascade bound to a PAM-containing dsDNA target at 3.6 angstrom resolution
Authors	:	Xiao, Y.; Lu, M.; Yu, C.; Zhang, Y.
Deposited on	:	2023-03-13
Resolution	:	3.60 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:

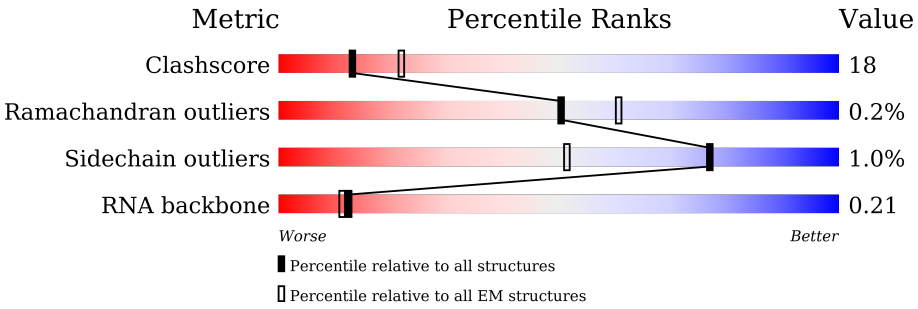
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 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
RNA backbone	4643	859

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 <=5%

Mol	Chain	Length	Quality of chain
1	J	551	67% 16% • 15%
2	A	237	57% 32% 11%
3	B	301	58% 41% •
3	C	301	65% 34% •
3	D	301	65% 34% •
3	H	301	65% 33% ••
3	I	301	66% 32% ••
3	N	301	69% 30% ••

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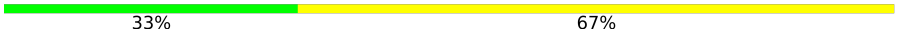
Mol	Chain	Length	Quality of chain
3	O	301	
4	E	15	
5	F	44	
6	G	41	
7	P	10	
8	K	124	
8	L	124	
8	M	124	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26526 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 Type I-MYXAN CRISPR-associated protein Cmx8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	467	3801	2462	637	695	7	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP A0A068N831
J	2	PRO	-	expression tag	UNP A0A068N831
J	3	LYS	-	expression tag	UNP A0A068N831
J	4	THR	-	expression tag	UNP A0A068N831
J	5	GLN	-	expression tag	UNP A0A068N831
J	6	ALA	-	expression tag	UNP A0A068N831
J	7	GLU	-	expression tag	UNP A0A068N831
J	8	ILE	-	expression tag	UNP A0A068N831
J	9	LEU	-	expression tag	UNP A0A068N831
J	10	THR	-	expression tag	UNP A0A068N831
J	11	LEU	-	expression tag	UNP A0A068N831
J	12	ASP	-	expression tag	UNP A0A068N831
J	13	PHE	-	expression tag	UNP A0A068N831
J	14	ASN	-	expression tag	UNP A0A068N831
J	15	LEU	-	expression tag	UNP A0A068N831
J	16	ALA	-	expression tag	UNP A0A068N831
J	17	GLU	-	expression tag	UNP A0A068N831
J	18	LEU	-	expression tag	UNP A0A068N831
J	19	PRO	-	expression tag	UNP A0A068N831
J	20	SER	-	expression tag	UNP A0A068N831
J	21	ALA	-	expression tag	UNP A0A068N831
J	22	GLN	-	expression tag	UNP A0A068N831
J	23	HIS	-	expression tag	UNP A0A068N831
J	24	ARG	-	expression tag	UNP A0A068N831
J	25	ALA	-	expression tag	UNP A0A068N831
J	26	GLY	-	expression tag	UNP A0A068N831
J	27	LEU	-	expression tag	UNP A0A068N831
J	28	ALA	-	expression tag	UNP A0A068N831

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Chain	Residue	Modelled	Actual	Comment	Reference
J	29	GLY	-	expression tag	UNP A0A068N831
J	30	LEU	-	expression tag	UNP A0A068N831
J	31	ILE	-	expression tag	UNP A0A068N831
J	32	LEU	-	expression tag	UNP A0A068N831

- Molecule 2 is a protein called Type I-MYXAN CRISPR-associated protein Cas5/Cmx5/DevS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	212	Total	C	N	O	S	0	0
			1695	1096	290	307	2		

- Molecule 3 is a protein called Fruiting body developmental protein R-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		
3	C	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		
3	D	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		
3	N	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		
3	O	241	Total	C	N	O	S	0	0
			1911	1225	325	352	9		
3	H	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		
3	I	299	Total	C	N	O	S	0	0
			2366	1501	407	449	9		

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*CP*CP*AP*TP*GP*TP*TP*TP*AP *TP*CP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	15	Total	C	N	O	P	0	0
			300	145	47	93	15		

- Molecule 5 is a RNA chain called RNA (44-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	44	Total	C	N	O	P	0	0
			925	414	152	315	44		

- Molecule 6 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	41	Total	C	N	O	P	0	0
			850	403	170	236	41		

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	10	Total	C	N	O	P	0	0
			210	100	50	50	10		

- Molecule 8 is a protein called CRISPR associated protein Cas11b.

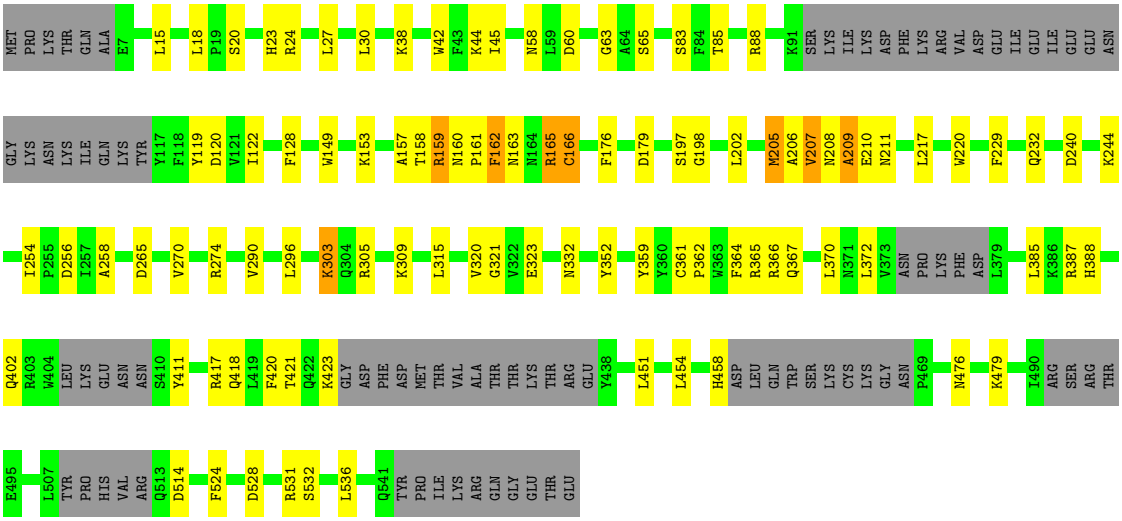
Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	110	Total	C	N	O	S	0	0
			918	591	155	171	1		
8	L	96	Total	C	N	O		0	0
			802	518	132	152			
8	M	110	Total	C	N	O	S	0	0
			918	591	155	171	1		

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.

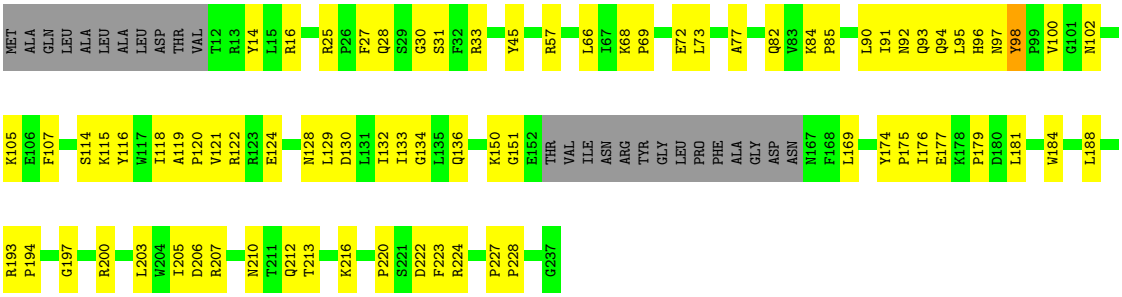
• Molecule 1: Type I-MYXAN CRISPR-associated protein Cmx8

Chain J:



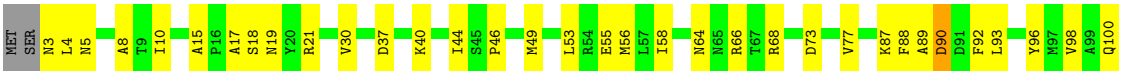
• Molecule 2: Type I-MYXAN CRISPR-associated protein Cas5/Cmx5/DevS

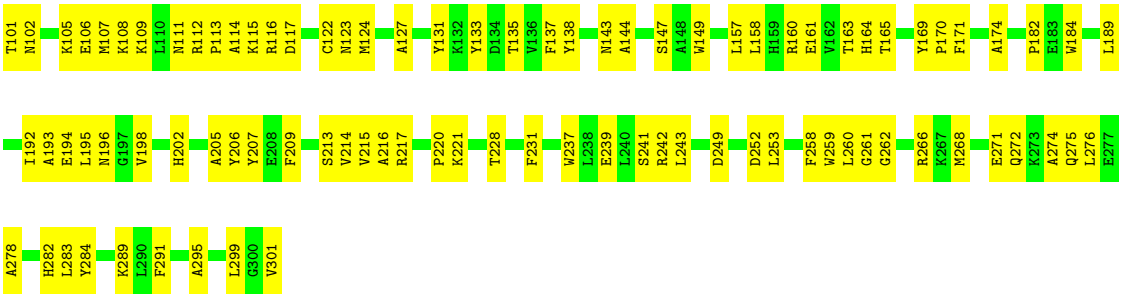
Chain A:



• Molecule 3: Fruiting body developmental protein R-like protein

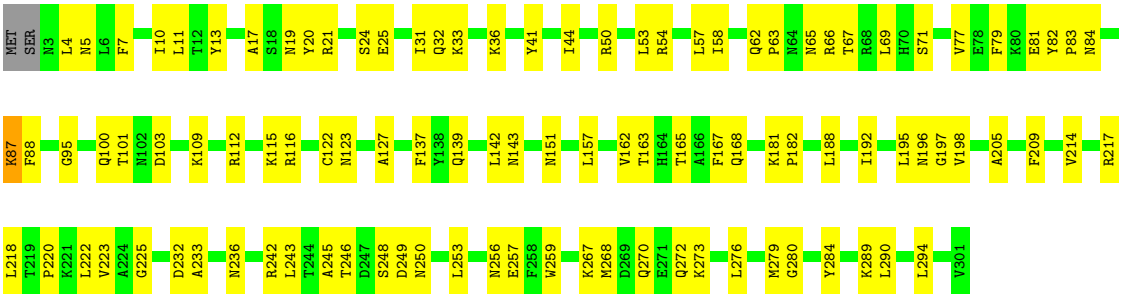
Chain B:





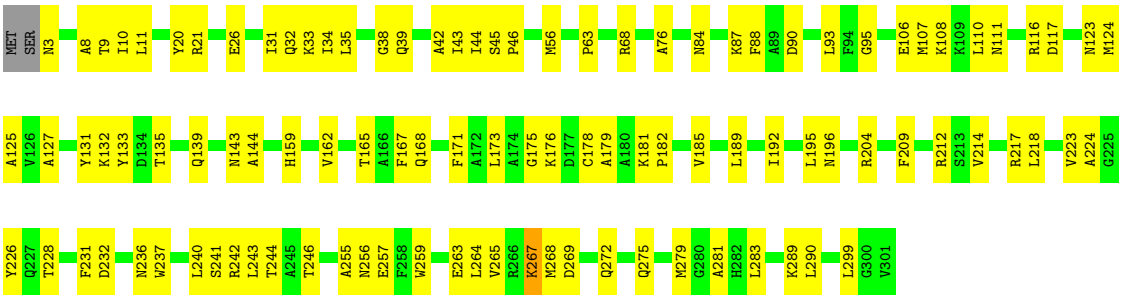
• Molecule 3: Fruiting body developmental protein R-like protein

Chain C:



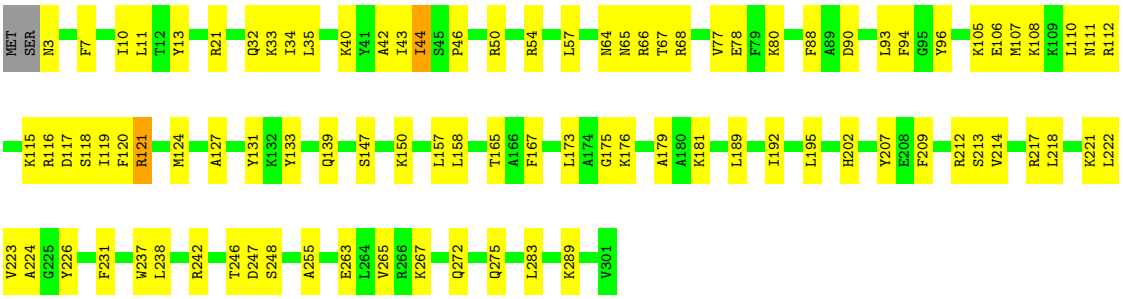
• Molecule 3: Fruiting body developmental protein R-like protein

