



## Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 02:28 PM JST

PDB ID : 8ZM3 / pdb\_00008zm3  
EMDB ID : EMD-60235  
Title : Cryo-EM strcuture of Cas5-HNH Cascade,apo-Conf2  
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.  
Deposited on : 2024-05-22  
Resolution : 3.10 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:

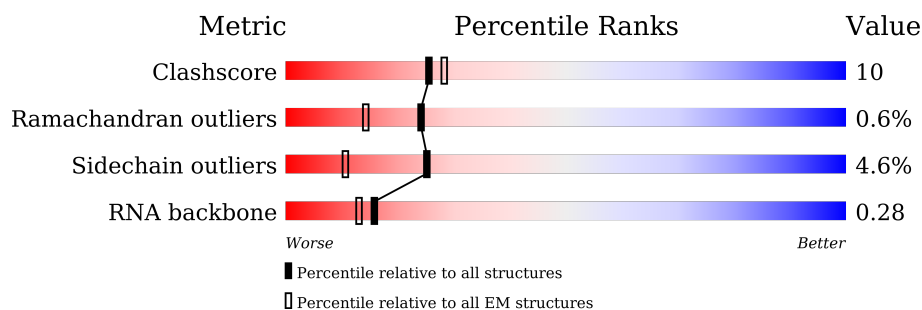
EMDB validation analysis : **FAILED**  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation 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 3.10 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	44% 43% 10% .
2	C	535	64% 19% 17%
3	E	174	75% 18% . 5%
4	F	378	80% 17% .
4	G	378	53% 13% 34%
4	H	378	78% 19% .
4	I	378	77% 19% .
4	J	378	72% 24% . .

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Mol	Chain	Length	Quality of chain
4	K	378	<div><div></div><div>37%37%15%•10%</div></div>
5	B	388	<div><div></div><div>75%22%••</div></div>
6	D	272	<div><div></div><div>78%20%•</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26938 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-associated protein Cse1 (CRISPR\_cse1).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	442	Total	C	N	O	S	0	0
			3476	2233	594	630	19		

- Molecule 3 is a protein called CRISPR-associated protein Cse2 (CRISPR\_cse2).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	165	Total	C	N	O	S	0	0
			1352	875	238	233	6		

- Molecule 4 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	367	Total	C	N	O	S	0	0
			2799	1772	485	530	12		
4	H	367	Total	C	N	O	S	0	0
			2833	1787	495	539	12		
4	I	364	Total	C	N	O	S	0	0
			2781	1760	484	525	12		
4	J	367	Total	C	N	O	S	0	0
			2804	1772	488	532	12		
4	K	341	Total	C	N	O	S	0	0
			2624	1660	463	490	11		
4	G	251	Total	C	N	O	S	0	0
			1919	1222	334	355	8		

- Molecule 5 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	378	Total	C	N	O	S	0	0
			2955	1866	546	522	21		

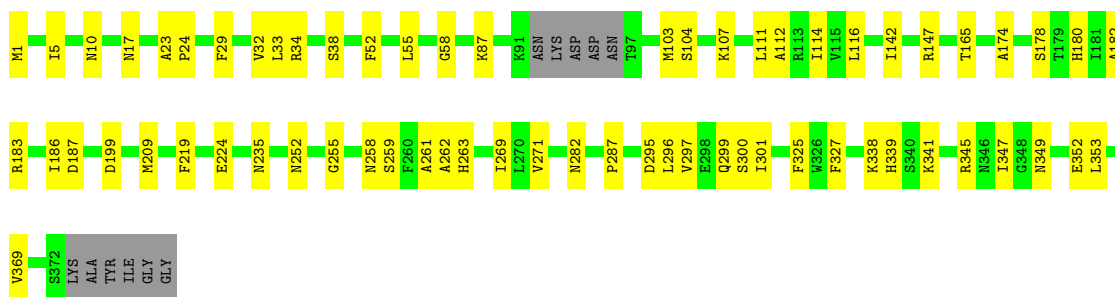
- Molecule 6 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	268	Total	C	N	O	S	0	0
			2135	1369	383	379	4		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

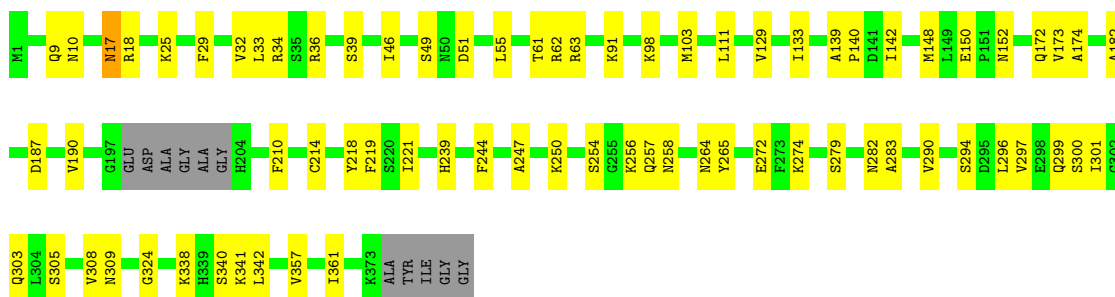
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	





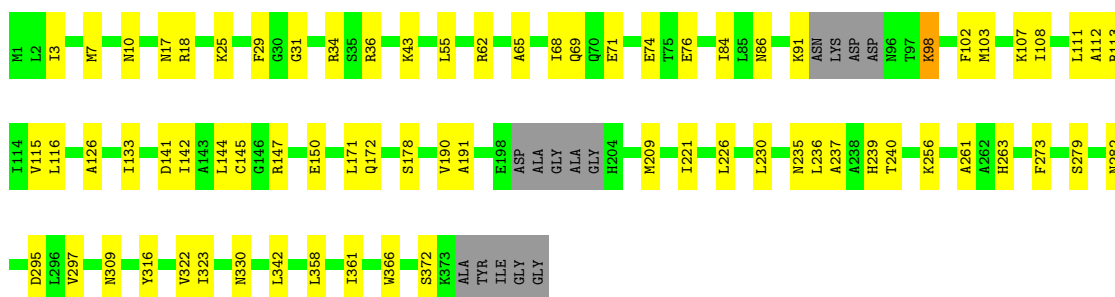
- Molecule 4: CRISPR system Cascade subunit CasC

Chain H: 78% 19%



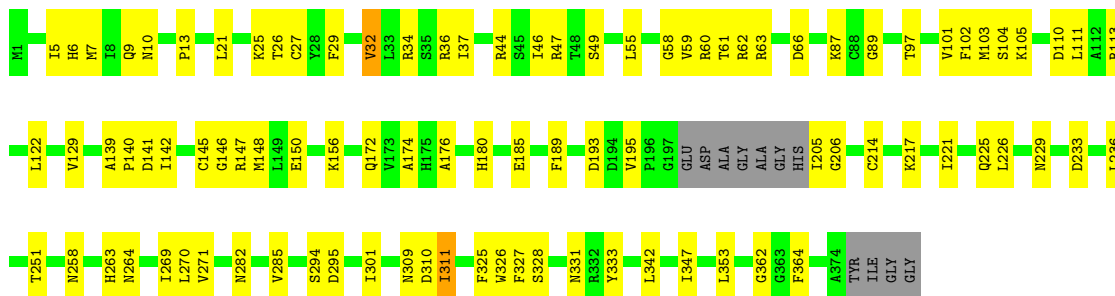
- Molecule 4: CRISPR system Cascade subunit CasC

Chain I: 77% 19%



- Molecule 4: CRISPR system Cascade subunit CasC

Chain J: 72% 24%



- Molecule 4: CRISPR system Cascade subunit CasC



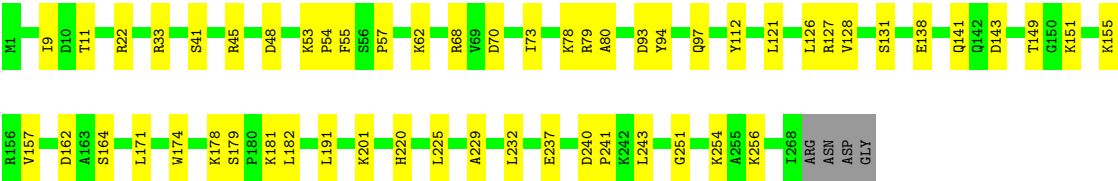


● Molecule 6: CRISPR-associated endoribonuclease Cse3

Chain D: 

