



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 02:13 PM JST

PDB ID : 8ZOL / pdb\_00008zol  
EMDB ID : EMD-60297  
Title : Cryo-EM strcuture of Cas5-HNH Cascade,Conf3  
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.  
Deposited on : 2024-05-28  
Resolution : 2.55 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](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:

EMDB validation analysis : **FAILED**  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

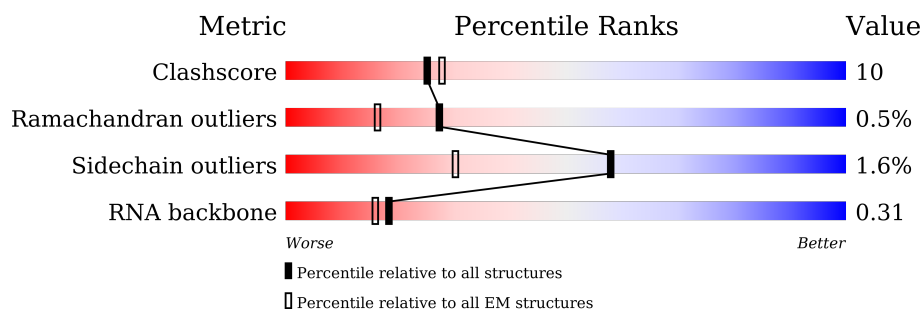
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.55 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	61	
2	F	378	
2	G	378	
2	H	378	
2	I	378	
2	J	378	
2	K	378	
3	B	388	

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Mol	Chain	Length	Quality of chain
4	D	272	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: a green segment on the left labeled '34%', a yellow segment in the middle labeled '7%', and a grey segment on the right labeled '59%'. The total length of the bar represents 100%.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19451 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	59	Total	C	N	O	P	0	0
			1258	562	225	413	58		

- Molecule 2 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	366	Total	C	N	O	S	0	0
			2797	1770	484	531	12		
2	H	367	Total	C	N	O	S	0	0
			2822	1778	494	538	12		
2	I	364	Total	C	N	O	S	0	0
			2775	1753	482	528	12		
2	J	365	Total	C	N	O	S	0	0
			2773	1749	483	529	12		
2	K	340	Total	C	N	O	S	0	0
			2591	1633	456	493	9		
2	G	258	Total	C	N	O	S	0	0
			1979	1259	342	370	8		

- Molecule 3 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	205	Total	C	N	O	S	0	0
			1591	1021	283	279	8		

- Molecule 4 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	112	Total	C	N	O	S	0	0
			865	562	155	147	1		

### 3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

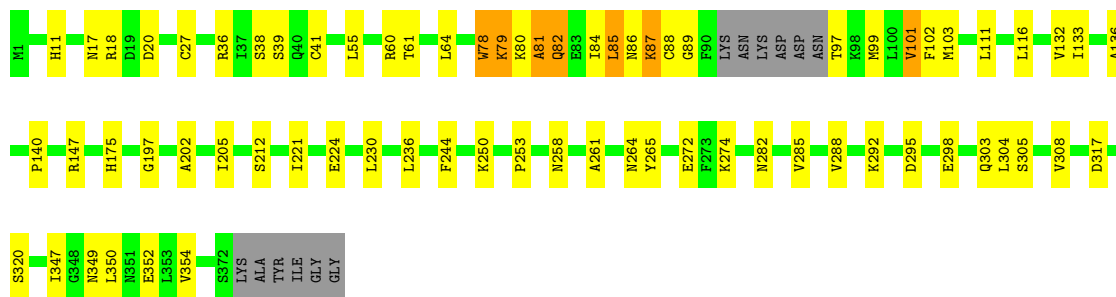
- Molecule 1: RNA (61-MER)

Chain A: 




- Molecule 2: CRISPR system Cascade subunit CasC

Chain F: 



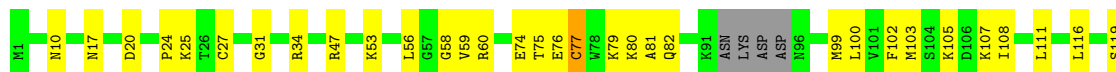
- Molecule 2: CRISPR system Cascade subunit CasC

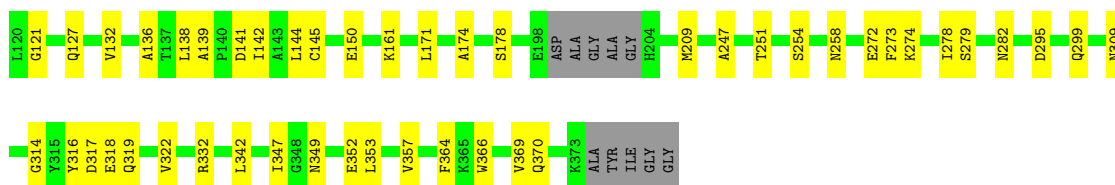
Chain H: 



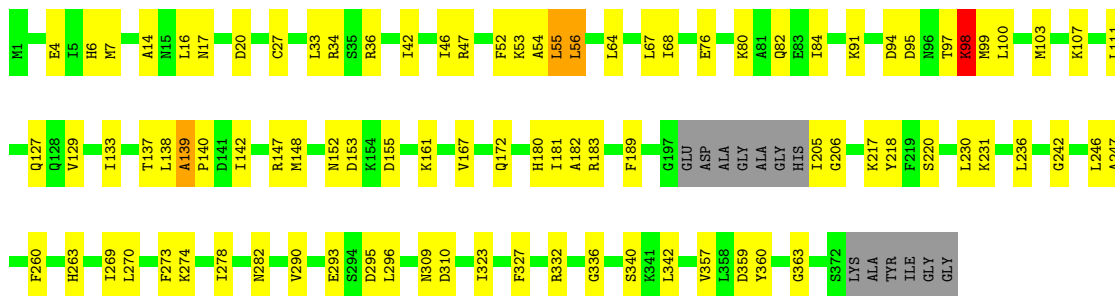
- Molecule 2: CRISPR system Cascade subunit CasC

Chain I: 