Chain D:



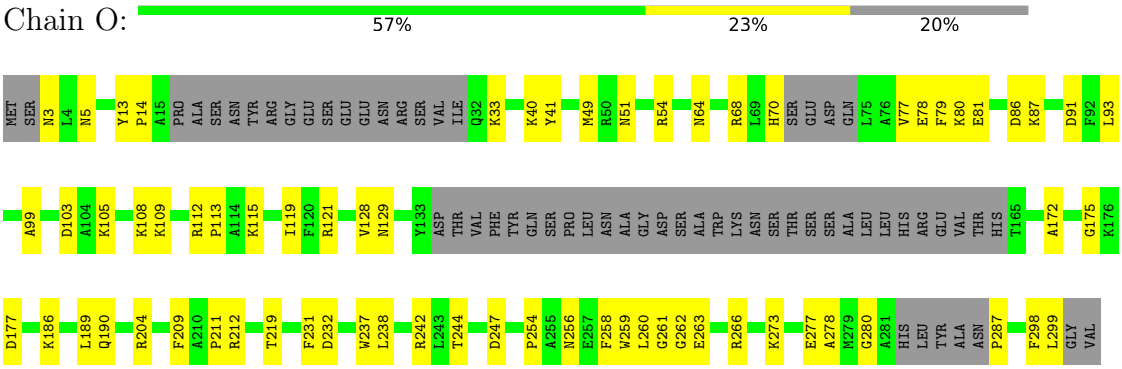
• Molecule 3: Fruiting body developmental protein R-like protein

Chain N:



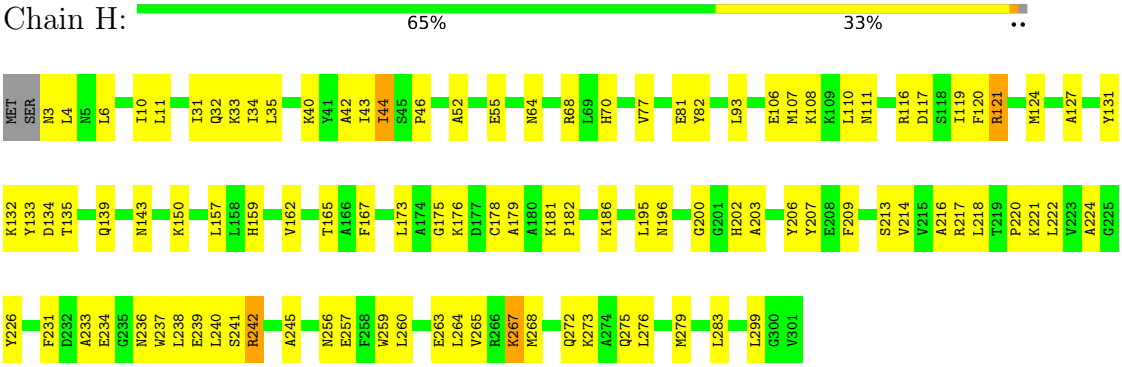
• Molecule 3: Fruiting body developmental protein R-like protein

Chain O:



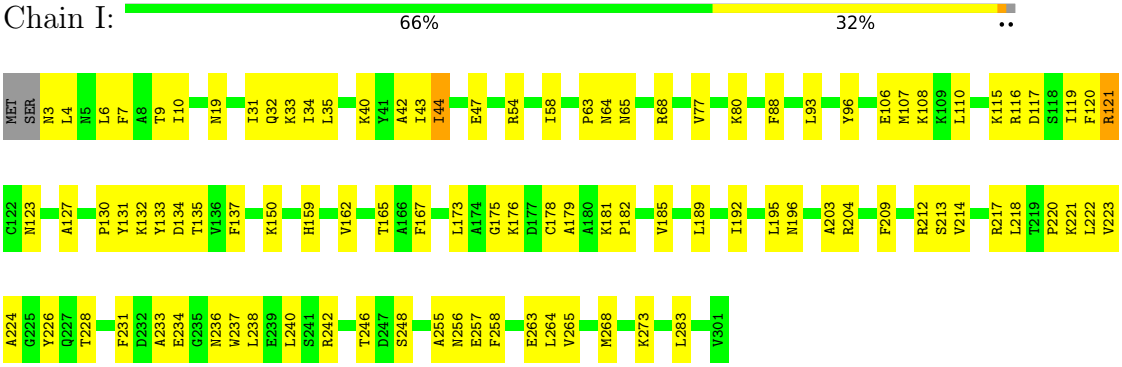
• Molecule 3: Fruiting body developmental protein R-like protein

Chain H:



• Molecule 3: Fruiting body developmental protein R-like protein

Chain I:

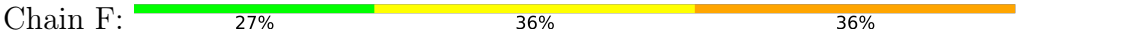


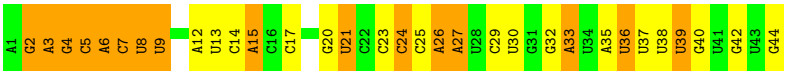
• Molecule 4: DNA (5'-D(P*TP*CP*CP*AP*TP*GP*TP*TP*TP*AP*TP*CP*AP*CP*C)-3')

Chain E:

• Molecule 5: RNA (44-MER)

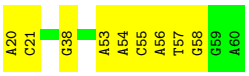
Chain F:





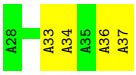
• Molecule 6: DNA (41-MER)

Chain G:



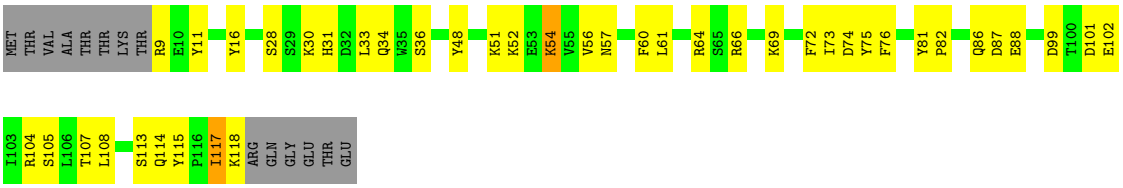
• Molecule 7: DNA (5'-D(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain P:



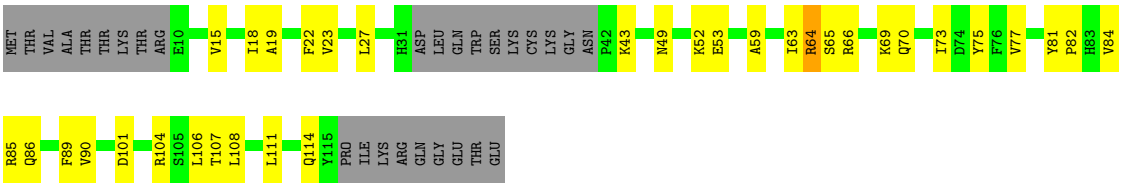
• Molecule 8: CRISPR associated protein Cas11b

Chain K:



• Molecule 8: CRISPR associated protein Cas11b

Chain L:



• Molecule 8: CRISPR associated protein Cas11b

Chain M:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	J	0.24	0/3887	0.45	0/5251
2	A	0.25	0/1741	0.52	0/2366
3	B	0.26	0/2421	0.55	0/3280
3	C	0.25	0/2421	0.51	0/3280
3	D	0.26	0/2421	0.53	0/3280
3	H	0.26	0/2421	0.54	0/3280
3	I	0.25	0/2421	0.54	0/3280
3	N	0.25	0/2421	0.53	0/3280
3	O	0.25	0/1951	0.52	0/2633
4	E	0.35	0/333	0.74	0/510
5	F	0.19	0/1030	0.75	0/1600
6	G	0.49	0/958	0.77	0/1477
7	P	0.41	0/239	0.62	0/366
8	K	0.26	0/937	0.50	0/1260
8	L	0.25	0/817	0.48	0/1097
8	M	0.26	0/937	0.52	0/1260
All	All	0.26	0/27356	0.54	0/37500

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3801	0	3766	187	0
2	A	1695	0	1705	94	0
3	B	2366	0	2305	102	0
3	C	2366	0	2305	78	0
3	D	2366	0	2305	111	0
3	H	2366	0	2305	79	0
3	I	2366	0	2305	81	0
3	N	2366	0	2305	78	0
3	O	1911	0	1890	50	0
4	E	300	0	172	44	0
5	F	925	0	469	45	0
6	G	850	0	459	25	0
7	P	210	0	111	7	0
8	K	918	0	920	37	0
8	L	802	0	798	45	0
8	M	918	0	920	36	0
All	All	26526	0	25040	943	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 18.

