



Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 02:22 PM JST

PDB ID : 8ZP7 / pdb_00008zp7
EMDB ID : EMD-60328
Title : Cryo-EM structure of Cas5-HNH Cascade bound with sDNA, Conf1
Authors : Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on : 2024-05-29
Resolution : 3.00 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 : 4-5-2 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

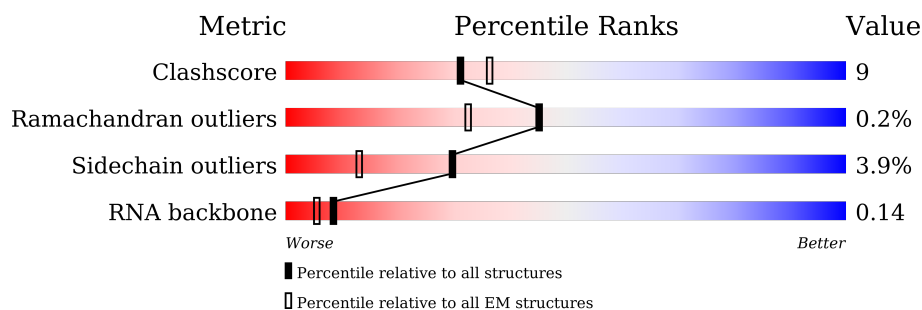
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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 ≥ 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	C	546	
3	E	174	
4	F	378	
4	G	378	
4	H	378	
4	I	378	
4	J	378	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	K	378	<div><div></div><div>78%</div><div>13%</div><div>• 7%</div></div>
5	B	388	<div><div></div><div>63%</div><div>24%</div><div>• 11%</div></div>
6	D	272	<div><div></div><div>63%</div><div>29%</div><div>• 6%</div></div>
7	M	60	<div><div></div><div>38%</div><div>17%</div><div>45%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27540 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	443	Total	C	N	O	S	0	0
			3495	2246	597	633	19		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP A0A1V6F8D1
C	-9	HIS	-	expression tag	UNP A0A1V6F8D1
C	-8	HIS	-	expression tag	UNP A0A1V6F8D1
C	-7	HIS	-	expression tag	UNP A0A1V6F8D1
C	-6	HIS	-	expression tag	UNP A0A1V6F8D1
C	-5	HIS	-	expression tag	UNP A0A1V6F8D1
C	-4	HIS	-	expression tag	UNP A0A1V6F8D1
C	-3	HIS	-	expression tag	UNP A0A1V6F8D1
C	-2	HIS	-	expression tag	UNP A0A1V6F8D1
C	-1	HIS	-	expression tag	UNP A0A1V6F8D1
C	0	HIS	-	expression tag	UNP A0A1V6F8D1
C	1	VAL	-	expression tag	UNP A0A1V6F8D1

- 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	368	Total	C	N	O	S	0	0
			2819	1782	489	536	12		
4	H	375	Total	C	N	O	S	0	0
			2878	1812	503	551	12		
4	I	373	Total	C	N	O	S	0	0
			2854	1800	498	544	12		
4	J	374	Total	C	N	O	S	0	0
			2845	1794	496	543	12		
4	K	350	Total	C	N	O	S	0	0
			2701	1708	474	508	11		
4	G	255	Total	C	N	O	S	0	0
			1927	1220	336	363	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	344	Total	C	N	O	S	0	0
			2701	1704	499	481	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	256	Total	C	N	O	S	0	0
			2039	1309	365	361	4		

- Molecule 7 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	33	Total	C	N	O	P	0	0
			669	319	119	198	33		

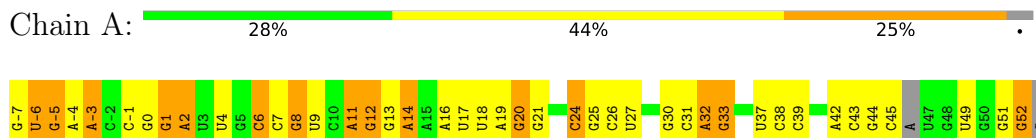
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