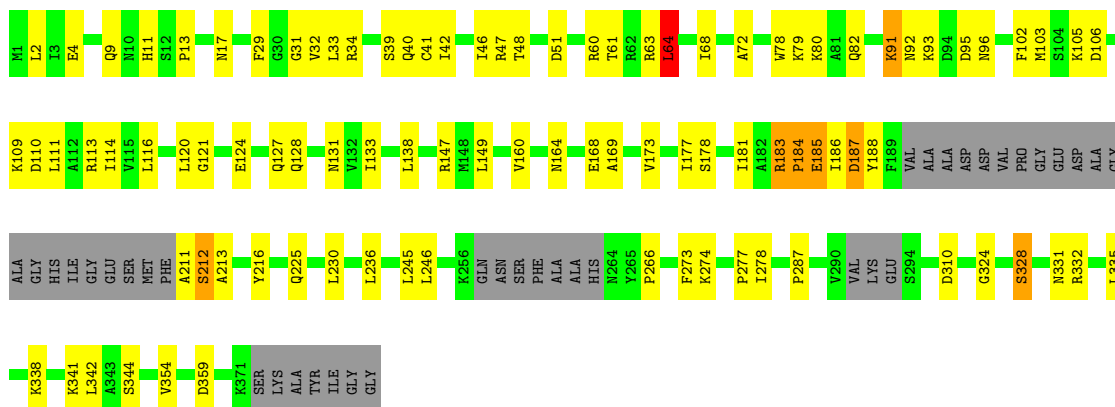




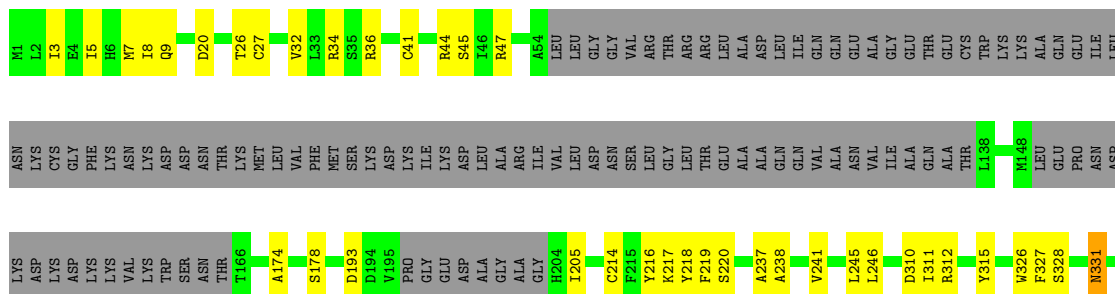
- Molecule 2: CRISPR system Cascade subunit CasC



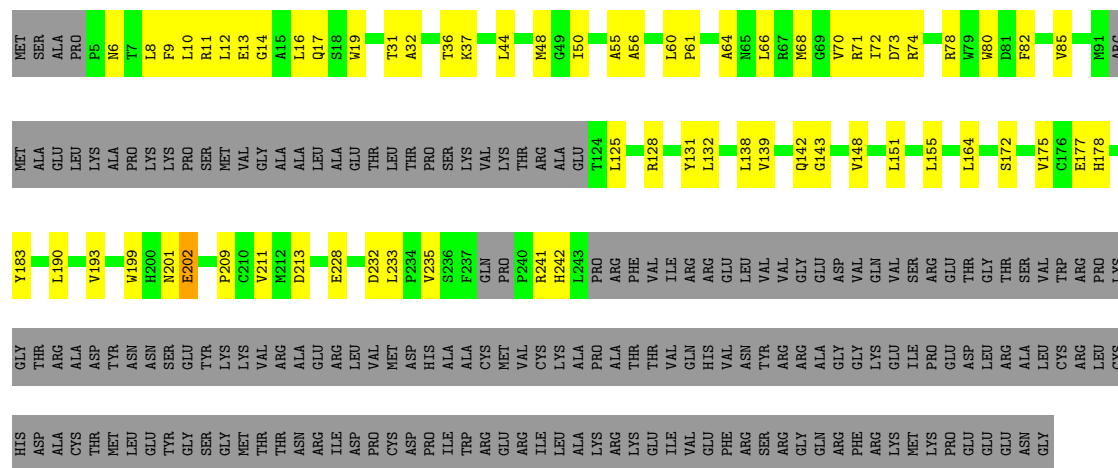
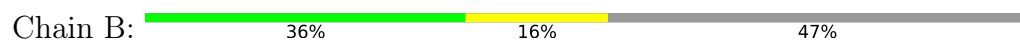
- Molecule 2: CRISPR system Cascade subunit CasC



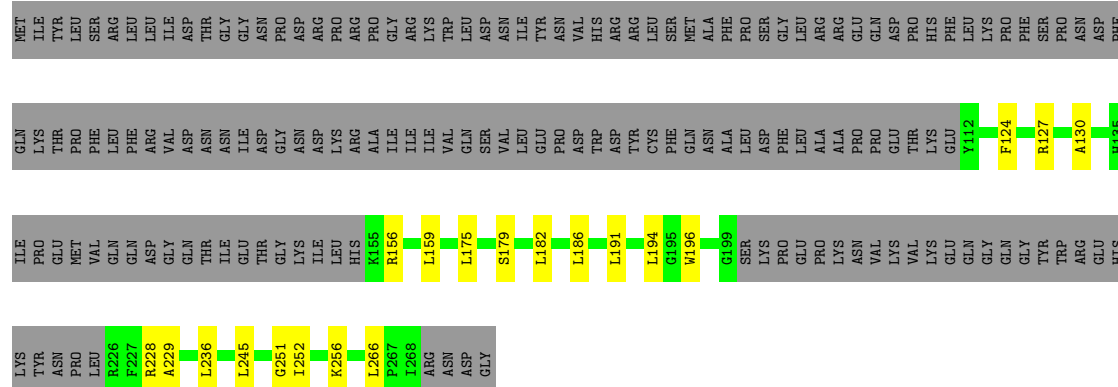
- Molecule 2: CRISPR system Cascade subunit CasC



- Molecule 3: CRISPR system Cascade subunit CasD



- Molecule 4: CRISPR-associated endoribonuclease Cse3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127239	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor



## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.16	0/1405	0.32	0/2187
2	F	0.36	2/2852 (0.1%)	0.51	4/3869 (0.1%)
2	G	0.20	0/2024	0.38	0/2748
2	H	0.18	0/2876	0.32	1/3898 (0.0%)
2	I	0.25	0/2830	0.35	0/3844
2	J	0.30	2/2826 (0.1%)	0.44	5/3836 (0.1%)
2	K	0.44	0/2638	0.60	7/3579 (0.2%)
3	B	0.15	0/1638	0.31	0/2231
4	D	0.16	0/883	0.27	0/1193
All	All	0.28	4/19972 (0.0%)	0.42	17/27385 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	54	ALA	CA-C	-6.84	1.43	1.52
2	F	86	ASN	CA-C	-6.62	1.44	1.53
2	F	78	TRP	CA-C	-6.35	1.46	1.53
2	J	55	LEU	CA-C	-5.23	1.46	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	84	ILE	N-CA-C	-13.97	95.78	111.00
2	F	88	CYS	N-CA-C	-9.39	101.08	112.54
2	J	100	LEU	N-CA-C	-8.35	97.94	109.71
2	F	81	ALA	N-CA-C	-7.84	101.55	112.45
2	K	187	ASP	N-CA-C	7.34	119.80	110.33
2	K	64	LEU	N-CA-C	-7.21	103.42	111.71
2	K	91	LYS	N-CA-C	-6.93	98.55	109.50
2	K	213	ALA	N-CA-C	6.91	119.67	109.24
2	K	177	ILE	N-CA-C	6.69	119.76	108.86
2	H	148	MET	CG-SD-CE	-6.43	86.76	100.90
2	K	80	LYS	N-CA-C	-6.03	104.63	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	54	ALA	CA-C-N	-5.97	114.28	122.87
2	J	54	ALA	C-N-CA	-5.97	114.28	122.87
2	J	54	ALA	N-CA-C	-5.43	107.02	113.97
2	J	98	LYS	N-CA-C	5.26	122.01	110.80
2	K	92	ASN	N-CA-C	5.26	118.74	109.80
2	F	82	GLN	N-CA-C	-5.04	106.96	113.01

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	A	1258	0	638	24	0
2	F	2797	0	2728	48	0
2	G	1979	0	1892	41	0
2	H	2822	0	2753	52	0
2	I	2775	0	2662	62	0
2	J	2773	0	2672	65	0
2	K	2591	0	2503	75	0
3	B	1591	0	1569	44	0
4	D	865	0	873	14	0
All	All	19451	0	18290	383	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 10.