All (943) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:LYS:CG	1:J:158:THR:HG21	1.14	1.58
3:D:44:ILE:CG1	3:D:125:ALA:HB3	1.29	1.56
1:J:149:TRP:HZ3	1:J:162:PHE:CD2	1.22	1.55
1:J:153:LYS:CB	1:J:158:THR:HG21	1.43	1.49
3:D:44:ILE:HG13	3:D:125:ALA:CB	1.43	1.46
1:J:149:TRP:CZ3	1:J:162:PHE:CD2	2.01	1.44
1:J:153:LYS:HD2	1:J:158:THR:CG2	1.52	1.39
1:J:153:LYS:CG	1:J:158:THR:CG2	1.98	1.37
1:J:153:LYS:CD	1:J:158:THR:CG2	2.05	1.33
1:J:157:ALA:O	1:J:161:PRO:CD	1.80	1.28
1:J:157:ALA:O	1:J:161:PRO:HD2	1.10	1.28
3:N:120:PHE:O	3:N:121:ARG:HD3	1.09	1.25
3:H:120:PHE:O	3:H:121:ARG:HD3	1.40	1.22
1:J:161:PRO:O	1:J:165:ARG:HG2	1.36	1.22
1:J:202:LEU:HD13	6:G:57:DT:OP1	1.37	1.21
1:J:153:LYS:HG3	1:J:158:THR:HG21	1.24	1.17
1:J:153:LYS:CD	1:J:158:THR:HG21	1.73	1.15
1:J:149:TRP:CZ3	1:J:162:PHE:HD2	1.49	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:TYR:CD2	4:E:4:DT:C4	2.34	1.14
1:J:210:GLU:C	2:A:98:TYR:HE2	1.50	1.14
1:J:153:LYS:HG3	1:J:158:THR:CG2	1.76	1.12
3:D:44:ILE:CG2	3:D:125:ALA:H	1.62	1.12
1:J:206:ALA:O	1:J:207:VAL:HG22	1.49	1.10
3:I:120:PHE:O	3:I:121:ARG:HD3	1.51	1.09
8:L:66:ARG:HB3	8:L:73:ILE:HG13	1.24	1.09
1:J:119:TYR:CG	4:E:4:DT:C4	2.40	1.09
2:A:95:LEU:HD12	2:A:121:VAL:HG12	1.33	1.08
1:J:206:ALA:HB2	2:A:100:VAL:CG2	1.84	1.07
4:E:-1:DC:O2	6:G:58:DG:N2	1.87	1.06
1:J:153:LYS:HD2	1:J:158:THR:HG23	1.37	1.06
3:N:120:PHE:O	3:N:121:ARG:CD	2.03	1.06
8:M:11:TYR:OH	8:M:103:ILE:CG2	2.03	1.05
8:M:11:TYR:OH	8:M:103:ILE:HG23	1.55	1.05
1:J:202:LEU:CD1	6:G:57:DT:OP1	2.07	1.03
1:J:153:LYS:CB	1:J:158:THR:CG2	2.31	1.02
8:L:66:ARG:HB3	8:L:73:ILE:CG1	1.89	1.00
1:J:206:ALA:HB2	2:A:100:VAL:HG22	1.00	0.99
1:J:208:ASN:CG	2:A:33:ARG:HH22	1.64	0.99
1:J:210:GLU:C	2:A:98:TYR:CE2	2.35	0.98
1:J:206:ALA:CB	2:A:100:VAL:HG22	1.93	0.98
1:J:161:PRO:O	1:J:165:ARG:CG	2.12	0.97
1:J:119:TYR:CE2	4:E:4:DT:C2	2.53	0.97
1:J:153:LYS:HB3	1:J:158:THR:HG21	1.41	0.97
1:J:149:TRP:HH2	1:J:162:PHE:CB	1.78	0.96
2:A:107:PHE:CE1	2:A:114:SER:OG	2.17	0.96
8:L:66:ARG:HG3	8:L:73:ILE:HG21	1.46	0.96
1:J:122:ILE:CD1	1:J:163:ASN:HD22	1.78	0.96
1:J:205:MET:HG2	6:G:57:DT:OP2	1.65	0.95
1:J:119:TYR:CZ	4:E:4:DT:C6	2.55	0.95
1:J:119:TYR:CD2	4:E:4:DT:N3	2.35	0.94
8:M:96:LEU:HA	8:M:101:ASP:H	1.34	0.93
3:D:43:ILE:O	3:D:43:ILE:HG22	1.66	0.93
1:J:153:LYS:CD	1:J:158:THR:HG22	1.95	0.93
3:I:119:ILE:HG22	3:I:119:ILE:O	1.67	0.92
1:J:160:ASN:HB3	1:J:161:PRO:HD3	1.52	0.92
1:J:153:LYS:HB3	1:J:158:THR:CG2	1.98	0.92
8:L:66:ARG:CG	8:L:73:ILE:HG21	1.99	0.92
3:D:44:ILE:CB	3:D:125:ALA:HB3	1.99	0.91
4:E:0:DA:N1	6:G:57:DT:O4	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:56:DA:H2"	6:G:57:DT:H5"	1.54	0.90
2:A:95:LEU:CD1	2:A:121:VAL:HG12	2.00	0.90
1:J:119:TYR:CD1	4:E:4:DT:C5	2.61	0.88
1:J:197:SER:OG	6:G:58:DG:OP1	1.92	0.88
1:J:149:TRP:NE1	1:J:159:ARG:CZ	2.36	0.88
1:J:159:ARG:NH1	4:E:3:DT:OP1	2.06	0.87
1:J:122:ILE:HD11	1:J:163:ASN:HD22	1.40	0.86
1:J:119:TYR:CD1	4:E:4:DT:C7	2.58	0.86
1:J:122:ILE:HD11	1:J:163:ASN:ND2	1.91	0.85
3:D:31:ILE:HG22	3:D:43:ILE:HD13	1.59	0.85
3:D:44:ILE:HG21	3:D:125:ALA:H	1.38	0.84
1:J:149:TRP:CH2	1:J:162:PHE:CB	2.60	0.84
2:A:93:GLN:HG2	2:A:94:GLN:H	1.43	0.84
8:L:66:ARG:CB	8:L:73:ILE:HG21	2.07	0.84
1:J:153:LYS:HD2	1:J:158:THR:HG22	1.50	0.84
4:E:-2:DC:H4'	4:E:-1:DC:OP1	1.77	0.83
1:J:149:TRP:HH2	1:J:162:PHE:HB2	1.40	0.83
8:M:96:LEU:HA	8:M:101:ASP:N	1.94	0.83
2:A:114:SER:O	5:F:7:C:N4	2.12	0.82
8:K:30:LYS:HD2	8:K:51:LYS:HB3	1.62	0.81
8:M:96:LEU:CB	8:M:101:ASP:HA	2.10	0.81
1:J:208:ASN:ND2	2:A:33:ARG:HH22	1.79	0.81
8:M:11:TYR:OH	8:M:103:ILE:HG21	1.80	0.80
8:L:66:ARG:CB	8:L:73:ILE:HG13	2.10	0.80
8:L:66:ARG:HE	8:L:73:ILE:HG23	1.46	0.80
1:J:208:ASN:O	1:J:209:ALA:HB2	1.83	0.79
3:D:44:ILE:CB	3:D:125:ALA:H	1.95	0.79
8:K:69:LYS:HG2	8:K:74:ASP:HB3	1.64	0.79
3:B:8:ALA:HA	3:B:216:ALA:HB3	1.63	0.79
2:A:98:TYR:OH	3:B:98:VAL:HB	1.83	0.78
1:J:208:ASN:CB	2:A:33:ARG:NH2	2.45	0.78
1:J:122:ILE:CD1	1:J:163:ASN:ND2	2.44	0.78
3:B:231:PHE:HB3	3:B:237:TRP:HB2	1.65	0.78
1:J:119:TYR:CE1	4:E:4:DT:C5	2.72	0.78
1:J:332:ASN:CG	4:E:2:DG:N2	2.37	0.78
3:B:89:ALA:O	3:B:90:ASP:OD1	2.01	0.77
7:P:36:DA:H62	8:K:87:ASP:CB	1.97	0.77
3:B:135:THR:HA	3:B:160:ARG:O	1.84	0.76
1:J:149:TRP:CH2	1:J:162:PHE:CD2	2.72	0.76
3:D:242:ARG:NH1	3:D:246:THR:O	2.19	0.76
3:D:31:ILE:HG22	3:D:43:ILE:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:217:ARG:NH1	3:H:226:TYR:O	2.16	0.75
1:J:119:TYR:CB	4:E:4:DT:O4	2.35	0.74
3:D:21:ARG:HH22	3:D:45:SER:HB3	1.52	0.74
1:J:149:TRP:HZ3	1:J:162:PHE:CE2	2.01	0.74
3:B:46:PRO:HD3	3:B:124:MET:HB2	1.69	0.74
8:K:60:PHE:HB3	8:K:64:ARG:HH21	1.53	0.74
1:J:122:ILE:HD13	1:J:163:ASN:HA	1.68	0.74
8:M:103:ILE:HG22	8:M:103:ILE:O	1.86	0.74
3:D:44:ILE:HB	3:D:125:ALA:N	2.01	0.74
3:H:242:ARG:NH2	3:H:279:MET:SD	2.61	0.74
3:C:79:PHE:O	3:C:84:ASN:ND2	2.21	0.73
8:L:65:SER:O	8:L:66:ARG:HD3	1.87	0.73
8:L:66:ARG:HG3	8:L:73:ILE:CG2	2.17	0.73
3:D:44:ILE:CG1	3:D:125:ALA:CB	2.25	0.73
3:D:44:ILE:O	3:D:124:MET:HB2	1.87	0.73
1:J:254:ILE:HB	1:J:323:GLU:HB2	1.70	0.73
3:B:138:TYR:OH	5:F:13:U:N3	2.22	0.73
3:O:242:ARG:HG2	3:O:254:PRO:HG3	1.71	0.73
3:D:44:ILE:CG2	3:D:125:ALA:N	2.46	0.73
8:M:96:LEU:CG	8:M:101:ASP:HA	2.19	0.73
3:I:130:PRO:O	3:I:132:LYS:NZ	2.21	0.72
3:C:103:ASP:HB3	3:C:109:LYS:HD2	1.70	0.72
1:J:119:TYR:CG	4:E:4:DT:C5	2.75	0.72
3:O:212:ARG:HH22	3:O:259:TRP:HD1	1.37	0.72
1:J:119:TYR:CE1	4:E:4:DT:C6	2.77	0.72
1:J:197:SER:OG	6:G:58:DG:P	2.48	0.72
3:B:10:ILE:HG12	3:B:169:TYR:HB3	1.72	0.71
1:J:149:TRP:CZ3	1:J:162:PHE:CG	2.78	0.71
1:J:157:ALA:O	1:J:161:PRO:CG	2.38	0.71
1:J:119:TYR:CG	4:E:4:DT:O4	2.44	0.71
8:L:70:GLN:HE21	8:L:101:ASP:HA	1.55	0.71
1:J:153:LYS:HB3	1:J:158:THR:CB	2.21	0.71
3:O:121:ARG:HB2	3:O:172:ALA:HB3	1.73	0.71
8:L:86:GLN:H	8:L:89:PHE:HE1	1.39	0.71
1:J:119:TYR:CD1	4:E:4:DT:H73	2.26	0.71
3:H:81:GLU:HG2	3:H:82:TYR:H	1.56	0.71
3:D:204:ARG:HH12	5:F:24:C:H5"	1.56	0.71
1:J:153:LYS:HB3	1:J:158:THR:OG1	1.90	0.70
1:J:149:TRP:HZ2	1:J:159:ARG:HG3	1.56	0.70
3:D:32:GLN:HB2	3:D:132:LYS:HE3	1.73	0.70
1:J:165:ARG:HH12	1:J:176:PHE:HB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:108:LEU:HD11	8:L:75:TYR:HB3	1.73	0.70
1:J:208:ASN:HB3	2:A:33:ARG:NH2	2.07	0.70
3:D:43:ILE:O	3:D:43:ILE:CG2	2.39	0.70
1:J:206:ALA:O	1:J:207:VAL:CG2	2.35	0.69
3:C:268:MET:SD	3:C:273:LYS:NZ	2.65	0.69
3:D:212:ARG:HD2	3:D:263:GLU:HG3	1.74	0.69
3:C:4:LEU:HD23	3:C:220:PRO:HB3	1.74	0.69
3:D:44:ILE:HG21	3:D:125:ALA:N	2.05	0.69
3:H:217:ARG:HG2	3:H:218:LEU:HG	1.74	0.69
3:O:189:LEU:HD12	3:O:190:GLN:HG3	1.73	0.69
1:J:122:ILE:HD13	1:J:163:ASN:HD22	1.57	0.68
3:D:32:GLN:HA	3:D:43:ILE:HD11	1.76	0.68
3:O:232:ASP:OD2	3:O:238:LEU:N	2.27	0.68
1:J:119:TYR:CE2	4:E:4:DT:N3	2.61	0.68
1:J:149:TRP:HH2	1:J:162:PHE:HB3	1.57	0.68
1:J:418:GLN:HG3	1:J:536:LEU:HD21	1.74	0.68
1:J:210:GLU:O	2:A:98:TYR:CE2	2.46	0.68
1:J:202:LEU:HD11	6:G:57:DT:P	2.33	0.68
1:J:208:ASN:CG	2:A:33:ARG:NH2	2.44	0.68
2:A:203:LEU:H	2:A:213:THR:HG21	1.59	0.67
1:J:158:THR:O	1:J:162:PHE:HB2	1.93	0.67
1:J:149:TRP:CH2	1:J:162:PHE:HB2	2.26	0.67
1:J:210:GLU:O	2:A:98:TYR:HE2	1.77	0.67
3:I:135:THR:HB	3:I:159:HIS:HB2	1.76	0.67
8:L:66:ARG:CG	8:L:73:ILE:CG2	2.72	0.67
3:B:194:GLU:HG3	3:C:222:LEU:HB2	1.77	0.67
7:P:36:DA:H62	8:K:87:ASP:HB3	1.58	0.67
1:J:524:PHE:HZ	8:L:106:LEU:HD22	1.59	0.67
3:I:119:ILE:O	3:I:119:ILE:CG2	2.40	0.67
8:L:66:ARG:HB3	8:L:73:ILE:HG21	1.77	0.67
1:J:206:ALA:CB	2:A:100:VAL:CG2	2.65	0.66
8:M:96:LEU:HG	8:M:101:ASP:CB	2.25	0.66
1:J:332:ASN:HB3	6:G:55:DC:O2	1.96	0.66
3:D:204:ARG:NH1	5:F:25:C:OP2	2.29	0.66
3:D:21:ARG:NH2	3:D:45:SER:HB3	2.09	0.66
2:A:97:ASN:ND2	2:A:119:ALA:HB3	2.10	0.66
3:C:196:ASN:OD1	3:C:197:GLY:N	2.29	0.66
3:D:21:ARG:HD2	5:F:21:U:H3'	1.78	0.66
3:N:217:ARG:HG2	3:N:218:LEU:HG	1.77	0.66
2:A:98:TYR:HE1	3:B:98:VAL:HG21	1.60	0.66
1:J:160:ASN:CB	1:J:161:PRO:HD3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:-1:DC:H2'	4:E:0:DA:C8	2.31	0.65
3:I:242:ARG:NH1	3:I:246:THR:O	2.29	0.65
3:B:8:ALA:H	3:B:171:PHE:HB3	1.61	0.65
3:N:179:ALA:O	3:N:181:LYS:NZ	2.25	0.65
2:A:206:ASP:OD1	2:A:210:ASN:ND2	2.30	0.65
3:D:259:TRP:HB3	3:D:290:LEU:HD11	1.79	0.65
8:K:105:SER:HB3	8:L:75:TYR:HD2	1.60	0.65
8:L:66:ARG:HD2	8:L:73:ILE:HD12	1.78	0.65
1:J:208:ASN:O	1:J:209:ALA:CB	2.45	0.65