78%

20%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20320	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

### 5.1 Standard geometry

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

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	0.43	0/2187
2	C	0.23	0/3575	0.50	0/4871
3	E	0.31	0/1382	0.59	1/1862 (0.1%)
4	F	0.23	0/2854	0.48	2/3872 (0.1%)
4	G	0.25	0/1960	0.51	2/2658 (0.1%)
4	H	0.18	0/2888	0.43	0/3913
4	I	0.26	0/2836	0.57	1/3848 (0.0%)
4	J	0.20	0/2858	0.51	0/3876
4	K	0.67	0/2670	1.17	29/3609 (0.8%)
5	B	0.25	0/3028	0.53	2/4107 (0.0%)
6	D	0.23	0/2193	0.52	0/2976
All	All	0.30	0/27649	0.60	37/37779 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	129	VAL	N-CA-C	-15.75	97.21	112.96
4	K	280	TYR	N-CA-C	-11.56	99.51	112.57
4	K	39	SER	N-CA-C	-11.24	99.61	113.20
4	K	235	ASN	N-CA-C	-10.70	99.40	111.71
4	K	181	ILE	N-CA-C	-10.12	96.53	109.58
4	K	19	ASP	N-CA-C	9.12	120.82	108.23
4	K	225	GLN	N-CA-C	-8.75	101.21	114.16
4	K	80	LYS	N-CA-C	-8.20	103.42	113.50
4	K	66	ASP	N-CA-C	-8.02	102.52	111.82
4	G	209	MET	CG-SD-CE	-7.92	83.47	100.90
4	K	126	ALA	N-CA-C	-7.40	103.29	111.36
4	K	111	LEU	N-CA-C	-6.94	104.07	112.54
4	K	12	SER	N-CA-C	6.91	121.11	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	253	PRO	CA-N-CD	-6.43	102.99	112.00
4	K	223	TRP	N-CA-C	6.29	124.20	110.80
5	B	303	ALA	N-CA-C	-6.24	102.83	110.31
4	K	138	LEU	N-CA-C	6.19	120.73	111.81
4	K	77	CYS	N-CA-C	6.17	118.22	108.79
4	K	62	ARG	N-CA-C	-6.10	104.00	112.30
4	G	329	PRO	CA-N-CD	-6.04	103.54	112.00
4	K	180	HIS	N-CA-C	6.04	117.41	108.60
4	K	137	THR	N-CA-C	5.83	120.08	113.15
4	K	297	VAL	N-CA-C	-5.82	107.07	112.83
4	K	26	THR	N-CA-C	5.80	118.17	108.02
4	K	301	ILE	N-CA-C	5.79	121.38	109.34
4	K	253	PRO	N-CD-CG	-5.60	94.81	103.20
4	I	98	LYS	CA-CB-CG	5.57	125.23	114.10
4	K	189	PHE	N-CA-C	-5.50	105.37	112.68
5	B	272	LYS	CB-CG-CD	5.49	123.92	111.30
4	F	87	LYS	CA-CB-CG	5.49	125.07	114.10
4	K	128	GLN	N-CA-C	-5.45	106.64	113.72
3	E	85	MET	CG-SD-CE	-5.44	88.93	100.90
4	K	79	LYS	N-CA-C	-5.40	106.57	112.72
4	K	290	VAL	N-CA-C	5.33	115.57	108.27
4	F	341	LYS	CA-CB-CG	5.14	124.37	114.10
4	K	105	LYS	N-CA-C	5.12	117.30	109.62
4	K	11	HIS	N-CA-C	5.05	116.96	109.69