All (383) 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)
2:K:13:PRO:CG	2:K:211:ALA:HB3	1.54	1.37
2:K:13:PRO:HG3	2:K:211:ALA:CB	1.77	1.12
2:K:13:PRO:HG3	2:K:212:SER:H	1.08	1.12
2:K:13:PRO:HG3	2:K:211:ALA:HB3	1.11	1.10
1:A:10:C:C2	2:H:148:MET:HE1	1.87	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:78:TRP:HE3	2:K:79:LYS:HD2	1.18	1.09
2:K:13:PRO:CB	2:K:211:ALA:HB3	1.83	1.07
2:K:79:LYS:HE3	2:K:79:LYS:CA	1.88	1.03
2:K:13:PRO:HB3	2:K:211:ALA:CB	1.92	1.00
2:K:79:LYS:HA	2:K:79:LYS:CE	1.92	0.99
2:K:79:LYS:HE3	2:K:79:LYS:HA	1.02	0.98
2:K:78:TRP:CE3	2:K:79:LYS:HD2	1.99	0.98
2:I:316:TYR:HE1	2:I:318:GLU:HG3	1.25	0.97
2:G:331:ASN:O	2:G:331:ASN:ND2	1.97	0.97
2:K:13:PRO:CB	2:K:211:ALA:CB	2.46	0.94
2:F:81:ALA:HB1	2:F:116:LEU:HD11	1.51	0.92
2:K:13:PRO:CG	2:K:211:ALA:CB	2.41	0.91
2:I:316:TYR:HD1	2:I:317:ASP:H	1.19	0.89
2:K:13:PRO:HG3	2:K:212:SER:N	1.87	0.89
2:K:13:PRO:CG	2:K:212:SER:H	1.86	0.88
2:I:316:TYR:OH	2:I:319:GLN:HB2	1.77	0.85
2:I:81:ALA:HB2	2:I:116:LEU:HD21	1.58	0.84
3:B:72:ILE:HB	3:B:209:PRO:HG2	1.57	0.84
1:A:10:C:O2	2:H:148:MET:HE1	1.77	0.84
2:K:328:SER:HB3	2:K:331:ASN:HA	1.60	0.82
2:I:353:LEU:O	2:I:357:VAL:HG23	1.79	0.81
2:J:91:LYS:HD3	2:J:98:LYS:HB2	1.61	0.81
2:I:47:ARG:HH12	2:I:60:ARG:HG3	1.44	0.81
3:B:155:LEU:HD21	3:B:175:VAL:HG12	1.60	0.81
2:I:316:TYR:CE1	2:I:318:GLU:HG3	2.14	0.80
3:B:17:GLN:HB3	3:B:164:LEU:HD13	1.63	0.80
2:K:13:PRO:HB3	2:K:211:ALA:HB3	1.55	0.80
2:G:358:LEU:HD12	2:G:364:PHE:HB2	1.64	0.79
2:K:78:TRP:CZ3	2:K:79:LYS:NZ	2.51	0.78
3:B:10:LEU:HB2	3:B:139:VAL:HB	1.66	0.76
2:H:110:ASP:O	2:H:114:ILE:HG22	1.86	0.75
2:I:316:TYR:HD1	2:I:317:ASP:N	1.86	0.74
2:G:7:MET:HE3	2:G:7:MET:C	2.13	0.73
3:B:12:LEU:HB3	3:B:164:LEU:HD21	1.71	0.73
2:K:121:GLY:N	2:K:124:GLU:OE2	2.22	0.72
2:J:129:VAL:O	2:J:133:ILE:HG13	1.89	0.72
2:I:103:MET:HE3	2:I:108:ILE:HB	1.71	0.71
1:A:10:C:C2	2:H:148:MET:CE	2.70	0.70
2:H:357:VAL:O	2:H:361:ILE:HG13	1.91	0.70
2:I:59:VAL:HG13	2:I:105:LYS:HG2	1.74	0.70
2:K:13:PRO:HB3	2:K:211:ALA:HB2	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:ASN:HA	2:H:172:GLN:HG2	1.73	0.69
2:J:52:PHE:HE1	2:J:55:LEU:HB2	1.55	0.69
2:K:78:TRP:HZ3	2:K:79:LYS:NZ	1.90	0.69
2:J:80:LYS:O	2:J:84:ILE:HG13	1.92	0.69
4:D:191:LEU:HD21	4:D:194:LEU:HB2	1.75	0.68
2:I:60:ARG:HH11	2:I:102:PHE:HB3	1.59	0.68
1:A:-4:A:H2'	1:A:-3:A:H8	1.58	0.68
2:G:34:ARG:HB3	2:G:178:SER:HB3	1.76	0.67
2:F:81:ALA:CB	2:F:116:LEU:HD11	2.24	0.67
2:J:137:THR:OG1	2:J:148:MET:SD	2.53	0.67
1:A:10:C:O2	2:H:148:MET:CE	2.42	0.66
3:B:48:MET:HE3	3:B:50:ILE:HD13	1.77	0.65
2:G:32:VAL:HG23	2:G:34:ARG:HE	1.62	0.65
3:B:6:ASN:ND2	3:B:142:GLN:OE1	2.31	0.64
3:B:60:LEU:HD23	3:B:61:PRO:HD3	1.79	0.64
2:H:91:LYS:HE3	2:H:93:LYS:HB3	1.78	0.64
2:F:11:HIS:HA	2:F:264:ASN:HD22	1.61	0.63
2:H:9:GLN:NE2	2:H:264:ASN:O	2.30	0.63
2:I:349:ASN:HB3	2:I:352:GLU:HG3	1.81	0.63
4:D:251:GLY:O	4:D:252:ILE:HD13	1.98	0.63
2:I:103:MET:CE	2:I:108:ILE:HB	2.29	0.63
2:G:26:THR:HG22	2:G:27:CYS:H	1.64	0.62
3:B:13:GLU:OE2	3:B:74:ARG:NH2	2.31	0.62
2:F:102:PHE:HB3	2:F:147:ARG:HD3	1.81	0.62
2:F:64:LEU:HD11	2:F:103:MET:HE1	1.81	0.62
3:B:201:ASN:O	3:B:202:GLU:HB3	2.00	0.61
2:K:4:GLU:HG3	2:K:274:LYS:HG3	1.82	0.61
2:F:111:LEU:HD23	2:F:132:VAL:HG22	1.82	0.61
2:K:78:TRP:CE3	2:K:79:LYS:CD	2.80	0.61
2:I:273:PHE:CZ	2:I:357:VAL:HG13	2.36	0.61
2:J:64:LEU:O	2:J:68:ILE:HG12	2.00	0.61
2:K:64:LEU:HD21	2:K:103:MET:HE1	1.83	0.61
2:K:188:TYR:HD2	4:D:266:LEU:HD13	1.64	0.61
2:F:224:GLU:N	2:F:224:GLU:OE1	2.33	0.61
2:I:247:ALA:O	2:I:251:THR:HG22	2.00	0.60
2:H:32:VAL:HG23	2:H:34:ARG:HE	1.65	0.60
2:F:261:ALA:HB3	2:H:174:ALA:HB2	1.83	0.60
3:B:11:ARG:NH1	3:B:73:ASP:OD2	2.34	0.60
2:J:263:HIS:CG	2:K:277:PRO:HB2	2.36	0.60
3:B:8:LEU:HB3	3:B:148:VAL:HG13	1.82	0.60
2:G:238:ALA:HB1	2:G:358:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:9:GLN:OE1	2:K:11:HIS:NE2	2.35	0.59
2:K:32:VAL:HG21	2:K:287:PRO:HG3	1.83	0.59
2:K:47:ARG:HG3	2:K:48:THR:HG23	1.83	0.59
2:H:358:LEU:HB3	2:H:364:PHE:HB2	1.83	0.59
2:G:5:ILE:HD12	2:G:219:PHE:HB2	1.83	0.59
3:B:44:LEU:HD22	3:B:151:LEU:HD22	1.85	0.59
2:J:46:ILE:HG23	2:J:247:ALA:CB	2.33	0.59
2:F:250:LYS:HA	2:F:265:TYR:CE1	2.38	0.58
2:I:273:PHE:HZ	2:I:357:VAL:HG13	1.67	0.58
2:F:282:ASN:O	2:F:285:VAL:HG23	2.03	0.58