2:A:222:ASP:OD1	2:A:224:ARG:NH2	2.28	0.65
3:C:50:ARG:NH1	5:F:13:U:OP1	2.29	0.65
3:C:67:THR:HG22	3:C:79:PHE:HB2	1.79	0.65
1:J:208:ASN:CB	2:A:33:ARG:HH22	2.06	0.65
3:D:44:ILE:HG21	3:D:125:ALA:CB	2.27	0.64
3:H:268:MET:O	3:H:273:LYS:NZ	2.29	0.64
2:A:107:PHE:HA	2:A:116:TYR:HD2	1.60	0.64
3:O:40:LYS:NZ	3:O:128:VAL:O	2.27	0.64
3:I:231:PHE:HB3	3:I:238:LEU:HD23	1.79	0.64
1:J:149:TRP:CH2	1:J:162:PHE:HB3	2.31	0.64
8:M:11:TYR:HH	8:M:103:ILE:HG23	1.62	0.64
1:J:149:TRP:CD1	1:J:159:ARG:NH2	2.66	0.63
8:L:66:ARG:NE	8:L:73:ILE:HG23	2.11	0.63
1:J:119:TYR:CE2	4:E:4:DT:N1	2.66	0.63
3:B:137:PHE:HD2	3:C:32:GLN:HE21	1.44	0.63
8:L:104:ARG:HD2	8:L:107:THR:HG21	1.81	0.63
3:B:102:ASN:ND2	3:B:106:GLU:OE2	2.30	0.63
8:L:23:VAL:HG11	8:L:111:LEU:HA	1.81	0.63
1:J:149:TRP:CD1	1:J:159:ARG:CZ	2.82	0.63
3:O:262:GLY:HA2	3:O:266:ARG:HH21	1.63	0.63
3:D:179:ALA:O	3:D:181:LYS:NZ	2.26	0.63
3:C:10:ILE:HG22	3:C:214:VAL:HG12	1.81	0.62
8:L:66:ARG:HB3	8:L:73:ILE:CG2	2.29	0.62
3:D:272:GLN:NE2	3:D:275:GLN:OE1	2.33	0.62
3:H:196:ASN:HD22	3:I:223:VAL:HG11	1.65	0.62
3:I:179:ALA:O	3:I:181:LYS:NZ	2.30	0.62
3:D:93:LEU:HB3	3:D:117:ASP:HB2	1.80	0.62
1:J:202:LEU:CD1	6:G:57:DT:P	2.87	0.62
8:M:96:LEU:HA	8:M:101:ASP:CA	2.29	0.62
8:K:73:ILE:HA	8:K:76:PHE:HD2	1.63	0.62
8:K:117:ILE:HG12	8:K:118:LYS:H	1.63	0.62
1:J:332:ASN:ND2	6:G:55:DC:N3	2.44	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:93:LEU:HD11	3:D:181:LYS:HD2	1.81	0.62
3:D:10:ILE:HG22	3:D:214:VAL:HG23	1.82	0.61
3:D:44:ILE:HB	3:D:125:ALA:H	1.61	0.61
1:J:210:GLU:CA	2:A:98:TYR:CE2	2.84	0.61
3:B:213:SER:HB2	3:B:262:GLY:HA2	1.82	0.61
3:H:179:ALA:O	3:H:181:LYS:NZ	2.28	0.61
3:I:236:ASN:HB3	3:I:264:LEU:HD22	1.82	0.61
3:D:217:ARG:HG2	3:D:218:LEU:HG	1.82	0.61
1:J:122:ILE:HD12	1:J:163:ASN:HB2	1.82	0.61
3:N:93:LEU:HB3	3:N:117:ASP:HB2	1.82	0.61
1:J:206:ALA:HB1	2:A:98:TYR:HB3	1.81	0.61
3:C:139:GLN:NE2	5:F:21:U:OP2	2.34	0.61
3:N:263:GLU:OE2	3:N:267:LYS:NZ	2.29	0.61
1:J:211:ASN:N	2:A:98:TYR:HE2	1.99	0.61
3:B:113:PRO:HB2	3:B:115:LYS:HG3	1.80	0.61
3:B:272:GLN:O	3:B:276:LEU:HG	2.01	0.61
3:O:244:THR:HB	3:O:254:PRO:HD2	1.81	0.61
3:C:20:TYR:HA	3:C:31:ILE:HG22	1.83	0.61
3:I:213:SER:HB3	3:I:263:GLU:HB3	1.82	0.61
3:O:261:GLY:O	3:O:266:ARG:NH2	2.34	0.60
1:J:421:THR:HA	1:J:531:ARG:HE	1.66	0.60
3:B:239:GLU:HG3	3:B:243:LEU:HD13	1.82	0.60
3:N:212:ARG:HD2	3:N:263:GLU:HG3	1.82	0.60
3:N:217:ARG:NH1	3:N:226:TYR:O	2.34	0.60
3:H:10:ILE:HG22	3:H:214:VAL:HG23	1.84	0.60
2:A:205:ILE:HD12	2:A:210:ASN:HD21	1.66	0.60
3:N:106:GLU:O	3:N:110:LEU:N	2.34	0.60
3:D:44:ILE:CB	3:D:125:ALA:N	2.59	0.60
4:E:4:DT:H2'	4:E:4:DT:O2	2.01	0.60
3:H:231:PHE:HA	3:H:237:TRP:HB3	1.83	0.60
8:K:66:ARG:NH2	8:K:104:ARG:O	2.34	0.60
3:N:94:PHE:HE1	3:N:118:SER:HA	1.67	0.60
1:J:332:ASN:CG	4:E:2:DG:H22	2.03	0.60
2:A:93:GLN:HG2	2:A:94:GLN:N	2.15	0.60
2:A:200:ARG:HE	2:A:216:LYS:HB3	1.65	0.60
3:N:32:GLN:HG2	3:N:40:LYS:HB3	1.83	0.60
3:H:119:ILE:O	3:H:119:ILE:HG22	2.02	0.59
3:I:217:ARG:HG2	3:I:218:LEU:HG	1.84	0.59
1:J:149:TRP:CH2	1:J:162:PHE:HD2	2.10	0.59
3:B:56:MET:HE3	3:B:195:LEU:HD12	1.83	0.59
1:J:153:LYS:HG3	1:J:158:THR:HG22	1.77	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:PHE:HE1	2:A:114:SER:HG	1.34	0.59
1:J:232:GLN:OE1	1:J:274:ARG:NH2	2.35	0.59
3:O:232:ASP:OD2	3:O:237:TRP:N	2.35	0.59
1:J:202:LEU:HD11	6:G:57:DT:OP2	2.02	0.59
3:B:5:ASN:HB3	3:B:174:ALA:HA	1.85	0.59
3:I:65:ASN:HD22	3:I:80:LYS:HB2	1.67	0.59
3:O:51:ASN:ND2	5:F:44:G:OP2	2.36	0.59
8:L:63:ILE:O	8:L:66:ARG:HG2	2.03	0.59
1:J:119:TYR:CE2	4:E:4:DT:C6	2.90	0.59
3:N:119:ILE:HG22	3:N:119:ILE:O	2.02	0.59
8:L:18:ILE:HG12	8:L:22:PHE:CZ	2.36	0.59
1:J:476:ASN:HA	1:J:479:LYS:HE2	1.85	0.58
1:J:20:SER:OG	1:J:23:HIS:ND1	2.28	0.58
1:J:385:LEU:O	1:J:388:HIS:ND1	2.29	0.58
3:N:88:PHE:HD1	3:N:90:ASP:H	1.50	0.58
3:H:218:LEU:HB3	3:H:221:LYS:HG2	1.84	0.58
3:C:248:SER:OG	3:C:250:ASN:OD1	2.20	0.58
1:J:119:TYR:CE2	4:E:4:DT:C4	2.91	0.58
8:M:74:ASP:HA	8:M:77:VAL:HG22	1.85	0.58
1:J:208:ASN:ND2	2:A:33:ARG:NH2	2.51	0.58
1:J:210:GLU:N	2:A:98:TYR:CE2	2.71	0.58
3:O:263:GLU:HA	3:O:266:ARG:HB2	1.85	0.58
3:B:205:ALA:HA	3:C:123:ASN:HA	1.86	0.58
3:D:44:ILE:CB	3:D:125:ALA:CB	2.75	0.58
1:J:258:ALA:HB2	1:J:320:VAL:HG23	1.86	0.58
2:A:94:GLN:HA	2:A:120:PRO:HB3	1.84	0.58
2:A:150:LYS:HD3	3:B:221:LYS:HE2	1.84	0.58
3:D:31:ILE:C	3:D:43:ILE:HD13	2.24	0.58
3:N:65:ASN:HA	3:N:80:LYS:HG2	1.86	0.58
3:H:106:GLU:O	3:H:110:LEU:N	2.36	0.58
1:J:119:TYR:CZ	4:E:4:DT:N1	2.72	0.58
2:A:176:ILE:HG22	2:A:179:PRO:HG2	1.85	0.58
5:F:23:C:O2'	3:H:116:ARG:NH1	2.33	0.58
3:I:131:TYR:CZ	3:I:133:TYR:HB2	2.39	0.58
1:J:149:TRP:HE1	1:J:159:ARG:CZ	2.16	0.57
3:N:213:SER:HB3	3:N:263:GLU:HB3	1.85	0.57
8:M:103:ILE:CG2	8:M:103:ILE:O	2.52	0.57
3:B:138:TYR:HH	5:F:13:U:H3	1.42	0.57
3:B:143:ASN:HB2	3:C:81:GLU:HG3	1.85	0.57
3:H:272:GLN:NE2	3:H:275:GLN:OE1	2.37	0.57
8:K:51:LYS:O	8:K:54:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:96:LEU:HB2	8:M:101:ASP:HA	1.86	0.57
3:B:115:LYS:HD3	5:F:4:G:H1	1.69	0.57
3:H:217:ARG:HH21	3:H:238:LEU:HD11	1.70	0.57
1:J:119:TYR:CZ	4:E:4:DT:C5	2.93	0.57
3:B:193:ALA:HB2	3:B:291:PHE:HD2	1.67	0.57
2:A:96:HIS:HB2	2:A:115:LYS:HD3	1.85	0.57
6:G:56:DA:C2'	6:G:57:DT:H5"	2.31	0.57
3:H:236:ASN:HB3	3:H:264:LEU:HD22	1.87	0.57
3:D:269:ASP:HB2	3:D:272:GLN:HB2	1.86	0.57
3:O:99:ALA:O	3:O:105:LYS:NZ	2.37	0.57
3:D:135:THR:HB	3:D:159:HIS:HB2	1.85	0.57
3:N:32:GLN:OE1	3:N:33:LYS:N	2.38	0.57
1:J:18:LEU:O	1:J:24:ARG:NH2	2.37	0.56
8:L:84:VAL:HG12	8:L:85:ARG:HG2	1.87	0.56
1:J:332:ASN:CB	6:G:55:DC:O2	2.53	0.56
3:C:31:ILE:O	3:C:33:LYS:NZ	2.30	0.56
3:D:31:ILE:CG2	3:D:43:ILE:HD13	2.32	0.56
3:D:131:TYR:CZ	3:D:133:TYR:HB2	2.41	0.56
3:N:120:PHE:CG	3:N:121:ARG:N	2.74	0.56
1:J:128:PHE:HE1	1:J:229:PHE:HB3	1.71	0.56
3:B:109:LYS:HZ3	3:B:111:ASN:HB2	1.69	0.56
8:L:81:TYR:HD1	8:L:82:PRO:HD2	1.69	0.56
2:A:205:ILE:HG12	5:F:3:A:C6	2.41	0.56
3:B:206:TYR:O	3:C:123:ASN:ND2	2.38	0.56
8:L:69:LYS:O	8:L:70:GLN:HG3	2.06	0.56
1:J:303:LYS:HB3	1:J:315:LEU:HD21	1.86	0.56
3:B:88:PHE:H	3:B:184:TRP:HH2	1.54	0.56
3:D:20:TYR:OH	5:F:23:C:OP2	2.22	0.56
3:D:106:GLU:O	3:D:110:LEU:N	2.38	0.56
3:C:5:ASN:O	3:C:217:ARG:NH2	2.38	0.56
3:N:242:ARG:NH1	3:N:246:THR:O	2.38	0.56
3:C:188:LEU:O	3:C:192:ILE:HG12	2.06	0.56
3:C:245:ALA:H	3:C:253:LEU:HD21	1.70	0.56
3:O:80:LYS:HG3	3:O:81:GLU:H	1.71	0.56
2:A:95:LEU:CD1	2:A:121:VAL:CG1	2.78	0.56
3:H:135:THR:HB	3:H:159:HIS:HB2	1.87	0.56
2:A:16:ARG:HG3	2:A:132:ILE:HG13	1.88	0.56
3:B:127:ALA:HB1	3:B:165:THR:HG21	1.87	0.56
7:P:36:DA:H2'	7:P:37:DA:C8	2.41	0.55
3:B:217:ARG:HD2	3:B:259:TRP:H	1.71	0.55
3:B:249:ASP:HB3	3:B:253:LEU:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:10:ILE:HG22	3:N:214:VAL:HG23	1.87	0.55
3:I:173:LEU:HD23	3:I:175:GLY:H	1.71	0.55
3:H:267:LYS:HD2	3:H:267:LYS:O	2.06	0.55
1:J:149:TRP:CZ2	1:J:159:ARG:HG3	2.40	0.55
2:A:94:GLN:HG3	5:F:8:U:OP2	2.06	0.55
3:B:143:ASN:OD1	3:B:144:ALA:N	2.39	0.55
3:N:120:PHE:CD2	3:N:121:ARG:N	2.75	0.55
3:I:32:GLN:OE1	3:I:33:LYS:N	2.38	0.55
3:I:10:ILE:HG22	3:I:214:VAL:HG23	1.89	0.55
3:D:46:PRO:HD3	3:D:124:MET:HB3	1.87	0.55
3:I:54:ARG:HH22	3:I:96:TYR:HE2	1.55	0.55
3:C:21:ARG:O	5:F:15:A:O2'	2.24	0.55
3:I:3:ASN:HD21	3:I:176:LYS:HB3	1.72	0.55
3:N:21:ARG:NH2	5:F:39:U:OP1	2.39	0.55
3:H:131:TYR:CZ	3:H:133:TYR:HB2	2.42	0.55
2:A:30:GLY:O	2:A:33:ARG:NH1	2.40	0.54
2:A:107:PHE:HE1	2:A:114:SER:OG	1.82	0.54
3:H:120:PHE:C	3:H:121:ARG:HD3	2.24	0.54
1:J:411:TYR:N	1:J:479:LYS:HE3	2.22	0.54
3:C:21:ARG:NH1	5:F:15:A:OP1	2.40	0.54
3:D:38:GLY:O	3:D:39:GLN:NE2	2.40	0.54
8:K:87:ASP:OD1	8:K:88:GLU:N	2.40	0.54
8:L:65:SER:O	8:L:66:ARG:CD	2.54	0.54
8:M:11:TYR:HH	8:M:103:ILE:CG2	2.14	0.54
1:J:119:TYR:CD2	4:E:4:DT:C5	2.95	0.54
3:C:142:LEU:HD23	3:C:143:ASN:HB2	1.88	0.54
3:I:217:ARG:NH1	3:I:226:TYR:O	2.39	0.54
3:O:209:PHE:CD2	3:O:211:PRO:HD2	2.43	0.54
8:M:103:ILE:O	8:M:107:THR:HG23	2.07	0.54
3:C:127:ALA:HB1	3:C:165:THR:HG21	1.90	0.54
3:D:182:PRO:HB3	3:D:299:LEU:HD21	1.89	0.54
3:I:93:LEU:HB3	3:I:117:ASP:HB2	1.90	0.54
3:C:62:GLN:OE1	3:C:63:PRO:HD2	2.08	0.54
3:I:237:TRP:NE1	3:I:240:LEU:HD11	2.23	0.54
8:L:15:VAL:HA	8:L:18:ILE:HG22	1.89	0.54
3:B:56:MET:HE1	3:B:196:ASN:H	1.73	0.54
8:M:101:ASP:O	8:M:103:ILE:HG13	2.08	0.54
1:J:149:TRP:NE1	1:J:159:ARG:NH1	2.56	0.54