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1258	0	638	26	0
2	C	3476	0	3376	62	0
3	E	1352	0	1387	25	0
4	F	2799	0	2728	42	0
4	G	1919	0	1852	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2833	0	2771	52	0
4	I	2781	0	2689	46	0
4	J	2804	0	2723	77	0
4	K	2624	0	2582	133	0
5	B	2955	0	2967	63	0
6	D	2135	0	2096	37	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
All	All	26938	0	25809	531	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 (531) 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)
4:G:185:GLU:O	4:G:209:MET:HG3	1.27	1.30
4:K:102:PHE:HB3	4:K:147:ARG:HG2	1.50	0.92
4:J:263:HIS:HB2	4:K:279:SER:H	1.39	0.87
1:A:30:G:H4'	4:K:41:CYS:HA	1.57	0.85
4:K:127:GLN:HA	4:K:130:ALA:HB3	1.56	0.85
1:A:42:A:H2	1:A:48:G:H1	1.20	0.83
4:K:17:ASN:HB3	4:K:25:LYS:HG3	1.63	0.80
4:K:147:ARG:HD3	4:K:148:MET:H	1.46	0.80
4:K:236:LEU:HD12	4:K:372:SER:HB3	1.63	0.79
4:J:29:PHE:O	4:J:34:ARG:NH1	2.16	0.78
4:J:62:ARG:HH21	4:J:97:THR:H	1.31	0.77
4:K:15:ASN:HB3	4:K:255:GLY:HA3	1.67	0.77
4:K:239:HIS:CD2	4:K:372:SER:HB2	2.20	0.76
4:K:239:HIS:HD2	4:K:372:SER:HB2	1.52	0.75
4:I:62:ARG:HD2	4:I:98:LYS:HB2	1.69	0.73
4:J:7:MET:HB2	4:J:217:LYS:HB2	1.71	0.73
4:G:41:CYS:O	4:G:45:SER:HB3	1.89	0.72
4:K:298:GLU:OE2	4:K:301:ILE:HD11	1.90	0.72
4:K:60:ARG:HG3	4:K:102:PHE:HB2	1.72	0.72
2:C:237:ILE:HG12	2:C:329:VAL:HG21	1.71	0.70
4:F:252:ASN:ND2	4:F:262:ALA:O	2.24	0.70
4:H:305:SER:O	4:H:309:ASN:ND2	2.25	0.70
4:K:183:ARG:HH21	4:K:213:ALA:HB2	1.57	0.69
2:C:199:HIS:O	5:B:121:ARG:NH2	2.26	0.68
4:K:38:SER:HB2	4:K:41:CYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:A:N1	1:A:48:G:O6	2.27	0.68
2:C:470:LYS:HE2	2:C:477:TYR:HB2	1.75	0.68
4:K:269:ILE:HB	4:K:327:PHE:HB3	1.75	0.68
4:I:68:ILE:HG22	4:I:76:GLU:HG3	1.75	0.67
4:K:298:GLU:OE2	4:K:301:ILE:CD1	2.41	0.67
3:E:151:PRO:HA	3:E:154:ARG:HB2	1.76	0.67
5:B:309:GLN:HE21	5:B:333:HIS:HA	1.59	0.67
4:G:27:CYS:HB3	4:G:36:ARG:HD3	1.75	0.67
5:B:8:LEU:HB3	5:B:148:VAL:HG13	1.76	0.67
4:J:263:HIS:HB2	4:K:279:SER:N	2.10	0.67
5:B:299:MET:HE3	5:B:326:ARG:HD2	1.77	0.67
4:K:71:GLU:HG2	4:K:109:LYS:NZ	2.09	0.66
4:F:33:LEU:HG	4:F:182:ALA:HB3	1.78	0.66
4:J:13:PRO:CG	4:K:29:PHE:HB2	2.25	0.66
4:K:55:LEU:HB3	4:K:140:PRO:HG2	1.76	0.66
1:A:-4:A:H2'	1:A:-3:A:H8	1.61	0.66
4:J:58:GLY:HA2	4:J:104:SER:HA	1.77	0.65
4:H:264:ASN:ND2	4:I:279:SER:OG	2.30	0.65
4:J:5:ILE:HG23	4:J:7:MET:HE3	1.79	0.65
4:K:33:LEU:O	4:K:181:ILE:HA	1.96	0.65
5:B:233:LEU:HB3	5:B:243:LEU:HB3	1.78	0.65
4:J:221:ILE:HD11	4:J:226:LEU:HD22	1.78	0.64
6:D:9:ILE:HB	6:D:80:ALA:HB3	1.79	0.63
4:F:261:ALA:HB3	4:H:174:ALA:HB2	1.81	0.63
4:I:358:LEU:HD23	4:I:361:ILE:HD12	1.81	0.63
4:K:29:PHE:CE2	4:K:285:VAL:HA	2.34	0.63
2:C:123:ASP:OD1	2:C:225:ARG:NH2	2.32	0.62
4:K:176:ALA:HB2	4:K:217:LYS:HG3	1.82	0.62
4:K:183:ARG:NH2	4:K:213:ALA:HB2	2.14	0.62
4:K:27:CYS:HB3	4:K:36:ARG:HD3	1.81	0.62
4:H:290:VAL:HG21	4:I:31:GLY:HA3	1.82	0.62
4:I:10:ASN:ND2	4:J:282:ASN:OD1	2.32	0.62
4:H:9:GLN:NE2	4:H:264:ASN:O	2.32	0.61
4:G:25:LYS:NZ	5:B:82:PHE:O	2.33	0.61
4:K:284:PHE:CZ	4:K:300:SER:HA	2.35	0.61
4:K:101:VAL:HA	4:K:149:LEU:HD21	1.81	0.61
4:I:65:ALA:HA	4:I:68:ILE:HD12	1.82	0.61
2:C:367:ALA:HB1	2:C:461:GLU:HG3	1.83	0.61
4:J:13:PRO:HD3	4:K:29:PHE:CD1	2.36	0.61
3:E:85:MET:HE1	3:E:127:LEU:HD13	1.82	0.61
4:J:37:ILE:HB	4:J:176:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:185:GLU:O	4:G:209:MET:CG	2.23	0.60
4:I:144:LEU:HD11	4:I:240:THR:HG21	1.83	0.60
4:J:328:SER:HB3	4:J:331:ASN:HA	1.82	0.60
4:K:110:ASP:HA	4:K:113:ARG:HB2	1.83	0.60
2:C:120:ASN:ND2	2:C:194:GLU:OE1	2.34	0.60
4:F:282:ASN:OD1	4:G:264:ASN:ND2	2.35	0.60
4:J:263:HIS:HB2	4:K:278:ILE:HA	1.82	0.60
4:K:176:ALA:HB1	4:K:215:PHE:HB3	1.84	0.60
4:J:195:VAL:HG21	4:K:67:LEU:HD11	1.85	0.59
2:C:177:PHE:HB3	2:C:223:LEU:HD13	1.85	0.59
4:J:145:CYS:SG	4:J:146:GLY:N	2.72	0.59
4:J:264:ASN:ND2	4:K:282:ASN:HB2	2.17	0.59
4:K:2:LEU:HD23	4:K:277:PRO:HD3	1.85	0.59
4:G:209:MET:HG2	4:G:210:PHE:N	2.18	0.59
2:C:93:VAL:HA	2:C:99:PRO:HA	1.85	0.59
4:K:74:GLU:HB2	4:K:116:LEU:HD12	1.84	0.59
2:C:138:CYS:O	2:C:142:THR:HB	2.02	0.58
4:H:62:ARG:HD2	4:H:98:LYS:HA	1.85	0.58
4:J:26:THR:O	4:J:36:ARG:NH1	2.36	0.58
4:J:180:HIS:HE1	4:J:214:CYS:H	1.49	0.58
4:K:35:SER:OG	4:K:178:SER:HB2	2.03	0.58
2:C:362:ASP:OD1	2:C:437:LYS:NZ	2.31	0.58
4:J:87:LYS:HZ2	4:J:122:LEU:HB3	1.69	0.58
4:J:233:ASP:OD1	4:J:236:LEU:N	2.33	0.58
4:F:187:ASP:OD1	4:H:25:LYS:NZ	2.34	0.58
5:B:233:LEU:HD22	5:B:243:LEU:HD23	1.85	0.58
4:K:2:LEU:CD2	4:K:277:PRO:HD3	2.34	0.57
5:B:257:ASP:OD1	5:B:257:ASP:N	2.36	0.57
4:F:1:MET:N	4:F:224:GLU:OE1	2.36	0.57
4:K:283:ALA:HB2	4:K:307:TYR:CD2	2.39	0.57
4:I:108:ILE:O	4:I:112:ALA:HB3	2.05	0.57
4:F:147:ARG:NH2	4:F:165:THR:OG1	2.38	0.57
4:I:34:ARG:HG2	4:I:178:SER:HB2	1.86	0.57
6:D:138:GLU:HG3	6:D:151:LYS:HE2	1.87	0.57
2:C:490:LEU:CD2	2:C:513:ILE:HA	2.35	0.57
5:B:10:LEU:HD21	5:B:44:LEU:HD21	1.86	0.57
4:K:37:ILE:HB	4:K:176:ALA:H	1.70	0.57
6:D:171:LEU:HD23	6:D:232:LEU:HD21	1.86	0.57
1:A:23:G:H1'	4:I:191:ALA:HB2	1.87	0.56
4:H:139:ALA:HB3	4:H:142:ILE:HG13	1.87	0.56
4:K:29:PHE:HE2	4:K:284:PHE:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:57:GLY:HA2	4:K:105:LYS:HG2	1.86	0.56
4:G:7:MET:HB3	4:G:217:LYS:HB2	1.87	0.56
4:G:270:LEU:HB2	4:G:326:TRP:HD1	1.70	0.56
5:B:66:LEU:HD23	5:B:141:LEU:HB3	1.87	0.56
4:K:37:ILE:HG13	4:K:176:ALA:HB3	1.88	0.56
4:K:328:SER:HB3	4:K:331:ASN:HA	1.87	0.56
4:G:47:ARG:NH2	4:G:146:GLY:O	2.35	0.56
5:B:90:ARG:HG2	5:B:122:ALA:HB2	1.87	0.56
4:H:29:PHE:HB3	4:H:34:ARG:HG3	1.87	0.55
2:C:171:GLY:O	2:C:175:ARG:NH1	2.37	0.55
5:B:287:ARG:NH2	5:B:306:THR:O	2.40	0.55
4:H:308:VAL:HG12	4:H:342:LEU:HD22	1.89	0.55
4:K:144:LEU:HB3	4:K:171:LEU:HD23	1.89	0.55
4:G:186:ILE:HG12	4:G:209:MET:HB2	1.87	0.55
2:C:459:HIS:HD2	2:C:489:LEU:HD11	1.72	0.55
4:I:141:ASP:O	4:I:145:CYS:HB3	2.07	0.55
4:K:60:ARG:HB2	4:K:102:PHE:HD1	1.72	0.55
4:J:263:HIS:CB	4:K:278:ILE:HA	2.37	0.54
4:G:7:MET:HG2	4:G:219:PHE:HE2	1.72	0.54
4:J:32:VAL:HG23	4:J:34:ARG:NH1	2.23	0.54
6:D:131:SER:OG	6:D:254:LYS:NZ	2.40	0.54
4:F:112:ALA:O	4:F:116:LEU:HB2	2.07	0.54
4:I:144:LEU:HD12	4:I:226:LEU:HD11	1.88	0.54
2:C:478:SER:H	2:C:481:ASP:HB2	1.71	0.54
4:F:259:SER:OG	4:H:39:SER:OG	2.25	0.54
4:J:104:SER:HB3	4:J:142:ILE:HD13	1.89	0.54
4:I:261:ALA:HB3	4:J:174:ALA:HB2	1.89	0.54
4:K:306:ASN:OD1	4:K:337:TYR:OH	2.26	0.54
5:B:207:ILE:HD11	5:B:251:GLU:HB3	1.90	0.54
4:F:10:ASN:ND2	4:H:282:ASN:OD1	2.36	0.53
4:H:283:ALA:O	4:H:303:GLN:NE2	2.41	0.53
5:B:93:MET:HE1	5:B:95:GLU:HB3	1.89	0.53
2:C:436:ARG:NH1	2:C:448:VAL:O	2.41	0.53
4:F:338:LYS:HD2	4:F:339:HIS:N	2.23	0.53
4:K:2:LEU:HB2	4:K:275:ASN:HA	1.90	0.53
4:K:183:ARG:HD2	4:K:211:ALA:HB1	1.90	0.53
5:B:85:VAL:HB	5:B:125:LEU:HB3	1.89	0.53
6:D:240:ASP:HB3	6:D:243:LEU:CB	2.38	0.53
4:F:325:PHE:CD1	4:F:345:ARG:HB3	2.43	0.53
4:H:10:ASN:ND2	4:I:282:ASN:OD1	2.37	0.53
3:E:153:LYS:HA	3:E:156:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:103:MET:HE2	4:H:133:ILE:HG13	1.90	0.53
4:I:18:ARG:HH21	4:I:256:LYS:HE2	1.74	0.53
2:C:318:SER:OG	2:C:319:GLU:N	2.34	0.53
4:F:349:ASN:HB3	4:F:352:GLU:HG3	1.90	0.53
2:C:467:ASN:HB2	2:C:470:LYS:HB3	1.91	0.53
4:J:46:ILE:O	4:J:49:SER:OG	2.25	0.53
4:J:264:ASN:HD22	4:K:282:ASN:HB2	1.74	0.53
2:C:376:PHE:HB3	2:C:426:ALA:HB2	1.90	0.52
4:H:296:LEU:O	4:H:300:SER:OG	2.27	0.52
5:B:29:ARG:HG3	5:B:129:ARG:HG2	1.91	0.52
4:H:111:LEU:HD22	4:H:129:VAL:HG22	1.92	0.52
4:I:69:GLN:NE2	4:I:74:GLU:OE1	2.33	0.52
6:D:57:PRO:O	6:D:62:LYS:NZ	2.43	0.52
2:C:159:TRP:O	2:C:163:ASN:ND2	2.42	0.52
4:K:230:LEU:O	4:K:231:LYS:C	2.52	0.52
6:D:127:ARG:HD3	6:D:229:ALA:HB1	1.91	0.52
1:A:-6:U:OP2	5:B:52:ARG:NH2	2.41	0.52
4:G:187:ASP:N	4:G:208:SER:O	2.31	0.52
4:I:263:HIS:NE2	4:J:172:GLN:OE1	2.42	0.52
4:I:295:ASP:OD1	4:I:297:VAL:N	2.43	0.52
2:C:512:PHE:HA	2:C:515:ARG:HE	1.75	0.52
3:E:19:ASP:HA	3:E:22:ILE:HG22	1.91	0.52
4:H:10:ASN:HA	4:H:214:CYS:HA	1.92	0.52
4:I:358:LEU:HD11	4:I:366:TRP:HE3	1.75	0.52
2:C:201:LEU:HD22	5:B:125:LEU:HD13	1.92	0.51
4:H:91:LYS:HD3	4:H:152:ASN:HD22	1.75	0.51