2:J:127:GLN:OE1	2:J:161:LYS:N	2.36	0.58
2:I:47:ARG:HE	2:I:56:LEU:HD11	1.69	0.57
2:J:290:VAL:HG22	2:J:296:LEU:HD13	1.85	0.57
2:H:84:ILE:HD12	2:H:115:VAL:HG23	1.87	0.57
3:B:82:PHE:CD1	3:B:82:PHE:O	2.56	0.57
1:A:51:G:O6	4:D:156:ARG:NH2	2.38	0.57
2:F:347:ILE:HG21	2:F:352:GLU:HB3	1.85	0.57
2:H:93:LYS:NZ	2:H:94:ASP:OD1	2.37	0.57
2:J:27:CYS:HB3	2:J:36:ARG:HD3	1.85	0.57
2:K:127:GLN:O	2:K:131:ASN:ND2	2.38	0.57
1:A:7:C:H5	2:F:20:ASP:HA	1.67	0.57
2:H:62:ARG:HD3	2:H:98:LYS:HA	1.87	0.56
2:H:309:ASN:HB2	2:H:342:LEU:HD11	1.87	0.56
2:J:46:ILE:HG23	2:J:247:ALA:HB3	1.88	0.56
2:K:32:VAL:HG23	2:K:34:ARG:HE	1.70	0.56
2:K:91:LYS:HG3	2:K:96:ASN:HA	1.87	0.56
2:I:316:TYR:CD1	2:I:317:ASP:N	2.71	0.56
3:B:44:LEU:O	3:B:48:MET:HG3	2.06	0.56
2:I:100:LEU:HD22	2:I:102:PHE:HE1	1.71	0.56
2:J:273:PHE:HZ	2:J:357:VAL:HG13	1.70	0.56
3:B:228:GLU:OE2	3:B:228:GLU:N	2.39	0.55
2:K:9:GLN:HG3	2:K:266:PRO:HA	1.88	0.55
2:F:304:LEU:O	2:F:308:VAL:HG12	2.06	0.55
2:J:33:LEU:HD23	2:J:182:ALA:HB3	1.88	0.55
2:I:258:ASN:HA	2:J:172:GLN:HG2	1.89	0.55
2:J:189:PHE:HB3	2:K:40:GLN:HE22	1.72	0.55
1:A:30:G:O2'	2:K:41:CYS:SG	2.59	0.55
3:B:14:GLY:HA2	3:B:172:SER:HB2	1.89	0.55
2:F:272:GLU:HB3	2:F:274:LYS:HE2	1.88	0.55
2:I:10:ASN:HB3	2:J:282:ASN:HD21	1.70	0.55
2:K:110:ASP:HA	2:K:113:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:U:H1'	1:A:38:C:H5	1.70	0.55
2:J:172:GLN:HB2	2:J:220:SER:HB3	1.89	0.55
3:B:155:LEU:HD11	3:B:175:VAL:HG11	1.89	0.55
4:D:251:GLY:C	4:D:252:ILE:HD13	2.31	0.55
3:B:213:ASP:OD1	3:B:213:ASP:N	2.40	0.55
2:H:347:ILE:HG22	2:H:349:ASN:H	1.72	0.54
2:H:264:ASN:ND2	2:I:279:SER:OG	2.40	0.54
2:J:91:LYS:HG3	2:J:152:ASN:HB2	1.89	0.54
2:K:110:ASP:O	2:K:114:ILE:HD13	2.08	0.54
2:J:16:LEU:C	2:J:17:ASN:HD22	2.16	0.54
2:I:47:ARG:NH1	2:I:60:ARG:HG3	2.18	0.54
2:K:39:SER:HB2	2:K:173:VAL:HG13	1.90	0.54
1:A:10:C:N3	2:H:148:MET:HE1	2.18	0.53
2:F:250:LYS:NZ	2:H:318:GLU:OE2	2.37	0.53
2:J:14:ALA:HA	2:J:260:PHE:HB3	1.89	0.53
2:J:76:GLU:C	2:J:76:GLU:OE1	2.52	0.53
2:I:111:LEU:HD23	2:I:132:VAL:HG22	1.91	0.53
2:G:347:ILE:HG22	2:G:349:ASN:H	1.74	0.53
2:I:34:ARG:HB3	2:I:178:SER:HB2	1.89	0.53
2:F:27:CYS:HB3	2:F:36:ARG:HD3	1.89	0.52
2:J:97:THR:HG22	2:J:97:THR:O	2.09	0.52
2:G:327:PHE:HB2	2:G:353:LEU:HD13	1.92	0.52
2:F:347:ILE:HG22	2:F:349:ASN:H	1.74	0.52
2:J:293:GLU:OE1	2:J:293:GLU:N	2.42	0.52
2:J:290:VAL:HG21	2:K:31:GLY:HA3	1.91	0.52
2:I:127:GLN:OE1	2:I:161:LYS:N	2.38	0.52
2:J:94:ASP:O	2:J:95:ASP:OD1	2.27	0.52
2:F:212:SER:OG	2:H:28:TYR:O	2.25	0.52
2:K:106:ASP:O	2:K:109:LYS:NZ	2.42	0.52
1:A:31:C:N4	2:J:205:ILE:HD11	2.25	0.52
2:G:26:THR:HG22	2:G:27:CYS:N	2.24	0.52
3:B:11:ARG:NH2	3:B:138:LEU:HB2	2.25	0.51
2:J:4:GLU:OE1	2:J:218:TYR:OH	2.22	0.51
2:J:309:ASN:HB2	2:J:342:LEU:HD11	1.92	0.51
2:J:6:HIS:HB2	2:J:270:LEU:HB3	1.91	0.51
2:F:79:LYS:C	2:F:81:ALA:H	2.16	0.51
2:K:34:ARG:HB3	2:K:178:SER:HB3	1.91	0.51
3:B:6:ASN:ND2	3:B:183:TYR:O	2.43	0.51
3:B:56:ALA:HA	3:B:60:LEU:HD22	1.93	0.51
2:H:290:VAL:HG21	2:I:31:GLY:HA3	1.92	0.51
2:F:197:GLY:HA3	2:H:63:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:295:ASP:N	2:F:295:ASP:OD1	2.42	0.51
2:I:254:SER:O	2:I:254:SER:OG	2.22	0.51
2:I:76:GLU:HB3	2:I:116:LEU:HD23	1.94	0.50
2:K:324:GLY:O	2:K:344:SER:N	2.29	0.50
2:G:20:ASP:N	2:G:20:ASP:OD1	2.44	0.50
3:B:55:ALA:O	3:B:60:LEU:HD22	2.11	0.50
2:H:359:ASP:HA	2:H:363:GLY:HA2	1.94	0.50
2:I:272:GLU:OE1	2:I:274:LYS:NZ	2.36	0.50
1:A:-1:C:OP1	2:G:47:ARG:NH1	2.44	0.50
3:B:60:LEU:HD23	3:B:60:LEU:H	1.76	0.50
2:K:133:ILE:HG12	2:K:133:ILE:O	2.12	0.50
2:I:366:TRP:O	2:I:370:GLN:HB2	2.12	0.50
2:F:230:LEU:HD21	2:F:236:LEU:HD22	1.94	0.50
2:H:172:GLN:HB2	2:H:220:SER:OG	2.12	0.50
2:J:274:LYS:HD3	2:J:278:ILE:HD12	1.93	0.50
2:G:7:MET:HE3	2:G:7:MET:O	2.10	0.50
4:D:175:LEU:HD23	4:D:186:LEU:HD11	1.93	0.49
2:I:60:ARG:HD2	2:I:102:PHE:CD2	2.48	0.49
2:J:138:LEU:HG	2:J:139:ALA:H	1.77	0.49
2:J:153:ASP:O	2:J:155:ASP:N	2.43	0.49
2:G:326:TRP:NE1	2:G:328:SER:HB2	2.27	0.49
2:K:168:GLU:HB3	2:K:225:GLN:HE22	1.77	0.49
3:B:71:ARG:HB2	3:B:190:LEU:HD22	1.93	0.49
2:K:61:THR:HG22	2:K:63:ARG:H	1.78	0.49
2:K:230:LEU:HD13	2:K:236:LEU:HD23	1.95	0.49
2:I:17:ASN:HB3	2:I:25:LYS:HG3	1.95	0.49
2:H:261:ALA:HB3	2:I:174:ALA:HB2	1.95	0.48
2:G:347:ILE:HD13	2:G:353:LEU:HD12	1.94	0.48