3:D:31:ILE:O	3:D:43:ILE:HD13	2.08	0.54
8:M:50:ASP:HB3	8:M:54:LYS:NZ	2.23	0.54
2:A:82:GLN:HE22	2:A:85:PRO:HA	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ILE:HD13	2:A:212:GLN:HG3	1.90	0.53
3:C:87:LYS:HD2	3:C:88:PHE:HB2	1.90	0.53
3:H:81:GLU:HG2	3:H:82:TYR:N	2.20	0.53
3:I:106:GLU:O	3:I:110:LEU:N	2.41	0.53
3:N:246:THR:HB	3:N:255:ALA:HA	1.89	0.53
3:O:256:ASN:ND2	3:O:278:ALA:O	2.39	0.53
3:O:68:ARG:HA	3:O:78:GLU:HG3	1.90	0.53
3:O:113:PRO:HD2	3:O:115:LYS:HG3	1.91	0.53
2:A:100:VAL:HG12	2:A:100:VAL:O	2.08	0.53
3:B:101:THR:HG22	3:B:105:LYS:HZ1	1.71	0.53
3:B:116:ARG:NH2	5:F:5:C:OP1	2.29	0.53
3:C:143:ASN:HD21	3:C:151:ASN:HA	1.73	0.53
3:H:173:LEU:HD23	3:H:175:GLY:H	1.73	0.53
8:K:66:ARG:HA	8:K:69:LYS:HB2	1.90	0.53
3:B:138:TYR:HD2	3:B:158:LEU:HB2	1.73	0.53
3:H:106:GLU:O	3:H:111:ASN:N	2.41	0.53
3:N:11:LEU:HD23	3:N:231:PHE:CE2	2.44	0.53
1:J:206:ALA:C	1:J:207:VAL:HG13	2.28	0.53
5:F:37:U:OP2	3:I:204:ARG:NH1	2.41	0.53
8:K:101:ASP:OD1	8:K:102:GLU:N	2.42	0.53
4:E:-1:DC:H5”	4:E:-1:DC:H6	1.74	0.53
3:H:106:GLU:HB3	3:H:110:LEU:HB2	1.91	0.53
3:B:68:ARG:HB3	3:B:77:VAL:HG22	1.91	0.52
1:J:85:THR:OG1	1:J:166:CYS:SG	2.67	0.52
3:B:215:VAL:HG11	3:B:261:GLY:HA2	1.92	0.52
3:C:66:ARG:NH2	5:F:14:C:OP2	2.39	0.52
3:H:32:GLN:OE1	3:H:33:LYS:N	2.42	0.52
1:J:165:ARG:HH12	1:J:176:PHE:CB	2.21	0.52
2:A:84:LYS:NZ	2:A:85:PRO:O	2.39	0.52
3:D:195:LEU:O	3:D:209:PHE:HB2	2.09	0.52
3:N:34:ILE:HG22	3:N:42:ALA:HB3	1.90	0.52
3:N:116:ARG:NH1	5:F:35:A:O3’	2.43	0.52
3:O:103:ASP:O	3:O:108:LYS:NZ	2.41	0.52
3:O:260:LEU:HB3	3:O:287:PRO:HB3	1.90	0.52
1:J:364:PHE:O	1:J:367:GLN:NE2	2.42	0.52
3:I:242:ARG:HH22	3:I:248:SER:HA	1.75	0.52
3:C:246:THR:OG1	3:C:279:MET:SD	2.65	0.52
3:D:127:ALA:HA	3:D:167:PHE:HB3	1.91	0.52
8:K:86:GLN:OE1	8:K:86:GLN:N	2.40	0.52
2:A:66:LEU:HB3	2:A:207:ARG:HG2	1.90	0.52
3:D:11:LEU:HD23	3:D:231:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:ASN:HD21	3:H:176:LYS:HB3	1.75	0.52
3:B:3:ASN:N	3:B:301:VAL:OXT	2.42	0.52
3:O:54:ARG:HH12	3:O:68:ARG:HH22	1.57	0.52
3:H:260:LEU:HD12	3:H:264:LEU:HD12	1.91	0.52
3:I:4:LEU:HD22	3:I:220:PRO:HA	1.92	0.52
2:A:57:ARG:HH22	2:A:73:LEU:HB2	1.74	0.51
3:B:17:ALA:N	3:B:163:THR:O	2.41	0.51
3:C:267:LYS:O	3:C:272:GLN:NE2	2.43	0.51
3:D:44:ILE:HB	3:D:125:ALA:O	2.10	0.51
3:N:50:ARG:NH1	3:I:203:ALA:O	2.43	0.51
1:J:149:TRP:HE1	1:J:159:ARG:NH1	2.09	0.51
2:A:151:GLY:H	3:B:221:LYS:NZ	2.08	0.51
3:B:278:ALA:HB3	3:B:282:HIS:HE2	1.75	0.51
3:H:34:ILE:HG22	3:H:42:ALA:HB3	1.91	0.51
8:L:86:GLN:HG2	8:L:89:PHE:CE1	2.46	0.51
8:L:107:THR:HG23	8:L:108:LEU:HG	1.92	0.51
1:J:119:TYR:HB2	4:E:4:DT:O4	2.10	0.51
3:C:54:ARG:O	3:C:58:ILE:HG12	2.10	0.51
3:C:82:TYR:HB3	3:C:83:PRO:HD3	1.92	0.51
3:D:106:GLU:O	3:D:111:ASN:N	2.43	0.51
2:A:66:LEU:HD22	2:A:207:ARG:HE	1.74	0.51
3:B:283:LEU:HD13	3:B:289:LYS:NZ	2.25	0.51
3:N:231:PHE:HB3	3:N:238:LEU:HD23	1.93	0.51
8:L:19:ALA:HA	8:L:22:PHE:CD2	2.46	0.51
1:J:290:VAL:HG13	1:J:366:ARG:HD3	1.92	0.51
1:J:387:ARG:O	1:J:423:LYS:NZ	2.44	0.51
3:C:112:ARG:NH2	3:C:115:LYS:O	2.41	0.51
3:N:106:GLU:HB3	3:N:110:LEU:HB2	1.91	0.51
8:M:96:LEU:CA	8:M:101:ASP:HA	2.41	0.51
8:M:116:PRO:HA	8:M:118:LYS:HZ2	1.75	0.51
1:J:157:ALA:O	1:J:161:PRO:HG2	2.11	0.51
3:B:164:HIS:NE2	3:C:36:LYS:HA	2.25	0.51
3:C:223:VAL:HG12	3:C:225:GLY:H	1.76	0.51
8:L:66:ARG:HB3	8:L:73:ILE:CB	2.41	0.51
2:A:14:TYR:CB	2:A:134:GLY:HA2	2.41	0.51
7:P:36:DA:N6	8:K:87:ASP:OD2	2.44	0.51
3:B:117:ASP:OD1	3:B:117:ASP:N	2.44	0.51
3:C:95:GLY:HA2	3:C:116:ARG:CZ	2.41	0.51
3:I:212:ARG:HD2	3:I:263:GLU:HG3	1.92	0.51
3:D:162:VAL:HG23	3:H:34:ILE:HD12	1.93	0.51
3:N:242:ARG:HH22	3:N:248:SER:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:36:DA:N6	8:K:87:ASP:CB	2.72	0.51
1:J:198:GLY:HA3	6:G:57:DT:OP1	2.11	0.50
2:A:130:ASP:OD1	2:A:130:ASP:N	2.43	0.50
8:M:96:LEU:HG	8:M:101:ASP:HB3	1.92	0.50
3:N:218:LEU:HD13	3:N:224:ALA:HB3	1.93	0.50
3:N:272:GLN:NE2	3:N:275:GLN:OE1	2.44	0.50
8:K:16:TYR:HD2	8:L:90:VAL:HG13	1.76	0.50
3:C:65:ASN:O	3:C:84:ASN:ND2	2.45	0.50
3:D:44:ILE:HB	3:D:125:ALA:CA	2.41	0.50
3:H:127:ALA:HB1	3:H:165:THR:HG21	1.93	0.50
3:D:44:ILE:HG13	3:D:125:ALA:HB3	0.56	0.50
4:E:0:DA:H5'	4:E:1:DT:OP2	2.12	0.50
1:J:149:TRP:CZ3	1:J:162:PHE:CE2	2.85	0.50
1:J:332:ASN:CB	4:E:2:DG:N2	2.75	0.50
3:D:178:CYS:H	3:D:181:LYS:HB2	1.76	0.50
3:N:54:ARG:HH22	3:N:96:TYR:HE2	1.58	0.50
3:N:223:VAL:HG21	3:I:196:ASN:HD22	1.77	0.50
3:I:58:ILE:HD12	3:I:64:ASN:HD22	1.75	0.50
8:K:30:LYS:HG2	8:K:31:HIS:HD2	1.77	0.50
2:A:121:VAL:HG13	2:A:122:ARG:N	2.27	0.50
3:B:260:LEU:O	3:B:284:TYR:OH	2.22	0.50
3:D:44:ILE:CG2	3:D:125:ALA:HB3	2.41	0.50
8:K:57:ASN:O	8:K:61:LEU:HG	2.12	0.50
3:C:19:ASN:HD21	3:C:21:ARG:NH2	2.09	0.50
3:C:122:CYS:SG	3:C:123:ASN:N	2.85	0.50
3:O:64:ASN:HD21	3:O:91:ASP:HA	1.77	0.50
3:D:26:GLU:HB2	6:G:38:DG:H8	1.77	0.49
3:D:44:ILE:CG2	3:D:125:ALA:CB	2.90	0.49
3:H:256:ASN:OD1	3:H:257:GLU:N	2.45	0.49
3:C:11:LEU:HB3	3:C:168:GLN:HB3	1.94	0.49
3:D:107:MET:SD	3:D:108:LYS:NZ	2.73	0.49
3:B:123:ASN:HB3	3:B:170:PRO:HG2	1.94	0.49
3:D:246:THR:HB	3:D:255:ALA:HA	1.95	0.49
3:N:131:TYR:CZ	3:N:133:TYR:HB2	2.48	0.49
8:K:52:LYS:O	8:K:56:VAL:HG23	2.13	0.49
1:J:149:TRP:CH2	1:J:162:PHE:CG	2.99	0.49
3:B:215:VAL:HG11	3:B:262:GLY:H	1.77	0.49
3:D:116:ARG:NH2	5:F:17:C:O2'	2.30	0.49
3:O:177:ASP:OD1	3:O:177:ASP:N	2.46	0.49
3:I:34:ILE:HG22	3:I:42:ALA:HB3	1.94	0.49
3:B:147:SER:OG	3:B:149:TRP:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:96:LEU:HA	8:M:101:ASP:HA	1.94	0.49
8:M:96:LEU:HG	8:M:101:ASP:HA	1.91	0.49
3:B:73:ASP:OD1	3:B:73:ASP:N	2.46	0.49
3:H:70:HIS:ND1	3:I:115:LYS:HG3	2.27	0.49
1:J:42:TRP:HA	1:J:45:ILE:HD12	1.94	0.49
1:J:372:LEU:HB3	1:J:385:LEU:HD12	1.94	0.49
3:C:205:ALA:O	3:D:123:ASN:ND2	2.45	0.49
3:N:46:PRO:HD3	3:N:124:MET:HB3	1.95	0.49
3:H:233:ALA:O	3:H:234:GLU:HG3	2.13	0.49
3:C:233:ALA:HB3	3:C:236:ASN:HB2	1.95	0.49
3:N:231:PHE:HA	3:N:237:TRP:HB3	1.94	0.49
8:K:113:SER:HA	8:L:89:PHE:CE2	2.48	0.49
3:D:231:PHE:HA	3:D:237:TRP:HB3	1.95	0.49
3:D:279:MET:HG3	3:D:281:ALA:H	1.78	0.49
3:N:265:VAL:HG11	3:N:283:LEU:HG	1.95	0.49
5:F:7:C:O2'	5:F:8:U:OP1	2.23	0.49
3:I:120:PHE:C	3:I:121:ARG:HD3	2.29	0.49
3:I:220:PRO:HG2	3:I:256:ASN:HD21	1.78	0.49
3:I:231:PHE:HA	3:I:237:TRP:HB3	1.95	0.49
3:B:266:ARG:NE	3:B:284:TYR:O	2.46	0.48
1:J:165:ARG:NH1	1:J:176:PHE:CB	2.76	0.48
4:E:6:DA:H2'	4:E:7:DT:H73	1.95	0.48
1:J:454:LEU:O	1:J:458:HIS:ND1	2.40	0.48
2:A:14:TYR:HB2	2:A:134:GLY:HA2	1.94	0.48
3:H:178:CYS:H	3:H:181:LYS:HB2	1.78	0.48
3:C:196:ASN:HB3	3:D:223:VAL:HG11	1.95	0.48
3:C:270:GLN:HA	3:C:273:LYS:HE2	1.95	0.48
3:D:90:ASP:OD2	3:D:95:GLY:N	2.45	0.48
3:B:115:LYS:HD3	5:F:4:G:N1	2.28	0.48
3:N:147:SER:HA	3:O:79:PHE:CG	2.49	0.48
2:A:118:ILE:HB	5:F:8:U:C5	2.48	0.48
3:H:127:ALA:HA	3:H:167:PHE:HB3	1.96	0.48
8:M:81:TYR:HB2	8:M:82:PRO:HD3	1.96	0.48
2:A:121:VAL:O	2:A:122:ARG:HG3	2.13	0.48
3:C:243:LEU:HA	3:C:253:LEU:HD13	1.96	0.48
3:H:4:LEU:HB3	3:H:220:PRO:HA	1.96	0.48
1:J:290:VAL:HG11	1:J:370:LEU:HD13	1.96	0.48
1:J:421:THR:HA	1:J:531:ARG:HH21	1.79	0.48
3:B:112:ARG:HD3	3:B:114:ALA:H	1.77	0.48
3:B:198:VAL:HG11	3:B:209:PHE:CD2	2.48	0.48
3:O:108:LYS:HG3	3:O:109:LYS:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:262:GLY:CA	3:O:266:ARG:HH21	2.27	0.48
3:I:35:LEU:HB3	3:I:40:LYS:HG2	1.94	0.48
1:J:38:LYS:O	1:J:44:LYS:NZ	2.47	0.47
1:J:332:ASN:HB2	6:G:55:DC:C2	2.49	0.47
2:A:31:SER:O	2:A:33:ARG:NH1	2.47	0.47
3:D:32:GLN:HA	3:D:43:ILE:CD1	2.44	0.47
3:H:31:ILE:HG22	3:H:43:ILE:HG12	1.96	0.47
3:B:271:GLU:O	3:B:274:ALA:N	2.46	0.47
3:D:139:GLN:OE1	5:F:27:A:H5"	2.14	0.47
3:N:107:MET:SD	3:N:108:LYS:HG3	2.54	0.47
3:O:40:LYS:HD3	3:O:40:LYS:HA	1.63	0.47
3:C:19:ASN:HD22	3:C:44:ILE:HG13	1.78	0.47
3:D:56:MET:HE3	3:D:196:ASN:O	2.14	0.47
8:M:70:GLN:HA	8:M:73:ILE:HD12	1.95	0.47
1:J:60:ASP:OD1	1:J:63:GLY:N	2.47	0.47
1:J:119:TYR:CE1	4:E:4:DT:C7	2.96	0.47
2:A:169:LEU:HD13	5:F:2:G:C5	2.49	0.47
3:D:11:LEU:HD23	3:D:231:PHE:CD2	2.50	0.47
3:D:139:GLN:NE2	5:F:26:A:O2'	2.47	0.47
3:I:268:MET:O	3:I:273:LYS:NZ	2.48	0.47
3:C:162:VAL:HG23	3:D:34:ILE:HD12	1.95	0.47
3:C:232:ASP:O	3:C:236:ASN:N	2.48	0.47
3:D:168:GLN:NE2	3:D:232:ASP:OD2	2.48	0.47
1:J:165:ARG:NH2	1:J:176:PHE:HB3	2.30	0.47
1:J:418:GLN:O	1:J:421:THR:OG1	2.31	0.47
2:A:92:ASN:OD1	2:A:122:ARG:HG2	2.14	0.47