4:K:171:LEU:HB2	4:K:221:ILE:HG23	1.92	0.51
4:F:271:VAL:HG11	4:F:353:LEU:HD11	1.91	0.51
4:J:193:ASP:OD1	4:J:195:VAL:N	2.39	0.51
4:K:71:GLU:HG2	4:K:109:LYS:HZ2	1.74	0.51
2:C:490:LEU:HD22	2:C:513:ILE:HA	1.93	0.51
4:J:225:GLN:NE2	4:J:229:ASN:OD1	2.44	0.51
4:J:301:ILE:HD13	4:J:333:TYR:HB3	1.93	0.51
4:G:247:ALA:O	4:G:251:THR:OG1	2.20	0.51
4:K:32:VAL:HG21	4:K:287:PRO:HG3	1.92	0.51
3:E:114:MET:HG3	3:E:115:GLN:HG3	1.93	0.51
4:J:32:VAL:HG23	4:J:34:ARG:HH12	1.75	0.51
5:B:11:ARG:HD2	5:B:173:ARG:HH21	1.75	0.51
3:E:32:ASP:N	3:E:32:ASP:OD1	2.43	0.51
3:E:55:ALA:O	5:B:275:ARG:NH2	2.44	0.51
4:K:42:ILE:HD11	4:K:173:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:78:LYS:O	6:D:79:ARG:NH1	2.44	0.51
2:C:360:SER:O	2:C:360:SER:OG	2.29	0.50
6:D:68:ARG:NH1	6:D:70:ASP:OD2	2.43	0.50
2:C:134:LEU:HD11	2:C:160:LEU:HD21	1.93	0.50
4:H:258:ASN:HA	4:I:172:GLN:HG2	1.93	0.50
4:J:55:LEU:HD22	4:J:140:PRO:HG2	1.94	0.50
4:J:104:SER:OG	4:J:105:LYS:N	2.45	0.50
4:F:5:ILE:HB	4:F:219:PHE:HB2	1.94	0.50
4:K:102:PHE:HE2	4:K:142:ILE:HG23	1.77	0.50
4:K:220:SER:CB	4:K:277:PRO:HB3	2.42	0.50
4:K:230:LEU:HD22	4:K:236:LEU:HD23	1.94	0.50
2:C:226:LEU:O	2:C:230:THR:OG1	2.28	0.50
4:K:42:ILE:HD12	4:K:219:PHE:HE2	1.77	0.50
4:F:263:HIS:HB2	4:H:279:SER:HB2	1.94	0.50
4:I:230:LEU:HD13	4:I:236:LEU:HB3	1.93	0.50
4:J:6:HIS:HB2	4:J:270:LEU:HB3	1.94	0.50
4:G:209:MET:CG	4:G:210:PHE:N	2.75	0.50
5:B:55:ALA:HB1	5:B:60:LEU:HG	1.93	0.50
4:F:103:MET:HA	4:F:142:ILE:HD11	1.94	0.49
4:G:7:MET:HE1	4:G:266:PRO:HB3	1.94	0.49
2:C:110:ASP:O	2:C:112:HIS:ND1	2.46	0.49
2:C:503:VAL:HG22	3:E:157:SER:HB3	1.93	0.49
4:K:104:SER:HB3	4:K:136:ALA:HB1	1.94	0.49
4:G:242:GLY:HA2	4:G:245:LEU:HD12	1.95	0.49
2:C:368:ASP:HA	5:B:30:ARG:HH22	1.77	0.49
4:I:235:ASN:OD1	4:I:372:SER:OG	2.27	0.49
4:K:13:PRO:HG2	4:K:210:PHE:HB2	1.94	0.49
4:G:312:ARG:NH2	4:G:322:VAL:O	2.45	0.49
4:G:24:PRO:HD3	4:G:209:MET:HE3	1.93	0.49
5:B:309:GLN:HE22	5:B:336:CYS:HB2	1.78	0.49
4:I:330:ASN:HD22	4:J:310:ASP:HA	1.78	0.49
4:K:147:ARG:HD3	4:K:148:MET:N	2.22	0.49
1:A:25:G:OP1	4:J:25:LYS:NZ	2.32	0.49
4:G:5:ILE:HB	4:G:219:PHE:HB2	1.94	0.49
4:K:12:SER:O	4:K:16:LEU:HB2	2.13	0.49
1:A:31:C:H41	4:J:205:ILE:HD11	1.78	0.48
2:C:376:PHE:HD1	2:C:422:LEU:HB3	1.77	0.48
3:E:19:ASP:O	3:E:23:LEU:HG	2.12	0.48
4:H:32:VAL:HG23	4:H:34:ARG:HE	1.78	0.48
4:G:337:TYR:CE2	5:B:272:LYS:HG3	2.47	0.48
4:F:338:LYS:HD2	4:F:339:HIS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:55:LEU:CB	4:K:140:PRO:HG2	2.43	0.48
4:K:102:PHE:CE2	4:K:142:ILE:HG23	2.48	0.48
4:K:1:MET:HE1	4:K:361:ILE:HA	1.94	0.48
4:K:47:ARG:HG2	4:K:56:LEU:HD11	1.96	0.48
4:G:285:VAL:HG21	5:B:198:ARG:HD2	1.96	0.48
4:H:18:ARG:HH12	4:H:256:LYS:HD3	1.79	0.48
6:D:121:LEU:HD23	6:D:237:GLU:HG3	1.94	0.48
2:C:501:GLN:NE2	3:E:154:ARG:HA	2.28	0.48
1:A:42:A:N1	1:A:48:G:C6	2.82	0.48
4:K:358:LEU:HG	4:K:364:PHE:HB2	1.94	0.48
1:A:30:G:C4'	4:K:41:CYS:HA	2.39	0.48
3:E:41:PHE:HE2	3:E:58:ARG:HG2	1.78	0.48
4:H:340:SER:O	4:H:341:LYS:NZ	2.45	0.48
4:K:13:PRO:HG3	4:K:211:ALA:O	2.13	0.48
6:D:22:ARG:O	6:D:22:ARG:NH1	2.40	0.48
4:J:13:PRO:HG3	4:K:29:PHE:HB2	1.95	0.48
3:E:27:ARG:HH21	3:E:117:GLU:HG2	1.78	0.48
4:K:72:ALA:HB1	4:K:116:LEU:HD11	1.94	0.48
4:I:102:PHE:HB3	4:I:142:ILE:HD11	1.95	0.47
4:I:171:LEU:HB2	4:I:221:ILE:HD11	1.96	0.47
5:B:274:THR:HG22	5:B:275:ARG:H	1.80	0.47
4:K:15:ASN:HA	4:K:254:SER:O	2.14	0.47
4:K:176:ALA:CB	4:K:215:PHE:HB3	2.44	0.47
1:A:14:A:H8	4:H:18:ARG:HH21	1.62	0.47
2:C:192:ILE:HG22	2:C:194:GLU:H	1.79	0.47
4:I:84:ILE:HG23	4:I:126:ALA:HB2	1.96	0.47
4:H:17:ASN:HD22	4:H:17:ASN:HA	1.58	0.47
4:J:59:VAL:HG22	4:J:61:THR:HG23	1.96	0.47
4:K:17:ASN:HD22	4:K:37:ILE:HD13	1.78	0.47
4:K:34:ARG:NH2	4:K:284:PHE:O	2.47	0.47
5:B:292:VAL:HG22	6:D:220:HIS:CD2	2.49	0.47
4:H:55:LEU:HD21	4:H:239:HIS:CD2	2.50	0.47
4:G:26:THR:O	5:B:79:TRP:NE1	2.47	0.47
5:B:358:ARG:NH2	6:D:97:GLN:O	2.47	0.47
4:J:63:ARG:NH1	4:J:97:THR:OG1	2.48	0.47
4:J:258:ASN:HA	4:K:172:GLN:HE21	1.79	0.47
4:K:68:ILE:HD13	4:K:68:ILE:HA	1.64	0.47
4:F:174:ALA:HB2	4:G:261:ALA:HB3	1.97	0.47
4:H:297:VAL:O	4:H:301:ILE:HG13	2.15	0.47
5:B:308:VAL:HG11	5:B:325:LEU:HD23	1.96	0.47
4:K:49:SER:HB3	4:K:52:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:46:ILE:HA	4:G:251:THR:HG21	1.97	0.46
4:K:282:ASN:O	4:K:284:PHE:N	2.48	0.46
4:K:1:MET:N	4:K:223:TRP:HB2	2.31	0.46
5:B:82:PHE:HZ	5:B:126:LEU:HD22	1.80	0.46
4:H:51:ASP:OD2	4:H:247:ALA:HA	2.15	0.46
4:J:139:ALA:O	4:J:142:ILE:HD12	2.15	0.46
4:J:147:ARG:NH2	4:J:150:GLU:HB2	2.31	0.46
4:K:173:VAL:HG12	4:K:219:PHE:HD2	1.80	0.46
6:D:251:GLY:HA3	6:D:256:LYS:HD3	1.98	0.46
1:A:17:U:O2'	4:H:190:VAL:O	2.34	0.46
4:H:309:ASN:ND2	4:H:342:LEU:HD11	2.30	0.46
4:I:111:LEU:O	4:I:115:VAL:HG12	2.15	0.46
4:G:209:MET:HB3	4:G:209:MET:HE2	1.72	0.46
4:J:111:LEU:HG	4:J:129:VAL:HG22	1.98	0.46
4:K:38:SER:C	4:K:40:GLN:N	2.70	0.46
4:G:234:THR:HG22	4:G:364:PHE:HZ	1.80	0.46
3:E:18:GLY:HA2	4:I:209:MET:HE2	1.98	0.46
3:E:23:LEU:HD21	3:E:40:LEU:HD23	1.96	0.46
4:H:294:SER:OG	4:H:299:GLN:NE2	2.47	0.46
4:J:269:ILE:HB	4:J:327:PHE:HD2	1.81	0.46
5:B:213:ASP:OD1	5:B:245:ARG:NH1	2.49	0.46
6:D:174:TRP:O	6:D:178:LYS:NZ	2.40	0.46
6:D:179:SER:HA	6:D:182:LEU:HD12	1.98	0.46
2:C:225:ARG:HB2	2:C:229:PHE:CD2	2.51	0.46
4:F:186:ILE:HG12	4:F:209:MET:SD	2.55	0.46
4:J:271:VAL:HG12	4:J:325:PHE:HB2	1.97	0.46
4:K:102:PHE:CB	4:K:147:ARG:HG2	2.35	0.46
6:D:45:ARG:NH2	6:D:93:ASP:OD1	2.49	0.46
2:C:390:LEU:HD23	2:C:410:ILE:HD11	1.97	0.46
2:C:440:LEU:HD12	2:C:440:LEU:H	1.80	0.46
4:F:17:ASN:HD22	4:F:38:SER:H	1.63	0.46
4:F:52:PHE:CE1	4:F:55:LEU:HD23	2.51	0.46
4:H:61:THR:HG23	4:H:63:ARG:H	1.79	0.46
4:J:347:ILE:HD12	4:J:353:LEU:HD12	1.98	0.45
5:B:40:VAL:HG21	5:B:139:VAL:HG21	1.98	0.45
4:J:102:PHE:CD2	4:J:146:GLY:HA2	2.51	0.45
5:B:333:HIS:O	5:B:337:THR:OG1	2.27	0.45
4:G:24:PRO:CD	4:G:209:MET:HE3	2.47	0.45
2:C:355:LYS:N	2:C:370:ASP:OD2	2.49	0.45
4:F:258:ASN:HA	4:H:172:GLN:HG2	1.98	0.45
4:J:101:VAL:HB	4:J:103:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:55:LEU:HB3	4:K:140:PRO:CG	2.44	0.45
4:J:309:ASN:HB2	4:J:342:LEU:HD11	1.99	0.45
4:K:27:CYS:HB3	4:K:36:ARG:HB3	1.99	0.45
4:K:282:ASN:O	4:K:283:ALA:C	2.60	0.45
1:A:35:A:H61	6:D:162:ASP:HA	1.81	0.45
3:E:34:LYS:HE2	3:E:36:PRO:HD2	1.99	0.45
4:I:86:ASN:OD1	4:I:86:ASN:N	2.50	0.45
4:J:27:CYS:HB3	4:J:36:ARG:HD3	1.98	0.45
4:K:227:VAL:HG22	4:K:237:ALA:HB1	1.99	0.45
4:K:298:GLU:OE2	4:K:301:ILE:HD12	2.15	0.45
5:B:73:ASP:HB2	5:B:136:SER:HB2	1.98	0.45
4:K:286:ARG:HE	4:K:286:ARG:HB2	1.54	0.45
5:B:334:ASP:OD2	5:B:372:ARG:NH2	2.38	0.45
6:D:48:ASP:O	6:D:94:TYR:OH	2.21	0.45
6:D:178:LYS:HA	6:D:181:LYS:HE2	1.97	0.45
3:E:88:ILE:HD12	3:E:130:HIS:ND1	2.32	0.45
4:K:103:MET:HE2	4:K:103:MET:HB3	1.82	0.45
5:B:121:ARG:NH1	5:B:123:GLU:OE1	2.50	0.45
1:A:30:G:H4'	4:K:41:CYS:CA	2.39	0.45
4:F:297:VAL:O	4:F:301:ILE:HG12	2.16	0.45
4:H:357:VAL:O	4:H:361:ILE:HG12	2.17	0.45
4:K:185:GLU:H	6:D:73:ILE:HD13	1.81	0.45
4:K:373:LYS:HE3	4:K:373:LYS:HB3	1.63	0.45
1:A:1:G:O5'	5:B:84:THR:OG1	2.32	0.44
4:K:3:ILE:H	4:K:3:ILE:HG13	1.42	0.44
4:K:26:THR:CB	6:D:78:LYS:HE2	2.47	0.44
4:K:185:GLU:H	4:K:185:GLU:HG3	1.51	0.44
5:B:41:LEU:HD22	5:B:63:LEU:HD22	1.99	0.44
2:C:359:MET:SD	2:C:360:SER:N	2.90	0.44
4:F:32:VAL:HG21	4:F:287:PRO:HG3	1.99	0.44
4:I:3:ILE:HG22	4:I:273:PHE:CD1	2.53	0.44
4:J:13:PRO:HG2	4:K:29:PHE:HB2	1.97	0.44
4:J:270:LEU:HB2	4:J:326:TRP:CZ3	2.52	0.44
4:K:85:LEU:HD12	4:K:85:LEU:HA	1.88	0.44
4:G:326:TRP:CE2	4:G:335:LEU:HB2	2.52	0.44
2:C:188:ILE:HG13	2:C:191:LEU:HD12	1.99	0.44
4:F:180:HIS:HD2	4:F:183:ARG:NH2	2.16	0.44
4:I:309:ASN:HA	4:I:342:LEU:HD11	2.00	0.44
2:C:105:VAL:HG13	2:C:157:ILE:HD12	1.99	0.44
2:C:300:TYR:HB2	2:C:326:SER:HB3	2.00	0.44
2:C:375:LEU:C	2:C:377:SER:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:33:LEU:HB3	4:H:182:ALA:HB3	1.98	0.44
4:J:66:ASP:OD1	4:J:66:ASP:N	2.50	0.44
5:B:147:LEU:HD12	5:B:147:LEU:HA	1.85	0.44
6:D:141:GLN:HG3	6:D:143:ASP:HB2	2.00	0.44
2:C:501:GLN:HE21	3:E:154:ARG:HG2	1.81	0.44
4:I:103:MET:HG3	4:I:133:ILE:HG23	1.98	0.44
5:B:231:TYR:HA	5:B:244:PRO:HA	1.99	0.44