2:I:20:ASP:N	2:I:20:ASP:OD1	2.45	0.48
2:J:111:LEU:HD22	2:J:129:VAL:HG12	1.94	0.48
2:K:127:GLN:HG3	2:K:131:ASN:HD21	1.78	0.48
2:I:60:ARG:HD2	2:I:102:PHE:CG	2.48	0.48
2:K:245:LEU:HD23	2:K:354:VAL:HG22	1.95	0.48
2:J:42:ILE:HG22	2:J:46:ILE:HD11	1.96	0.48
2:G:7:MET:HE1	2:G:9:GLN:HB2	1.95	0.48
2:F:292:LYS:NZ	2:F:292:LYS:HB3	2.29	0.48
2:I:141:ASP:O	2:I:145:CYS:HB2	2.14	0.48
2:G:27:CYS:HB3	2:G:36:ARG:CD	2.44	0.48
1:A:12:G:H2'	1:A:12:G:N3	2.29	0.48
2:K:102:PHE:HB3	2:K:147:ARG:HG3	1.96	0.48
2:F:317:ASP:OD2	2:F:320:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:144:LEU:HD22	2:H:171:LEU:HB2	1.96	0.47
3:B:9:PHE:HB2	3:B:178:HIS:HB2	1.96	0.47
2:K:128:GLN:HA	2:K:131:ASN:HD22	1.77	0.47
2:F:264:ASN:OD1	2:H:279:SER:OG	2.32	0.47
2:G:310:ASP:O	2:G:312:ARG:N	2.46	0.47
1:A:12:G:O2'	1:A:13:G:H4'	2.15	0.47
2:I:139:ALA:HB3	2:I:142:ILE:HG13	1.97	0.47
2:I:309:ASN:HA	2:I:342:LEU:HD11	1.97	0.47
2:J:183:ARG:NH1	2:K:31:GLY:HA2	2.30	0.47
2:G:216:TYR:CE1	2:G:218:TYR:HB2	2.50	0.47
4:D:127:ARG:HD3	4:D:229:ALA:HB1	1.97	0.47
1:A:7:C:C4	2:G:205:ILE:HD11	2.49	0.47
2:I:295:ASP:O	2:I:299:GLN:HG3	2.15	0.47
2:J:52:PHE:CE1	2:J:55:LEU:HB2	2.43	0.47
2:J:138:LEU:O	2:J:142:ILE:HB	2.15	0.47
2:J:82:GLN:OE1	2:J:82:GLN:O	2.33	0.47
2:K:120:LEU:HB3	2:K:124:GLU:OE2	2.14	0.47
2:K:359:ASP:OD1	2:K:359:ASP:C	2.58	0.47
2:H:311:ILE:HD12	2:H:315:TYR:OH	2.15	0.46
2:J:295:ASP:OD1	2:J:295:ASP:N	2.49	0.46
2:H:110:ASP:OD1	2:H:110:ASP:N	2.47	0.46
2:J:140:PRO:HA	2:J:230:LEU:HD21	1.95	0.46
1:A:22:U:H1'	2:J:147:ARG:HG2	1.97	0.46
2:I:81:ALA:HA	2:I:116:LEU:HD11	1.96	0.46
2:H:221:ILE:HD11	2:H:244:PHE:CD2	2.51	0.46
2:H:336:GLY:HA3	2:H:339:HIS:CD2	2.51	0.46
2:J:64:LEU:HD23	2:J:67:LEU:HD13	1.97	0.46
2:F:87:LYS:C	2:F:89:GLY:N	2.67	0.46
2:I:77:CYS:O	2:I:82:GLN:HB2	2.16	0.46
3:B:12:LEU:HD13	3:B:19:TRP:CZ2	2.51	0.46
1:A:31:C:OP1	2:K:17:ASN:ND2	2.49	0.46
1:A:-4:A:H2'	1:A:-3:A:C8	2.46	0.46
2:F:61:THR:OG1	2:G:193:ASP:OD1	2.33	0.46
1:A:8:G:N2	2:F:18:ARG:HH12	2.13	0.46
2:F:350:LEU:O	2:F:354:VAL:HG23	2.15	0.46
2:K:29:PHE:O	2:K:34:ARG:NH2	2.49	0.46
2:K:63:ARG:O	2:K:64:LEU:C	2.55	0.46
2:G:246:LEU:HD23	2:G:350:LEU:HD23	1.97	0.46
2:K:147:ARG:HD3	2:K:149:LEU:HD12	1.99	0.45
3:B:68:MET:H	3:B:213:ASP:CG	2.24	0.45
3:B:13:GLU:O	3:B:172:SER:N	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:2:LEU:O	2:K:273:PHE:HA	2.17	0.45
2:G:3:ILE:O	2:G:220:SER:HA	2.16	0.45
3:B:177:GLU:OE2	3:B:178:HIS:NE2	2.49	0.45
2:G:41:CYS:O	2:G:45:SER:HB3	2.17	0.45
4:D:124:PHE:HB3	4:D:236:LEU:HD22	1.99	0.45
2:H:10:ASN:ND2	2:I:282:ASN:OD1	2.39	0.45
2:K:60:ARG:HG3	2:K:102:PHE:CD1	2.52	0.45
3:B:233:LEU:O	3:B:242:HIS:HA	2.17	0.45
2:K:72:ALA:HB1	2:K:116:LEU:HD11	1.98	0.45
3:B:235:VAL:HB	3:B:241:ARG:HG2	2.00	0.44
2:I:10:ASN:HB3	2:J:282:ASN:ND2	2.32	0.44
2:J:189:PHE:CZ	2:J:206:GLY:HA3	2.52	0.44
2:J:269:ILE:HD13	2:J:327:PHE:CD2	2.52	0.44
2:K:51:ASP:HB3	2:K:246:LEU:HD23	1.98	0.44
2:G:327:PHE:HA	2:G:347:ILE:O	2.17	0.44
2:K:110:ASP:O	2:K:114:ILE:CD1	2.65	0.44
4:D:179:SER:HA	4:D:182:LEU:HD12	2.00	0.44
2:J:103:MET:SD	2:J:133:ILE:HG23	2.58	0.44
2:J:140:PRO:HG3	2:J:236:LEU:HD21	1.99	0.44
2:G:311:ILE:O	2:G:315:TYR:HB2	2.17	0.44
2:F:39:SER:OG	2:F:175:HIS:ND1	2.48	0.44
2:I:144:LEU:HD13	2:I:171:LEU:HD22	2.00	0.44
2:G:174:ALA:HB3	2:G:218:TYR:HB3	2.00	0.44
2:H:76:GLU:HB3	2:H:77:CYS:H	1.56	0.44
2:H:348:GLY:O	2:I:314:GLY:HA2	2.18	0.44
2:F:41:CYS:SG	2:F:253:PRO:HB3	2.58	0.43
2:F:221:ILE:HD11	2:F:244:PHE:CE2	2.53	0.43
2:I:74:GLU:CD	2:I:74:GLU:H	2.25	0.43
2:I:107:LYS:HD2	2:I:136:ALA:HA	2.00	0.43
2:K:274:LYS:NZ	2:K:278:ILE:HB	2.33	0.43
2:H:55:LEU:HD12	2:H:55:LEU:H	1.83	0.43
2:H:59:VAL:HG13	2:H:105:LYS:HG3	2.00	0.43
2:H:358:LEU:HD23	2:H:361:ILE:HD12	1.99	0.43
2:H:366:TRP:O	2:H:370:GLN:HG3	2.17	0.43
3:B:37:LYS:NZ	3:B:64:ALA:O	2.39	0.43
1:A:37:U:H6	1:A:38:C:H41	1.65	0.43
2:H:336:GLY:HA3	2:H:339:HIS:HD2	1.83	0.43
2:I:58:GLY:H	2:I:105:LYS:HE3	1.82	0.43
2:J:20:ASP:N	2:J:20:ASP:OD1	2.49	0.43
2:J:359:ASP:HA	2:J:363:GLY:HA2	2.00	0.43
2:K:164:ASN:OD1	2:K:164:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:A:N7	2:H:205:ILE:HD11	2.34	0.43
2:I:209:MET:HE2	2:I:209:MET:HB3	1.74	0.43
2:I:79:LYS:O	2:I:80:LYS:C	2.62	0.43
2:G:326:TRP:CE2	2:G:335:LEU:HB2	2.54	0.43
2:J:148:MET:HE2	2:J:167:VAL:HG22	2.00	0.43