2:A:197:GLY:HA2	2:A:220:PRO:HD3	1.96	0.47
3:I:32:GLN:HG2	3:I:40:LYS:HB3	1.96	0.47
1:J:217:LEU:HD12	1:J:220:TRP:H	1.80	0.47
3:H:213:SER:HB3	3:H:263:GLU:HB3	1.97	0.47
8:M:55:VAL:O	8:M:58:GLU:HG3	2.15	0.47
8:M:102:GLU:O	8:M:102:GLU:HG3	2.15	0.47
1:J:160:ASN:HB3	1:J:161:PRO:CD	2.34	0.47
1:J:514:ASP:OD1	1:J:514:ASP:N	2.47	0.47
3:B:205:ALA:N	3:C:122:CYS:O	2.47	0.47
3:C:142:LEU:HD13	3:D:76:ALA:HB2	1.97	0.47
3:C:137:PHE:HZ	3:C:157:LEU:HD21	1.80	0.46
3:C:249:ASP:OD1	3:C:250:ASN:N	2.48	0.46
3:D:33:LYS:HG2	3:D:43:ILE:HG23	1.96	0.46
3:N:68:ARG:NH2	5:F:38:U:OP1	2.48	0.46
3:O:112:ARG:HA	3:O:115:LYS:HZ3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:244:THR:OG1	3:O:247:ASP:OD1	2.32	0.46
5:F:30:U:H5'	3:I:116:ARG:NE	2.30	0.46
3:H:35:LEU:HB3	3:H:40:LYS:HG2	1.97	0.46
3:C:57:LEU:HD12	3:C:62:GLN:HG2	1.97	0.46
8:K:34:GLN:NE2	8:K:36:SER:HB3	2.31	0.46
3:O:244:THR:N	3:O:277:GLU:OE2	2.47	0.46
8:K:48:TYR:OH	8:K:52:LYS:NZ	2.36	0.46
1:J:332:ASN:CB	6:G:55:DC:C2	2.98	0.46
2:A:14:TYR:O	2:A:177:GLU:HB3	2.15	0.46
3:B:66:ARG:NH2	5:F:7:C:O2'	2.46	0.46
3:B:157:LEU:HD23	3:B:157:LEU:H	1.80	0.46
3:C:242:ARG:C	3:C:253:LEU:HD22	2.36	0.46
3:D:256:ASN:OD1	3:D:257:GLU:N	2.48	0.46
1:J:332:ASN:HB3	4:E:2:DG:N2	2.31	0.46
3:D:267:LYS:HD2	3:D:267:LYS:O	2.15	0.46
3:N:106:GLU:O	3:N:111:ASN:N	2.48	0.46
3:N:202:HIS:CE1	3:N:207:TYR:H	2.34	0.46
3:H:218:LEU:HD13	3:H:224:ALA:HB3	1.97	0.46
3:H:265:VAL:HG11	3:H:283:LEU:HG	1.98	0.46
3:I:195:LEU:O	3:I:209:PHE:HB2	2.15	0.46
2:A:206:ASP:OD1	2:A:206:ASP:N	2.49	0.46
5:F:33:A:OP2	3:H:139:GLN:NE2	2.49	0.46
3:B:4:LEU:HB3	3:B:220:PRO:HG3	1.97	0.46
3:B:249:ASP:HB3	3:B:252:ASP:HB2	1.96	0.46
3:D:241:SER:HA	3:D:244:THR:HG22	1.96	0.46
3:N:110:LEU:HD13	3:N:112:ARG:HH21	1.81	0.46
3:H:120:PHE:O	3:H:121:ARG:CD	2.34	0.46
3:I:246:THR:HB	3:I:255:ALA:HA	1.98	0.46
3:D:44:ILE:HD11	3:D:167:PHE:CE2	2.51	0.46
3:N:67:THR:OG1	3:N:78:GLU:OE2	2.34	0.46
3:H:32:GLN:HB2	3:H:132:LYS:HE3	1.97	0.46
3:H:93:LEU:HB3	3:H:117:ASP:HB2	1.98	0.46
8:L:27:LEU:HG	8:L:114:GLN:HG2	1.98	0.46
8:L:63:ILE:HD12	8:L:77:VAL:HG22	1.98	0.46
1:J:18:LEU:HD13	1:J:23:HIS:HB3	1.98	0.46
1:J:122:ILE:CD1	1:J:163:ASN:CB	2.94	0.46
2:A:223:PHE:HZ	2:A:227:PRO:HA	1.81	0.46
3:B:58:ILE:HD12	3:B:64:ASN:HD21	1.81	0.46
3:B:49:MET:HE1	3:B:169:TYR:CE1	2.51	0.46
3:B:241:SER:OG	3:B:242:ARG:NH1	2.48	0.46
3:D:63:PRO:HG2	3:D:88:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:107:MET:SD	3:H:108:LYS:HG3	2.56	0.46
1:J:83:SER:O	1:J:166:CYS:HA	2.15	0.45
3:O:5:ASN:OD1	3:O:175:GLY:N	2.48	0.45
5:F:29:C:O2'	3:I:116:ARG:NH2	2.47	0.45
3:I:178:CYS:H	3:I:181:LYS:HB2	1.80	0.45
8:K:72:PHE:O	8:K:75:TYR:HB3	2.16	0.45
8:L:59:ALA:O	8:L:63:ILE:HG12	2.16	0.45
1:J:58:ASN:H	1:J:65:SER:HB2	1.81	0.45
3:B:30:VAL:HA	3:B:161:GLU:OE2	2.16	0.45
3:N:3:ASN:HD21	3:N:176:LYS:HB3	1.81	0.45
3:N:127:ALA:HB1	3:N:165:THR:HG21	1.99	0.45
3:O:232:ASP:CG	3:O:237:TRP:H	2.19	0.45
3:I:218:LEU:HD13	3:I:224:ALA:HB3	1.98	0.45
3:B:15:ALA:HB3	3:B:207:TYR:CE2	2.51	0.45
3:C:192:ILE:O	3:C:195:LEU:HD23	2.17	0.45
3:D:173:LEU:HD23	3:D:175:GLY:H	1.81	0.45
3:N:105:LYS:HB3	3:N:107:MET:HG3	1.98	0.45
2:A:181:LEU:HD13	2:A:224:ARG:HA	1.98	0.45
3:B:96:TYR:HE2	5:F:6:A:C8	2.34	0.45
3:I:6:LEU:HD23	3:I:6:LEU:H	1.82	0.45
3:I:221:LYS:HZ3	3:I:222:LEU:HB3	1.81	0.45
1:J:210:GLU:HA	2:A:98:TYR:OH	2.17	0.45
3:D:218:LEU:HD13	3:D:224:ALA:HB3	1.98	0.45
3:N:158:LEU:HD13	6:G:20:DA:C6	2.52	0.45
3:I:265:VAL:HA	3:I:268:MET:HE1	1.99	0.45
2:A:121:VAL:HG13	2:A:122:ARG:H	1.81	0.45
3:N:94:PHE:CE1	3:N:118:SER:HA	2.49	0.45
3:O:298:PHE:HD2	3:O:299:LEU:HD22	1.81	0.45
3:H:206:TYR:O	3:I:123:ASN:ND2	2.50	0.45
3:C:198:VAL:HG13	3:C:198:VAL:O	2.16	0.45
3:I:127:ALA:HA	3:I:167:PHE:HB3	1.99	0.45
8:M:53:GLU:O	8:M:57:ASN:ND2	2.49	0.45
1:J:122:ILE:CD1	1:J:163:ASN:HB2	2.46	0.45
1:J:256:ASP:HB3	1:J:321:GLY:H	1.80	0.45
2:A:66:LEU:HD23	2:A:207:ARG:H	1.81	0.45
3:C:284:TYR:HB2	3:C:290:LEU:HD12	1.99	0.45
3:H:11:LEU:HD23	3:H:231:PHE:CE2	2.52	0.45
3:H:143:ASN:HD21	3:H:150:LYS:HA	1.81	0.45
8:M:96:LEU:HG	8:M:101:ASP:CA	2.46	0.45
3:C:13:TYR:CZ	3:D:226:TYR:HB2	2.52	0.45
3:C:217:ARG:HB2	3:C:259:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:150:LYS:HA	3:N:150:LYS:HD3	1.73	0.45
3:I:173:LEU:HD23	3:I:175:GLY:N	2.32	0.45
8:L:18:ILE:HD11	8:L:86:GLN:HB2	1.99	0.45
1:J:119:TYR:CE2	4:E:4:DT:C5	3.04	0.44
3:H:182:PRO:HB3	3:H:299:LEU:HD21	1.99	0.44
3:H:237:TRP:HE3	3:H:238:LEU:HD22	1.82	0.44
3:H:93:LEU:HD11	3:H:181:LYS:HD2	2.00	0.44
8:L:52:LYS:HD3	8:L:52:LYS:HA	1.76	0.44
3:B:87:LYS:HE2	3:B:92:PHE:HZ	1.82	0.44
3:C:7:PHE:HZ	3:C:218:LEU:HD12	1.82	0.44
4:E:0:DA:N1	6:G:57:DT:C4	2.82	0.44
1:J:209:ALA:O	1:J:210:GLU:HB2	2.17	0.44
3:B:37:ASP:N	3:B:37:ASP:OD1	2.51	0.44
1:J:332:ASN:HB3	4:E:2:DG:H22	1.82	0.44
3:C:24:SER:OG	3:C:25:GLU:OE1	2.19	0.44
1:J:332:ASN:CB	4:E:2:DG:H22	2.30	0.44
2:A:184:TRP:CE2	2:A:227:PRO:HD3	2.52	0.44
3:D:44:ILE:CB	3:D:125:ALA:CA	2.96	0.44
3:N:147:SER:HA	3:O:79:PHE:CD2	2.53	0.44
5:F:38:U:O4	5:F:40:G:O2'	2.33	0.44
6:G:53:DA:H2'	6:G:54:DA:C8	2.53	0.44
8:M:53:GLU:HA	8:M:56:VAL:HG22	1.99	0.44
2:A:14:TYR:HB2	2:A:133:ILE:O	2.17	0.44
3:C:7:PHE:CZ	3:C:223:VAL:HG13	2.52	0.44
3:H:32:GLN:HG2	3:H:40:LYS:HD3	2.00	0.44
3:I:7:PHE:CE2	3:I:217:ARG:HB3	2.53	0.44
1:J:15:LEU:O	1:J:24:ARG:NH1	2.50	0.44
2:A:207:ARG:HH12	5:F:4:G:H5'	1.82	0.44
3:D:3:ASN:HD21	3:D:176:LYS:HB3	1.82	0.44
3:D:44:ILE:HG21	3:D:125:ALA:HB2	2.00	0.44
3:N:35:LEU:HB3	3:N:40:LYS:HG2	2.00	0.44
3:O:68:ARG:HD2	3:O:77:VAL:HG13	1.99	0.44
3:I:19:ASN:HD22	3:I:44:ILE:HG12	1.83	0.44
3:I:65:ASN:HD21	3:I:88:PHE:HZ	1.62	0.44
3:I:150:LYS:HA	3:I:150:LYS:HD3	1.68	0.44
3:D:127:ALA:HB1	3:D:165:THR:HG21	1.98	0.44
1:J:359:TYR:HD1	1:J:365:ARG:HB3	1.82	0.43
1:J:528:ASP:HA	1:J:532:SER:HB3	1.99	0.43
3:D:237:TRP:CE2	3:D:240:LEU:HD11	2.53	0.43
3:N:43:ILE:HG22	3:N:44:ILE:N	2.33	0.43
6:G:21:DC:H6	6:G:21:DC:H2'	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:107:MET:SD	3:I:108:LYS:HG3	2.58	0.43
8:L:43:LYS:HA	8:L:43:LYS:HD3	1.85	0.43
1:J:179:ASP:OD1	1:J:179:ASP:N	2.51	0.43
1:J:361:CYS:HB3	1:J:362:PRO:HD3	2.00	0.43
3:B:122:CYS:HB2	3:B:169:TYR:OH	2.18	0.43
3:H:218:LEU:HD23	3:H:256:ASN:HB3	1.99	0.43
3:C:100:GLN:NE2	3:C:101:THR:HG22	2.34	0.43
3:C:273:LYS:HA	3:C:276:LEU:HD12	1.99	0.43
3:D:31:ILE:O	3:D:43:ILE:CD1	2.66	0.43
3:D:182:PRO:HA	3:D:185:VAL:HG12	2.00	0.43
3:N:7:PHE:CE2	3:N:217:ARG:HB3	2.54	0.43
7:P:36:DA:N6	8:K:87:ASP:CG	2.72	0.43
1:J:210:GLU:N	2:A:98:TYR:CZ	2.87	0.43
3:B:100:GLN:H	3:B:100:GLN:HG3	1.72	0.43
3:B:144:ALA:HA	3:C:77:VAL:O	2.18	0.43
3:C:217:ARG:HG3	3:C:257:GLU:HB3	2.00	0.43
3:N:68:ARG:HA	3:N:77:VAL:HG12	2.01	0.43
5:F:8:U:O2'	5:F:9:U:OP1	2.29	0.43
3:H:162:VAL:HG23	3:I:34:ILE:HD12	2.00	0.43
3:I:7:PHE:HZ	3:I:218:LEU:HD12	1.82	0.43
3:I:63:PRO:HG2	3:I:88:PHE:HB2	1.99	0.43
8:K:114:GLN:O	8:K:114:GLN:HG3	2.18	0.43
8:L:64:ARG:HD3	8:L:64:ARG:HA	1.62	0.43
2:A:45:TYR:HE2	2:A:73:LEU:HD21	1.83	0.43
3:B:53:LEU:HD11	3:B:192:ILE:HG12	2.01	0.43
3:C:181:LYS:N	3:C:182:PRO:HD3	2.33	0.43
3:D:44:ILE:HG22	3:D:125:ALA:H	1.69	0.43
3:N:195:LEU:O	3:N:209:PHE:HB2	2.19	0.43
3:H:120:PHE:CD2	3:H:121:ARG:N	2.86	0.43
3:I:189:LEU:O	3:I:192:ILE:HG22	2.19	0.43
1:J:160:ASN:CB	1:J:161:PRO:CD	2.95	0.43
2:A:174:TYR:HA	2:A:175:PRO:HD3	1.86	0.43
3:D:31:ILE:C	3:D:43:ILE:CD1	2.86	0.43
3:O:86:ASP:N	3:O:86:ASP:OD1	2.51	0.43
1:J:240:ASP:OD1	1:J:244:LYS:N	2.51	0.43
1:J:451:LEU:HD12	1:J:454:LEU:HD11	2.00	0.43
3:D:84:ASN:ND2	3:D:87:LYS:HD3	2.33	0.43
3:N:13:TYR:CE1	3:N:212:ARG:HD3	2.54	0.43
3:H:231:PHE:HB3	3:H:238:LEU:HD23	2.01	0.43
3:I:182:PRO:HA	3:I:185:VAL:HG12	2.00	0.43
3:I:256:ASN:OD1	3:I:257:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:LYS:HB3	3:C:41:TYR:CD1	2.53	0.43
3:D:32:GLN:OE1	3:D:34:ILE:N	2.52	0.43
3:D:106:GLU:HB3	3:D:110:LEU:HB2	2.01	0.43
3:O:13:TYR:HD1	3:O:209:PHE:CG	2.37	0.43
3:D:189:LEU:O	3:D:192:ILE:HG22	2.18	0.43
3:H:43:ILE:HG22	3:H:44:ILE:N	2.34	0.43
3:I:137:PHE:HA	3:I:159:HIS:HB3	2.00	0.43
1:J:120:ASP:OD1	1:J:120:ASP:N	2.49	0.42
2:A:128:ASN:OD1	2:A:129:LEU:N	2.51	0.42
3:B:40:LYS:HB2	3:B:131:TYR:HB3	2.01	0.42
3:B:109:LYS:NZ	3:B:111:ASN:HB2	2.33	0.42
1:J:208:ASN:HB3	2:A:33:ARG:HH21	1.82	0.42
1:J:364:PHE:HZ	1:J:402:GLN:HG2	1.84	0.42
3:B:18:SER:HB2	3:B:202:HIS:CE1	2.54	0.42