6:D:178:LYS:HE3	6:D:178:LYS:HB3	1.83	0.44
2:C:221:LYS:HD2	2:C:221:LYS:C	2.43	0.44
4:H:173:VAL:HG22	4:H:219:PHE:HD1	1.83	0.44
4:I:29:PHE:O	4:I:34:ARG:NH1	2.51	0.44
4:J:110:ASP:HA	4:J:113:ARG:HE	1.82	0.44
4:G:186:ILE:HG13	4:G:209:MET:SD	2.58	0.44
1:A:35:A:H4'	1:A:36:U:H5''	1.99	0.44
1:A:38:C:OP2	6:D:155:LYS:NZ	2.45	0.44
2:C:187:ALA:HA	2:C:324:SER:HA	2.00	0.44
6:D:33:ARG:CZ	6:D:55:PHE:HE2	2.31	0.44
1:A:17:U:OP1	4:I:43:LYS:NZ	2.34	0.43
2:C:179:ALA:HB3	2:C:298:LYS:HB2	1.99	0.43
4:H:148:MET:SD	4:H:150:GLU:HG3	2.58	0.43
4:K:220:SER:HB2	4:K:277:PRO:HB3	2.00	0.43
4:G:289:SER:O	4:G:299:GLN:NE2	2.46	0.43
4:H:250:LYS:HA	4:H:265:TYR:HE1	1.83	0.43
4:J:9:GLN:NE2	4:J:264:ASN:O	2.51	0.43
4:K:279:SER:C	4:K:281:ALA:H	2.25	0.43
1:A:-1:C:O2	5:B:129:ARG:NH2	2.51	0.43
4:F:199:ASP:H	4:H:63:ARG:HH12	1.67	0.43
4:F:235:ASN:HB3	4:F:369:VAL:HG12	1.99	0.43
4:J:147:ARG:HH22	4:J:150:GLU:HB2	1.83	0.43
4:G:312:ARG:HH21	4:G:322:VAL:HG23	1.83	0.43
6:D:149:THR:HG22	6:D:151:LYS:HG2	1.99	0.43
2:C:346:THR:HG22	2:C:352:LEU:HD13	2.01	0.43
3:E:22:ILE:HD13	3:E:22:ILE:HG21	1.83	0.43
4:H:221:ILE:HD11	4:H:244:PHE:CD2	2.54	0.43
4:I:107:LYS:HE2	4:I:107:LYS:HB2	1.71	0.43
4:I:230:LEU:HD12	4:I:237:ALA:HB2	1.99	0.43
4:K:16:LEU:HG	4:K:215:PHE:HE1	1.82	0.43
4:K:38:SER:C	4:K:40:GLN:H	2.24	0.43
4:K:140:PRO:HB3	4:K:240:THR:HG23	1.99	0.43
4:K:287:PRO:O	4:K:288:VAL:C	2.59	0.43
1:A:42:A:C2	1:A:48:G:N1	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:376:PHE:CE1	2:C:423:ALA:HB2	2.53	0.43
4:J:6:HIS:C	4:J:7:MET:HE2	2.44	0.43
4:K:143:ALA:HA	4:K:229:ASN:HD22	1.83	0.43
5:B:199:TRP:NE1	5:B:201:ASN:O	2.52	0.43
1:A:8:G:H5'	4:F:255:GLY:HA2	1.99	0.43
3:E:116:MET:HE3	3:E:116:MET:HB2	1.79	0.43
4:F:24:PRO:HD3	4:F:209:MET:HB2	2.01	0.43
4:F:263:HIS:HD2	4:H:218:TYR:HE2	1.66	0.43
4:J:103:MET:H	4:J:103:MET:HG2	1.63	0.43
4:F:111:LEU:HA	4:F:114:ILE:HG12	2.01	0.43
4:J:101:VAL:HA	4:J:148:MET:O	2.19	0.43
6:D:11:THR:HG23	6:D:22:ARG:HD3	2.00	0.43
4:I:55:LEU:HD21	4:I:239:HIS:HB3	2.00	0.43
4:K:62:ARG:HE	4:K:62:ARG:HB2	1.44	0.43
6:D:126:LEU:HG	6:D:128:VAL:HG22	2.01	0.43
2:C:265:GLN:HA	2:C:266:PRO:HD3	1.91	0.43
4:K:29:PHE:HE2	4:K:284:PHE:C	2.27	0.43
5:B:61:PRO:HA	5:B:64:ALA:HB3	2.00	0.43
1:A:36:U:H4'	6:D:157:VAL:HG11	2.00	0.42
4:H:46:ILE:O	4:H:49:SER:OG	2.36	0.42
4:H:254:SER:HA	4:H:257:GLN:HG3	2.01	0.42
4:J:139:ALA:O	4:J:141:ASP:N	2.52	0.42
4:J:295:ASP:OD1	4:J:295:ASP:N	2.43	0.42
2:C:259:MET:O	2:C:263:ASN:ND2	2.52	0.42
4:F:29:PHE:HB3	4:F:34:ARG:HE	1.83	0.42
4:H:187:ASP:HB2	4:H:210:PHE:HE2	1.84	0.42
4:I:91:LYS:O	4:I:98:LYS:HD3	2.19	0.42
4:J:294:SER:OG	4:J:295:ASP:N	2.52	0.42
4:J:362:GLY:HA3	4:J:364:PHE:CZ	2.53	0.42
4:K:16:LEU:HB3	4:K:17:ASN:H	1.69	0.42
2:C:251:TRP:CZ2	2:C:386:ARG:HG2	2.55	0.42
4:K:16:LEU:HD21	4:K:215:PHE:CE1	2.55	0.42
2:C:492:LYS:HA	2:C:492:LYS:HD3	1.64	0.42
5:B:235:VAL:HB	5:B:241:ARG:HG2	2.01	0.42
2:C:198:ALA:HA	5:B:95:GLU:HB2	2.01	0.42
2:C:370:ASP:OD1	2:C:370:ASP:N	2.38	0.42
4:K:142:ILE:H	4:K:142:ILE:HG12	1.51	0.42
4:K:149:LEU:HD13	4:K:149:LEU:HA	1.54	0.42
4:G:20:ASP:OD2	5:B:128:ARG:NH1	2.52	0.42
4:G:312:ARG:HE	4:G:322:VAL:HG22	1.85	0.42
4:G:341:LYS:HD3	4:G:341:LYS:HA	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:301:CYS:SG	5:B:365:ARG:NH1	2.89	0.42
6:D:48:ASP:OD1	6:D:48:ASP:N	2.51	0.42
4:F:296:LEU:O	4:F:300:SER:OG	2.31	0.42
4:K:192:ALA:HA	6:D:112:TYR:HE1	1.84	0.42
5:B:45:CYS:HA	5:B:50:ILE:HD12	2.02	0.42
6:D:164:SER:O	6:D:164:SER:OG	2.38	0.42
4:H:338:LYS:H	4:H:338:LYS:HG2	1.54	0.42
4:I:323:ILE:H	4:I:323:ILE:HD12	1.85	0.42
5:B:229:ILE:O	5:B:230:HIS:ND1	2.52	0.42
6:D:151:LYS:HB2	6:D:151:LYS:HE3	1.87	0.42
4:F:34:ARG:HB3	4:F:178:SER:HB3	2.01	0.42
4:F:58:GLY:HA2	4:F:104:SER:HA	2.01	0.42
4:K:148:MET:HG3	4:K:166:THR:HG23	2.02	0.42
6:D:191:LEU:HA	6:D:232:LEU:HD23	2.02	0.42
2:C:145:GLU:HG2	2:C:264:TRP:HE1	1.85	0.41
2:C:424:GLN:CD	2:C:519:PRO:HB2	2.45	0.41
2:C:433:ASN:O	2:C:437:LYS:HB2	2.20	0.41
4:F:269:ILE:HD13	4:F:327:PHE:CD2	2.55	0.41
4:J:10:ASN:HB3	4:K:282:ASN:HD21	1.85	0.41
4:J:44:ARG:HD2	4:J:47:ARG:HH21	1.85	0.41
4:J:282:ASN:HA	4:J:285:VAL:HG23	2.01	0.41
4:K:29:PHE:HB3	4:K:34:ARG:HD2	2.02	0.41
4:G:326:TRP:CH2	4:G:328:SER:HB2	2.55	0.41
4:J:263:HIS:N	4:K:279:SER:HB3	2.36	0.41
4:K:283:ALA:HB2	4:K:307:TYR:CE2	2.55	0.41
4:G:337:TYR:CZ	5:B:272:LYS:HG3	2.56	0.41
5:B:84:THR:HG22	5:B:126:LEU:HD23	2.02	0.41
4:J:46:ILE:HA	4:J:251:THR:HG21	2.01	0.41
4:J:185:GLU:OE2	4:K:27:CYS:HA	2.20	0.41
4:K:49:SER:O	4:K:50:ASN:C	2.62	0.41
4:K:313:LEU:HD23	4:K:313:LEU:HA	1.91	0.41
5:B:62:LYS:HE2	5:B:147:LEU:HD11	2.02	0.41
6:D:53:LYS:HE3	6:D:54:PRO:HD2	2.01	0.41
1:A:12:G:O2'	1:A:13:G:H4'	2.19	0.41
3:E:63:LEU:HA	3:E:66:LYS:HE2	2.02	0.41
4:F:23:ALA:HA	4:F:209:MET:HB2	2.01	0.41
4:H:25:LYS:HD2	4:H:36:ARG:NH2	2.36	0.41
4:G:34:ARG:HH22	4:G:287:PRO:HB3	1.85	0.41
4:G:209:MET:CG	4:G:210:PHE:H	2.34	0.41
5:B:338:MET:HE2	5:B:338:MET:HB2	1.86	0.41
1:A:1:G:OP1	4:G:17:ASN:ND2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:116:MET:HE1	3:E:147:TRP:CD1	2.55	0.41
4:I:226:LEU:HA	4:I:226:LEU:HD12	1.53	0.41
4:J:311:ILE:HD13	4:J:311:ILE:HA	1.98	0.41
4:K:274:LYS:HE2	4:K:274:LYS:HB2	1.70	0.41
5:B:253:VAL:HG13	5:B:256:GLU:HG2	2.02	0.41
5:B:290:ARG:NH1	5:B:322:PRO:O	2.51	0.41
4:F:347:ILE:HG22	4:F:349:ASN:H	1.86	0.41
4:J:63:ARG:HD3	4:J:63:ARG:HA	1.92	0.41
4:K:217:LYS:HB2	4:K:217:LYS:HE3	1.64	0.41
2:C:188:ILE:HG12	2:C:214:LEU:HD12	2.01	0.41
3:E:120:LEU:O	3:E:124:MET:HG2	2.21	0.41
4:H:103:MET:HE1	4:H:111:LEU:HD11	2.03	0.41
4:K:27:CYS:SG	4:K:36:ARG:HB3	2.60	0.41
2:C:109:LYS:HB2	2:C:109:LYS:HE3	1.86	0.41
3:E:113:ILE:H	3:E:113:ILE:HD12	1.86	0.41
1:A:24:C:H5"	4:I:190:VAL:O	2.21	0.41
3:E:74:GLU:OE1	3:E:76:ARG:HB2	2.21	0.41
4:H:272:GLU:OE1	4:H:274:LYS:NZ	2.48	0.41
4:I:25:LYS:HB3	4:I:36:ARG:NH2	2.36	0.41
4:J:47:ARG:HH12	4:J:60:ARG:HH21	1.69	0.41
4:J:189:PHE:CZ	4:J:206:GLY:HA3	2.56	0.41
4:K:161:LYS:HA	4:K:161:LYS:HD3	1.55	0.41
4:K:358:LEU:HD12	4:K:358:LEU:HA	1.89	0.41
4:G:236:LEU:HD12	4:G:236:LEU:HA	1.91	0.41
5:B:28:LEU:HD12	5:B:28:LEU:HA	1.93	0.41
6:D:201:LYS:HE2	6:D:225:LEU:HD11	2.03	0.41
2:C:93:VAL:HG12	2:C:117:ALA:HB2	2.02	0.41
4:F:295:ASP:O	4:F:299:GLN:HG3	2.21	0.41
4:H:272:GLU:HG2	4:H:324:GLY:HA3	2.02	0.41
4:J:89:GLY:HA3	4:J:156:LYS:HB3	2.02	0.41
4:K:151:PRO:O	4:K:152:ASN:C	2.63	0.41
5:B:7:THR:HB	5:B:142:GLN:HG3	2.03	0.41
5:B:309:GLN:NE2	5:B:336:CYS:HB2	2.35	0.41
5:B:354:ASP:HA	5:B:355:PRO:HD3	1.96	0.41
2:C:128:PHE:CZ	2:C:132:LEU:HD22	2.56	0.40
2:C:469:GLY:O	2:C:475:ARG:NH2	2.55	0.40
4:I:112:ALA:O	4:I:116:LEU:HG	2.21	0.40
3:E:71:PHE:CZ	3:E:124:MET:HB2	2.56	0.40
4:I:71:GLU:HG3	4:I:113:ARG:HE	1.85	0.40
4:K:79:LYS:H	4:K:79:LYS:HG3	1.60	0.40
4:F:199:ASP:H	4:H:63:ARG:NH1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:142:ILE:HD12	4:I:147:ARG:HB2	2.04	0.40
4:K:16:LEU:CG	4:K:215:PHE:HE1	2.33	0.40
4:K:46:ILE:HD12	4:K:46:ILE:HA	1.86	0.40
4:K:209:MET:HE2	4:K:209:MET:HB2	1.46	0.40
4:G:274:LYS:HG2	4:G:322:VAL:HG11	2.03	0.40
2:C:192:ILE:HG13	2:C:195:ILE:HD12	2.04	0.40
2:C:365:THR:OG1	2:C:433:ASN:OD1	2.37	0.40
4:K:1:MET:H3	4:K:223:TRP:HB2	1.86	0.40
5:B:307:THR:OG1	5:B:308:VAL:N	2.54	0.40
1:A:-4:A:P	5:B:29:ARG:HH21	2.44	0.40
4:F:107:LYS:O	4:F:111:LEU:HB2	2.22	0.40
4:H:55:LEU:HB3	4:H:140:PRO:HG2	2.04	0.40
4:J:21:LEU:HA	5:B:379:ARG:CZ	2.52	0.40
4:K:180:HIS:CD2	4:K:296:LEU:HD22	2.56	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	C	438/535 (82%)	378 (86%)	59 (14%)	1 (0%)	44	74
3	E	163/174 (94%)	156 (96%)	7 (4%)	0	100	100
4	F	363/378 (96%)	337 (93%)	26 (7%)	0	100	100
4	G	241/378 (64%)	223 (92%)	18 (8%)	0	100	100
4	H	363/378 (96%)	332 (92%)	31 (8%)	0	100	100
4	I	358/378 (95%)	324 (90%)	33 (9%)	1 (0%)	37	68
4	J	363/378 (96%)	327 (90%)	36 (10%)	0	100	100
4	K	329/378 (87%)	239 (73%)	75 (23%)	15 (5%)	2	12
5	B	376/388 (97%)	350 (93%)	25 (7%)	1 (0%)	37	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	266/272 (98%)	248 (93%)	17 (6%)	1 (0%)	30	63
All	All	3260/3637 (90%)	2914 (89%)	327 (10%)	19 (1%)	24	53