2:G:326:TRP:CE2	2:G:328:SER:HB2	2.53	0.43
2:F:60:ARG:HA	2:F:101:VAL:O	2.18	0.43
2:H:103:MET:HE3	2:H:103:MET:HB2	1.90	0.43
2:K:169:ALA:O	2:K:225:GLN:NE2	2.41	0.43
2:G:7:MET:HB3	2:G:217:LYS:HB2	2.01	0.43
2:G:36:ARG:NH1	3:B:16:LEU:HD11	2.34	0.43
2:F:55:LEU:HB3	2:F:140:PRO:HG2	2.00	0.43
2:G:27:CYS:SG	2:G:34:ARG:HB2	2.59	0.43
3:B:66:LEU:HG	3:B:143:GLY:HA3	2.01	0.43
3:B:80:TRP:HB3	3:B:128:ARG:NH2	2.34	0.43
2:F:103:MET:SD	2:F:133:ILE:HG12	2.59	0.42
3:B:70:VAL:HB	3:B:211:VAL:HG23	2.01	0.42
4:D:251:GLY:HA3	4:D:256:LYS:HD3	2.01	0.42
1:A:13:G:C5	2:F:205:ILE:HD11	2.54	0.42
2:F:17:ASN:ND2	2:F:38:SER:HB3	2.33	0.42
2:I:332:ARG:HB2	2:J:310:ASP:OD2	2.19	0.42
2:J:332:ARG:HD2	2:K:310:ASP:OD2	2.19	0.42
2:K:184:PRO:HB2	2:K:185:GLU:H	1.68	0.42
2:F:79:LYS:HB2	2:F:79:LYS:HE2	1.34	0.42
2:F:85:LEU:HD23	2:F:85:LEU:HA	1.80	0.42
2:H:358:LEU:HA	2:H:361:ILE:HD12	2.01	0.42
2:I:99:MET:HE1	2:I:150:GLU:C	2.44	0.42
2:I:364:PHE:HB3	2:I:369:VAL:HG21	2.00	0.42
2:K:105:LYS:HB2	2:K:105:LYS:HE2	1.65	0.42
2:G:44:ARG:HA	2:G:47:ARG:HB3	2.00	0.42
2:J:242:GLY:O	2:J:246:LEU:HG	2.20	0.42
2:J:269:ILE:HD13	2:J:327:PHE:CE2	2.54	0.42
2:J:138:LEU:HD22	2:J:231:LYS:HZ2	1.84	0.42
1:A:41:C:H2'	1:A:42:A:C8	2.54	0.42
2:J:336:GLY:HA3	2:J:340:SER:O	2.19	0.42
2:K:183:ARG:HE	2:K:183:ARG:HB3	1.68	0.42
2:G:7:MET:SD	2:G:8:ILE:N	2.92	0.42
2:F:82:GLN:HA	2:F:85:LEU:HB2	2.02	0.42
2:F:103:MET:HB2	2:F:136:ALA:HB3	2.01	0.42
2:G:7:MET:C	2:G:7:MET:CE	2.89	0.42
2:K:111:LEU:HD23	2:K:111:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:245:LEU:HD12	4:D:245:LEU:HA	1.86	0.42
2:H:62:ARG:HG3	2:H:100:LEU:HG	2.02	0.42
2:H:185:GLU:OE2	2:I:27:CYS:HA	2.20	0.42
2:J:107:LYS:H	2:J:107:LYS:HG2	1.68	0.42
2:J:323:ILE:HD12	2:J:360:TYR:HE2	1.84	0.42
2:H:180:HIS:CD2	2:H:296:LEU:HD21	2.55	0.42
2:J:342:LEU:HD23	2:J:342:LEU:HA	1.86	0.42
2:H:64:LEU:HD12	2:H:101:VAL:HG11	2.02	0.41
2:H:335:LEU:HD12	2:H:335:LEU:HA	1.82	0.41
2:I:53:LYS:HB2	2:I:53:LYS:HE3	1.85	0.41
2:I:274:LYS:HE2	2:I:278:ILE:HD12	2.02	0.41
2:K:33:LEU:HD12	2:K:33:LEU:HA	1.90	0.41
2:F:288:VAL:HG22	2:F:303:GLN:NE2	2.36	0.41
2:J:7:MET:HE3	2:J:217:LYS:HD3	2.02	0.41
3:B:31:THR:OG1	3:B:32:ALA:N	2.53	0.41
4:D:130:ALA:HB1	4:D:159:LEU:HB3	2.03	0.41
2:K:138:LEU:HD12	2:K:138:LEU:HA	1.88	0.41
1:A:13:G:N1	2:F:202:ALA:O	2.39	0.41
2:F:87:LYS:HB3	2:F:87:LYS:HE3	1.75	0.41
2:F:265:TYR:HD2	2:H:315:TYR:CZ	2.39	0.41
2:J:47:ARG:HE	2:J:56:LEU:HD21	1.85	0.41
4:D:252:ILE:O	4:D:252:ILE:HG22	2.21	0.41
3:B:78:ARG:HA	3:B:131:TYR:O	2.20	0.41
3:B:199:TRP:CZ2	3:B:202:GLU:HB2	2.56	0.41
2:I:17:ASN:O	2:I:24:PRO:HA	2.21	0.41
2:I:136:ALA:O	2:I:138:LEU:N	2.54	0.41
2:I:317:ASP:N	2:I:317:ASP:OD1	2.54	0.41
2:K:42:ILE:O	2:K:46:ILE:HG12	2.21	0.41
2:K:78:TRP:CZ3	2:K:79:LYS:CD	3.04	0.41
3:B:85:VAL:HB	3:B:125:LEU:HB3	2.03	0.41
2:F:305:SER:HA	2:F:308:VAL:CG1	2.51	0.41
2:J:180:HIS:ND1	2:J:181:ILE:O	2.38	0.41
2:G:338:LYS:HG3	2:G:339:HIS:H	1.86	0.41
3:B:128:ARG:HG3	3:B:128:ARG:HH11	1.86	0.41
4:D:196:TRP:HE1	4:D:228:ARG:HH11	1.67	0.41
2:F:295:ASP:OD1	2:F:298:GLU:HB3	2.21	0.40
2:H:99:MET:SD	2:H:151:PRO:HA	2.61	0.40
2:H:307:TYR:O	2:H:311:ILE:HG12	2.21	0.40
2:I:347:ILE:HG21	2:I:352:GLU:HB2	2.03	0.40
2:G:178:SER:HA	2:G:214:CYS:O	2.21	0.40
2:H:102:PHE:HD2	2:H:147:ARG:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:ARG:HD3	2:J:180:HIS:O	2.21	0.40
2:I:119:SER:O	2:I:121:GLY:N	2.52	0.40
3:B:36:THR:HB	3:B:232:ASP:HB2	2.02	0.40
3:B:71:ARG:NH1	3:B:193:VAL:O	2.30	0.40
2:J:147:ARG:HG3	2:J:147:ARG:O	2.21	0.40
2:K:64:LEU:O	2:K:68:ILE:HD12	2.22	0.40
2:G:237:ALA:O	2:G:241:VAL:HG23	2.22	0.40
2:G:245:LEU:HD12	2:G:245:LEU:HA	1.88	0.40
2:G:365:LYS:HE2	2:G:365:LYS:HB2	1.84	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	
2	F	362/378 (96%)	339 (94%)	23 (6%)	0	100	100
2	G	250/378 (66%)	221 (88%)	28 (11%)	1 (0%)	30	40
2	H	363/378 (96%)	336 (93%)	27 (7%)	0	100	100
2	I	358/378 (95%)	322 (90%)	34 (10%)	2 (1%)	22	29
2	J	361/378 (96%)	324 (90%)	35 (10%)	2 (1%)	22	29
2	K	332/378 (88%)	294 (89%)	33 (10%)	5 (2%)	8	11
3	B	199/388 (51%)	185 (93%)	13 (6%)	1 (0%)	25	34
4	D	106/272 (39%)	105 (99%)	1 (1%)	0	100	100
All	All	2331/2928 (80%)	2126 (91%)	194 (8%)	11 (0%)	27	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	98	LYS