3:N:247:ASP:OD1	3:N:248:SER:N	2.52	0.42
3:I:120:PHE:CD2	3:I:121:ARG:N	2.87	0.42
8:K:66:ARG:HA	8:K:66:ARG:HD2	1.94	0.42
3:B:18:SER:HB2	3:B:202:HIS:HE1	1.84	0.42
3:B:112:ARG:HH12	3:B:116:ARG:H	1.67	0.42
3:B:182:PRO:HB3	3:B:299:LEU:HD13	2.02	0.42
3:B:214:VAL:HG13	3:B:214:VAL:O	2.20	0.42
3:O:3:ASN:N	3:O:219:THR:O	2.52	0.42
3:O:70:HIS:HE2	5:F:44:G:H5”	1.84	0.42
3:I:31:ILE:HG22	3:I:43:ILE:HG12	2.01	0.42
3:I:68:ARG:HA	3:I:77:VAL:HG12	2.01	0.42
3:I:265:VAL:HG11	3:I:283:LEU:HG	2.01	0.42
8:K:28:SER:HB2	8:K:33:LEU:HD21	2.00	0.42
8:M:100:THR:O	8:M:101:ASP:CG	2.58	0.42
2:A:223:PHE:HZ	2:A:228:PRO:HD3	1.84	0.42
3:C:195:LEU:HB3	3:C:209:PHE:HB2	2.00	0.42
3:O:41:TYR:OH	3:O:129:ASN:O	2.34	0.42
3:H:139:GLN:HB3	3:H:157:LEU:HD13	2.02	0.42
3:H:173:LEU:HD23	3:H:175:GLY:N	2.34	0.42
3:H:239:GLU:HG2	3:H:240:LEU:N	2.34	0.42
1:J:205:MET:HG2	6:G:57:DT:P	2.59	0.42
3:C:53:LEU:HD11	3:C:192:ILE:HD13	2.01	0.42
3:D:217:ARG:NH1	3:D:226:TYR:O	2.53	0.42
3:D:265:VAL:HG11	3:D:283:LEU:HG	2.01	0.42
1:J:417:ARG:HA	1:J:420:PHE:HD2	1.83	0.42
3:D:34:ILE:CG2	3:D:42:ALA:HB3	2.49	0.42
3:D:68:ARG:NH1	5:F:20:G:N7	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:173:LEU:HD23	3:N:175:GLY:H	1.84	0.42
3:H:52:ALA:O	3:H:55:GLU:HG3	2.18	0.42
3:I:233:ALA:O	3:I:234:GLU:HG3	2.19	0.42
8:K:117:ILE:HG23	8:K:118:LYS:N	2.34	0.42
8:L:66:ARG:HB3	8:L:73:ILE:CD1	2.46	0.42
8:M:50:ASP:HB3	8:M:54:LYS:HZ1	1.84	0.42
2:A:25:ARG:NH1	5:F:3:A:O2'	2.49	0.42
2:A:93:GLN:N	2:A:93:GLN:OE1	2.53	0.42
3:B:131:TYR:CZ	3:B:133:TYR:HA	2.55	0.42
3:I:236:ASN:N	3:I:236:ASN:OD1	2.52	0.42
8:M:93:ALA:O	8:M:96:LEU:HB3	2.19	0.42
3:D:236:ASN:HB3	3:D:264:LEU:HD22	2.02	0.42
1:J:205:MET:O	1:J:207:VAL:HG13	2.20	0.42
3:B:217:ARG:HB2	3:B:258:PHE:HA	2.02	0.42
3:C:69:LEU:HG	3:C:71:SER:H	1.85	0.42
3:D:26:GLU:HB2	6:G:38:DG:C8	2.54	0.42
3:D:237:TRP:CE3	3:D:240:LEU:HD21	2.55	0.42
3:N:64:ASN:HD22	3:N:67:THR:HG22	1.85	0.42
3:O:258:PHE:H	3:O:280:GLY:HA3	1.85	0.42
3:I:93:LEU:HD22	3:I:119:ILE:HD12	2.02	0.42
8:M:50:ASP:HA	8:M:53:GLU:OE1	2.19	0.42
1:J:149:TRP:CD1	1:J:159:ARG:NH1	2.87	0.42
2:A:57:ARG:HD2	2:A:69:PRO:HD2	2.02	0.42
2:A:90:LEU:HA	2:A:124:GLU:HA	2.02	0.42
3:B:19:ASN:ND2	3:B:21:ARG:HD3	2.35	0.42
3:B:112:ARG:HH12	3:B:117:ASP:N	2.17	0.42
3:B:189:LEU:HD23	3:B:295:ALA:HB2	2.00	0.42
3:B:268:MET:SD	3:B:268:MET:N	2.93	0.42
3:N:54:ARG:HD2	3:N:66:ARG:HH21	1.83	0.42
3:N:57:LEU:HD23	3:N:57:LEU:HA	1.90	0.42
3:O:298:PHE:CD2	3:O:299:LEU:HD22	2.54	0.42
3:H:46:PRO:HD3	3:H:124:MET:HB3	2.01	0.42
1:J:27:LEU:O	1:J:30:LEU:HG	2.20	0.41
3:B:170:PRO:HB3	3:B:228:THR:HB	2.02	0.41
3:N:32:GLN:HG2	3:N:40:LYS:HD3	2.02	0.41
3:O:113:PRO:HD2	3:O:115:LYS:HZ3	1.85	0.41
3:O:231:PHE:CG	3:O:232:ASP:N	2.88	0.41
7:P:33:DA:H2"	7:P:34:DA:H5"	2.02	0.41
3:I:58:ILE:HD12	3:I:64:ASN:ND2	2.34	0.41
8:K:99:ASP:OD2	8:K:102:GLU:HB3	2.19	0.41
2:A:57:ARG:HE	2:A:68:LYS:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:19:ASN:HD21	3:B:21:ARG:NH1	2.18	0.41
3:H:241:SER:O	3:H:245:ALA:N	2.48	0.41
3:H:276:LEU:O	3:H:276:LEU:HD23	2.20	0.41
8:L:49:ASN:O	8:L:53:GLU:HG2	2.20	0.41
3:B:217:ARG:NH2	3:B:284:TYR:OH	2.49	0.41
3:H:221:LYS:HZ3	3:H:222:LEU:HG	1.85	0.41
3:I:127:ALA:HB1	3:I:165:THR:HG21	2.02	0.41
8:K:60:PHE:HE1	8:K:115:TYR:HE2	1.68	0.41
1:J:88:ARG:NH1	4:E:5:DT:OP1	2.53	0.41
3:B:90:ASP:OD2	3:B:93:LEU:N	2.51	0.41
3:D:8:ALA:HB3	3:D:171:PHE:CE1	2.55	0.41
3:D:35:LEU:HD23	3:D:35:LEU:H	1.85	0.41
3:N:221:LYS:HZ3	3:N:222:LEU:HG	1.85	0.41
3:H:195:LEU:O	3:H:209:PHE:HB2	2.21	0.41
8:K:9:ARG:HG3	8:K:11:TYR:H	1.85	0.41
8:K:30:LYS:HG2	8:K:31:HIS:CD2	2.56	0.41
2:A:27:PHE:HD2	2:A:28:GLN:HG2	1.85	0.41
2:A:72:GLU:O	2:A:72:GLU:HG2	2.20	0.41
2:A:91:ILE:HD12	2:A:93:GLN:HE22	1.84	0.41
3:B:44:ILE:O	3:B:124:MET:HG3	2.20	0.41
3:B:55:GLU:O	3:B:58:ILE:HG22	2.20	0.41
3:B:283:LEU:HD13	3:B:289:LYS:HZ3	1.85	0.41
3:N:116:ARG:NH1	5:F:35:A:O2'	2.49	0.41
4:E:3:DT:H2'	4:E:4:DT:H5'	2.02	0.41
5:F:26:A:C2	3:H:200:GLY:HA2	2.56	0.41
3:H:6:LEU:H	3:H:6:LEU:HD23	1.86	0.41
2:A:188:LEU:HD13	2:A:194:PRO:HB3	2.02	0.41
3:B:138:TYR:CD2	3:B:158:LEU:HB2	2.54	0.41
3:D:46:PRO:HB3	3:D:124:MET:N	2.35	0.41
3:D:265:VAL:HA	3:D:268:MET:HG2	2.03	0.41
3:N:34:ILE:HD13	3:I:162:VAL:HG23	2.02	0.41
3:N:189:LEU:O	3:N:192:ILE:HG22	2.20	0.41
3:O:49:MET:SD	3:O:49:MET:N	2.92	0.41
3:H:203:ALA:HA	3:I:121:ARG:HG3	2.03	0.41
3:I:106:GLU:OE1	3:I:110:LEU:HD13	2.20	0.41
2:A:77:ALA:HB3	2:A:136:GLN:HB3	2.02	0.41
2:A:107:PHE:HD1	2:A:116:TYR:HB2	1.86	0.41
3:B:10:ILE:HG22	3:B:214:VAL:HG23	2.02	0.41
3:C:127:ALA:HA	3:C:167:PHE:HB3	2.03	0.41
3:D:143:ASN:OD1	3:D:144:ALA:N	2.42	0.41
3:N:34:ILE:HD12	3:I:134:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:202:HIS:O	3:N:202:HIS:ND1	2.54	0.41
3:O:14:PRO:HD2	3:O:209:PHE:CD2	2.56	0.41
3:I:43:ILE:HG22	3:I:44:ILE:HG13	2.02	0.41
2:A:223:PHE:CZ	2:A:228:PRO:HD3	2.55	0.41
3:B:21:ARG:HA	3:B:21:ARG:HD2	1.87	0.41
3:B:112:ARG:HH11	3:B:114:ALA:HA	1.86	0.41
3:B:275:GLN:HG2	3:B:276:LEU:N	2.35	0.41
3:N:107:MET:HA	3:N:111:ASN:HA	2.03	0.41
3:O:33:LYS:HA	3:O:33:LYS:HD3	1.89	0.41
3:H:268:MET:SD	3:H:272:GLN:HB3	2.60	0.41
8:K:69:LYS:HA	8:K:74:ASP:HB3	2.02	0.41
8:L:63:ILE:O	8:L:66:ARG:CG	2.68	0.41
1:J:158:THR:O	1:J:162:PHE:N	2.37	0.41
3:B:105:LYS:O	3:B:107:MET:HE3	2.21	0.41
3:B:147:SER:HA	3:C:82:TYR:HD1	1.85	0.41
3:C:17:ALA:N	3:C:163:THR:O	2.49	0.41
3:C:256:ASN:HA	3:C:280:GLY:HA3	2.02	0.41
3:N:11:LEU:HD23	3:N:231:PHE:CD2	2.55	0.41
3:O:189:LEU:CD1	3:O:190:GLN:HG3	2.47	0.41
5:F:32:G:H4'	3:I:47:GLU:OE1	2.20	0.41
5:F:36:U:H2'	5:F:37:U:C6	2.56	0.41
3:I:212:ARG:HB2	3:I:263:GLU:HB2	2.02	0.41
8:M:27:LEU:HD21	8:M:35:TRP:HB3	2.03	0.41
8:M:71:ALA:HB1	8:M:104:ARG:HH21	1.86	0.41
1:J:296:LEU:HB3	1:J:352:TYR:HE1	1.86	0.41
3:C:7:PHE:CZ	3:C:218:LEU:HD12	2.56	0.41
3:D:9:THR:HG21	3:D:228:THR:O	2.21	0.41
3:O:93:LEU:HD21	3:O:119:ILE:H	1.86	0.41
4:E:-2:DC:H2"	4:E:-1:DC:C5	2.56	0.41
3:H:216:ALA:HB3	3:H:259:TRP:HB2	2.03	0.41
8:K:66:ARG:HH12	8:K:107:THR:C	2.24	0.41
2:A:115:LYS:C	5:F:7:C:H41	2.24	0.40
2:A:188:LEU:H	2:A:188:LEU:HD23	1.86	0.40
3:D:289:LYS:HE2	3:D:289:LYS:HB2	1.88	0.40
2:A:184:TRP:CG	2:A:227:PRO:HB3	2.56	0.40
3:N:115:LYS:HZ2	3:N:116:ARG:HG2	1.86	0.40
3:N:242:ARG:NH2	3:N:248:SER:HA	2.36	0.40
3:H:186:LYS:HB2	3:H:186:LYS:HE3	1.82	0.40
3:I:9:THR:HG21	3:I:228:THR:O	2.21	0.40
1:J:270:VAL:HG22	1:J:305:ARG:HG2	2.03	0.40
3:B:113:PRO:HG2	3:B:115:LYS:HZ2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:217:ARG:CZ	3:B:259:TRP:HB2	2.51	0.40
3:B:220:PRO:O	3:B:221:LYS:HD2	2.20	0.40
3:D:240:LEU:HA	3:D:243:LEU:HG	2.03	0.40
3:N:11:LEU:HD23	3:N:231:PHE:HE2	1.85	0.40
4:E:4:DT:H2"	4:E:5:DT:OP2	2.21	0.40
8:K:81:TYR:N	8:K:82:PRO:HD3	2.35	0.40
1:J:265:ASP:O	1:J:309:LYS:NZ	2.35	0.40
3:C:65:ASN:HD22	3:C:84:ASN:CG	2.25	0.40
3:C:259:TRP:CD2	3:C:294:LEU:HD21	2.57	0.40
3:N:127:ALA:HA	3:N:167:PHE:HB3	2.03	0.40
4:E:3:DT:H6	4:E:3:DT:H5"	1.86	0.40
3:H:64:ASN:OD1	3:H:64:ASN:N	2.51	0.40
3:H:134:ASP:OD2	3:I:34:ILE:HG13	2.21	0.40
3:H:236:ASN:OD1	3:H:236:ASN:N	2.54	0.40
3:I:242:ARG:HD3	3:I:258:PHE:CD2	2.57	0.40
1:J:122:ILE:HD13	1:J:163:ASN:CA	2.45	0.40
3:N:64:ASN:ND2	3:N:67:THR:HG22	2.35	0.40
3:N:139:GLN:HB3	3:N:157:LEU:HD13	2.04	0.40
3:N:289:LYS:HE2	3:N:289:LYS:HB2	1.96	0.40
3:O:93:LEU:CD2	3:O:119:ILE:H	2.35	0.40
3:H:68:ARG:HA	3:H:77:VAL:HG12	2.04	0.40
3:H:202:HIS:CE1	3:H:207:TYR:H	2.40	0.40
8:L:63:ILE:HG23	8:L:77:VAL:HG21	2.03	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	J	451/551 (82%)	430 (95%)	19 (4%)	2 (0%)	34 71
2	A	208/237 (88%)	189 (91%)	19 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	297/301 (99%)	271 (91%)	26 (9%)	0	100	100
3	C	297/301 (99%)	260 (88%)	37 (12%)	0	100	100
3	D	297/301 (99%)	268 (90%)	29 (10%)	0	100	100
3	H	297/301 (99%)	266 (90%)	30 (10%)	1 (0%)	41	75
3	I	297/301 (99%)	269 (91%)	27 (9%)	1 (0%)	41	75
3	N	297/301 (99%)	264 (89%)	32 (11%)	1 (0%)	41	75
3	O	231/301 (77%)	206 (89%)	25 (11%)	0	100	100
8	K	108/124 (87%)	100 (93%)	7 (6%)	1 (1%)	17	57
8	L	92/124 (74%)	83 (90%)	9 (10%)	0	100	100
8	M	108/124 (87%)	96 (89%)	12 (11%)	0	100	100
All	All	2980/3267 (91%)	2702 (91%)	272 (9%)	6 (0%)	50	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	209	ALA
1	J	207	VAL
8	K	117	ILE
3	N	44	ILE
3	H	44	ILE
3	I	44	ILE