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	310	ALA
4	I	322	VAL
4	K	20	ASP
4	K	301	ILE
5	B	346	THR
4	K	78	TRP
4	K	283	ALA
4	K	288	VAL
6	D	241	PRO
4	K	76	GLU
4	K	83	GLU
4	K	106	ASP
4	K	231	LYS
4	K	155	ASP
4	K	362	GLY
4	K	118	ASN
4	K	160	VAL
4	K	164	ASN
4	K	369	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	
2	C	366/459 (80%)	364 (100%)	2 (0%)	86	92
3	E	143/153 (94%)	139 (97%)	4 (3%)	38	66
4	F	291/313 (93%)	291 (100%)	0	100	100
4	G	199/313 (64%)	196 (98%)	3 (2%)	60	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	300/313 (96%)	299 (100%)	1 (0%)	91	95
4	I	288/313 (92%)	284 (99%)	4 (1%)	62	81
4	J	291/313 (93%)	289 (99%)	2 (1%)	81	90
4	K	275/313 (88%)	169 (62%)	106 (38%)	0	0
5	B	308/322 (96%)	307 (100%)	1 (0%)	91	95
6	D	223/238 (94%)	222 (100%)	1 (0%)	89	94
All	All	2684/3050 (88%)	2560 (95%)	124 (5%)	25	52