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Mol	Chain	Res	Type
2	K	184	PRO
3	B	202	GLU
2	I	77	CYS
2	K	95	ASP
2	G	361	ILE
2	K	212	SER
2	I	322	VAL
2	K	342	LEU
2	K	160	VAL
2	J	139	ALA

### 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	
2	F	292/313 (93%)	284 (97%)	8 (3%)	40	57
2	G	205/313 (66%)	203 (99%)	2 (1%)	73	84
2	H	298/313 (95%)	297 (100%)	1 (0%)	91	96
2	I	287/313 (92%)	286 (100%)	1 (0%)	91	96
2	J	286/313 (91%)	282 (99%)	4 (1%)	62	77
2	K	268/313 (86%)	254 (95%)	14 (5%)	19	27
3	B	163/322 (51%)	162 (99%)	1 (1%)	84	92
4	D	87/238 (37%)	87 (100%)	0	100	100
All	All	1886/2438 (77%)	1855 (98%)	31 (2%)	58	75

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	78	TRP
2	F	79	LYS
2	F	80	LYS
2	F	85	LEU
2	F	87	LYS

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Mol	Chain	Res	Type
2	F	97	THR
2	F	99	MET
2	F	101	VAL
2	H	110	ASP
2	I	75	THR
2	J	53	LYS
2	J	56	LEU
2	J	98	LYS
2	J	99	MET
2	K	64	LEU
2	K	82	GLN
2	K	93	LYS
2	K	181	ILE
2	K	183	ARG
2	K	185	GLU
2	K	186	ILE
2	K	187	ASP
2	K	216	TYR
2	K	328	SER
2	K	332	ARG
2	K	335	LEU
2	K	338	LYS
2	K	341	LYS
2	G	331	ASN
2	G	365	LYS
3	B	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	264	ASN
2	F	299	GLN
2	F	306	ASN
2	H	339	HIS
2	I	9	GLN
2	I	257	GLN
2	I	264	ASN
2	J	86	ASN
2	J	299	GLN
2	J	351	ASN
2	K	6	HIS
2	K	70	GLN

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Mol	Chain	Res	Type
2	K	118	ASN
2	K	131	ASN
2	K	252	ASN
2	K	264	ASN
2	K	275	ASN
2	K	309	ASN
2	K	331	ASN
2	G	349	ASN
3	B	200	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/61 (93%)	18 (31%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	0	G
1	A	1	G
1	A	5	G
1	A	6	C
1	A	7	C
1	A	13	G
1	A	18	U
1	A	19	A
1	A	20	G
1	A	23	G
1	A	25	G
1	A	26	C
1	A	28	U
1	A	29	A
1	A	31	C
1	A	38	C
1	A	45	C
1	A	52	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.