5.3.2 Protein sidechains (i)

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	J	409/487 (84%)	403 (98%)	6 (2%)	65	84
2	A	185/204 (91%)	181 (98%)	4 (2%)	52	77
3	B	245/247 (99%)	243 (99%)	2 (1%)	81	91
3	C	245/247 (99%)	243 (99%)	2 (1%)	81	91
3	D	245/247 (99%)	244 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	245/247 (99%)	242 (99%)	3 (1%)	71 87
3	I	245/247 (99%)	244 (100%)	1 (0%)	91 97
3	N	245/247 (99%)	244 (100%)	1 (0%)	91 97
3	O	195/247 (79%)	191 (98%)	4 (2%)	53 78
8	K	101/113 (89%)	100 (99%)	1 (1%)	76 88
8	L	88/113 (78%)	87 (99%)	1 (1%)	73 88
8	M	101/113 (89%)	101 (100%)	0	100 100
All	All	2549/2759 (92%)	2523 (99%)	26 (1%)	77 88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	159	ARG
1	J	162	PHE
1	J	165	ARG
1	J	166	CYS
1	J	205	MET
1	J	303	LYS
2	A	98	TYR
2	A	102	ASN
2	A	105	LYS
2	A	193	ARG
3	B	90	ASP
3	B	108	LYS
3	C	87	LYS
3	C	289	LYS
3	D	267	LYS
3	N	121	ARG
3	O	87	LYS
3	O	186	LYS
3	O	204	ARG
3	O	273	LYS
3	H	121	ARG
3	H	242	ARG
3	H	267	LYS
3	I	121	ARG
8	K	54	LYS
8	L	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	J	163	ASN
1	J	208	ASN
2	A	82	GLN
2	A	97	ASN
3	C	19	ASN
3	C	65	ASN
3	C	84	ASN
3	C	139	GLN
3	D	129	ASN
3	D	272	GLN
3	N	65	ASN
3	O	3	ASN
3	O	51	ASN
8	K	31	HIS
8	L	20	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	F	43/44 (97%)	18 (41%)	3 (6%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	F	2	G
5	F	3	A
5	F	4	G
5	F	5	C
5	F	6	A
5	F	7	C
5	F	8	U
5	F	9	U
5	F	12	A
5	F	15	A
5	F	21	U
5	F	24	C
5	F	26	A
5	F	27	A
5	F	33	A
5	F	36	U
5	F	39	U

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Mol	Chain	Res	Type
5	F	42	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	F	5	C
5	F	7	C
5	F	8	U

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)

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.