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	252	HIS
2	C	379	LEU
3	E	127	LEU
3	E	153	LYS
3	E	157	SER
3	E	158	ASP
4	H	17	ASN
4	I	7	MET
4	I	17	ASN
4	I	150	GLU
4	I	316	TYR
4	J	32	VAL
4	J	311	ILE
4	K	3	ILE
4	K	4	GLU
4	K	5	ILE
4	K	8	ILE
4	K	9	GLN
4	K	10	ASN
4	K	11	HIS
4	K	12	SER
4	K	15	ASN
4	K	16	LEU
4	K	18	ARG
4	K	21	LEU
4	K	26	THR
4	K	32	VAL
4	K	33	LEU
4	K	35	SER

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Mol	Chain	Res	Type
4	K	36	ARG
4	K	37	ILE
4	K	38	SER
4	K	39	SER
4	K	43	LYS
4	K	44	ARG
4	K	45	SER
4	K	46	ILE
4	K	47	ARG
4	K	48	THR
4	K	51	ASP
4	K	55	LEU
4	K	59	VAL
4	K	62	ARG
4	K	63	ARG
4	K	64	LEU
4	K	68	ILE
4	K	69	GLN
4	K	75	THR
4	K	76	GLU
4	K	78	TRP
4	K	79	LYS
4	K	82	GLN
4	K	83	GLU
4	K	88	CYS
4	K	101	VAL
4	K	104	SER
4	K	106	ASP
4	K	107	LYS
4	K	108	ILE
4	K	110	ASP
4	K	113	ARG
4	K	114	ILE
4	K	116	LEU
4	K	120	LEU
4	K	122	LEU
4	K	127	GLN
4	K	129	VAL
4	K	131	ASN
4	K	135	GLN
4	K	141	ASP
4	K	142	ILE

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Mol	Chain	Res	Type
4	K	147	ARG
4	K	149	LEU
4	K	154	LYS
4	K	157	ASP
4	K	161	LYS
4	K	165	THR
4	K	167	VAL
4	K	168	GLU
4	K	171	LEU
4	K	172	GLN
4	K	173	VAL
4	K	177	ILE
4	K	179	THR
4	K	183	ARG
4	K	185	GLU
4	K	186	ILE
4	K	187	ASP
4	K	190	VAL
4	K	209	MET
4	K	210	PHE
4	K	212	SER
4	K	217	LYS
4	K	220	SER
4	K	221	ILE
4	K	222	ASP
4	K	225	GLN
4	K	228	LYS
4	K	233	ASP
4	K	234	THR
4	K	272	GLU
4	K	274	LYS
4	K	276	SER
4	K	278	ILE
4	K	280	TYR
4	K	285	VAL
4	K	286	ARG
4	K	289	SER
4	K	290	VAL
4	K	291	VAL
4	K	292	LYS
4	K	293	GLU
4	K	295	ASP

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Mol	Chain	Res	Type
4	K	298	GLU
4	K	299	GLN
4	K	301	ILE
4	K	361	ILE
4	K	367	GLU
4	K	373	LYS
4	G	2	LEU
4	G	278	ILE
4	G	347	ILE
5	B	147	LEU
6	D	41	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	243	ASN
2	C	308	GLN
2	C	501	GLN
3	E	50	GLN
4	F	17	ASN
4	F	239	HIS
4	F	257	GLN
4	F	351	ASN
4	H	252	ASN
4	H	331	ASN
4	I	40	GLN
4	I	225	GLN
4	I	309	ASN
4	I	339	HIS
4	J	10	ASN
4	J	264	ASN
4	J	351	ASN
4	J	370	GLN
4	K	15	ASN
4	K	17	ASN
4	K	69	GLN
4	K	82	GLN
4	K	96	ASN
4	K	131	ASN
4	K	135	GLN
4	K	172	GLN
4	K	225	GLN

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Mol	Chain	Res	Type
4	K	229	ASN
4	K	239	HIS
5	B	22	ASN
5	B	89	GLN
5	B	206	GLN
5	B	309	GLN
5	B	310	HIS
6	D	113	ASN
6	D	135	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	-4	A
1	A	0	G
1	A	1	G
1	A	6	C
1	A	7	C
1	A	8	G
1	A	11	A
1	A	13	G
1	A	18	U
1	A	19	A
1	A	20	G
1	A	25	G
1	A	29	A
1	A	31	C
1	A	37	U
1	A	44	G
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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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](#)

There are no chain breaks in this entry.