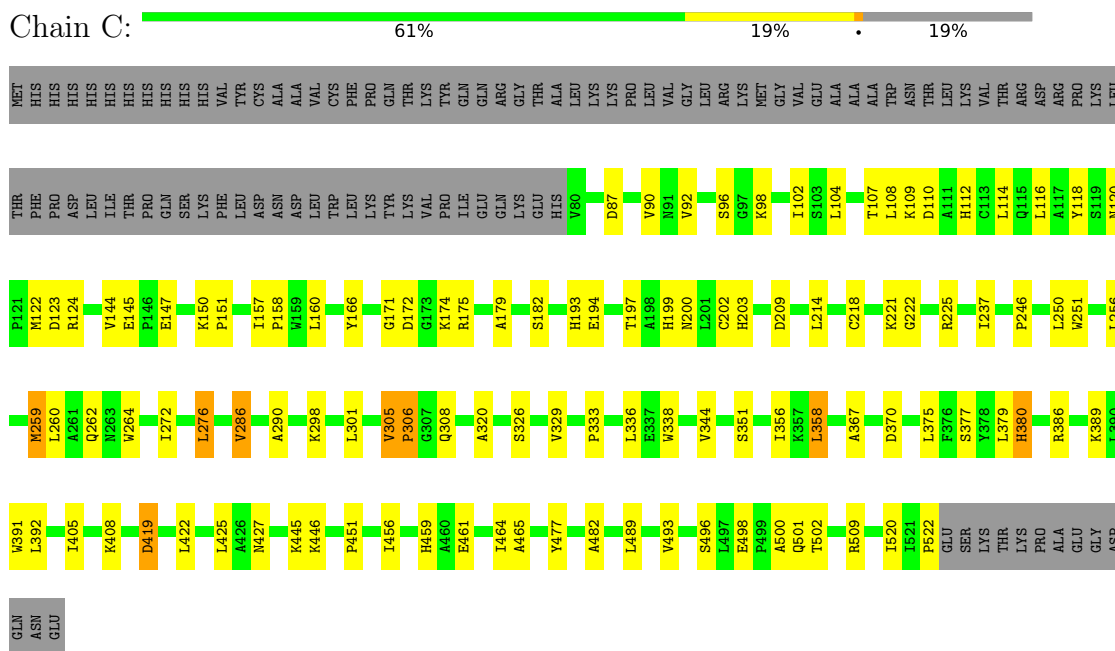
3 Residue-property plots

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.

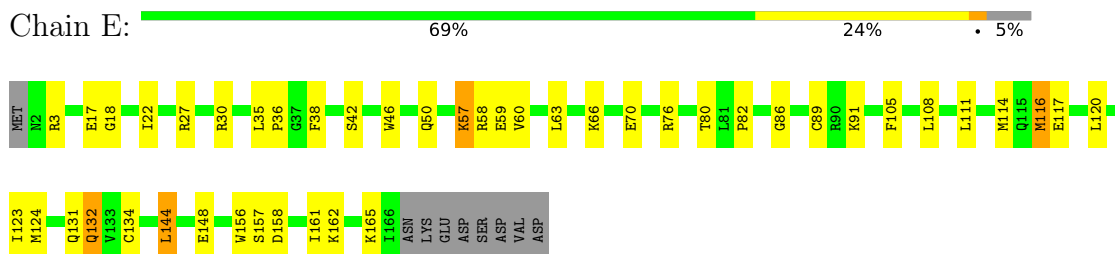
- Molecule 1: RNA (61-MER)




- Molecule 2: CRISPR-associated protein Cse1 (CRISPR_cse1)

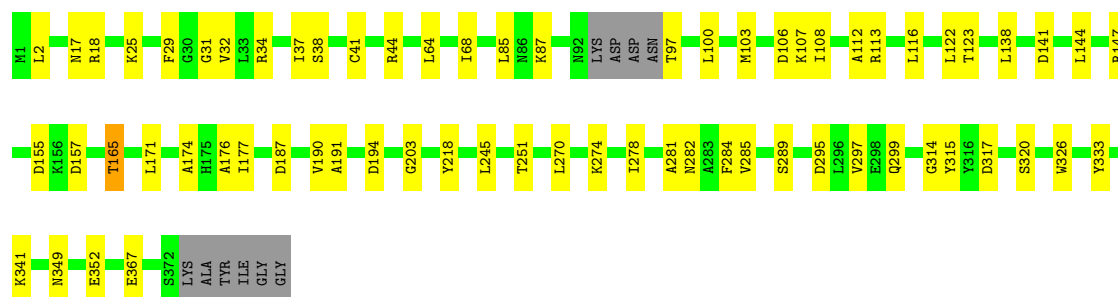


- Molecule 3: CRISPR-associated protein Cse2 (CRISPR_cse2)




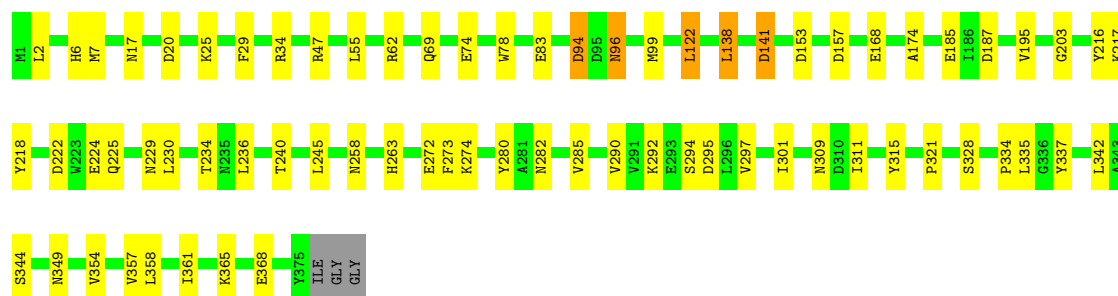
- Molecule 4: CRISPR system Cascade subunit CasC

Chain F:  80% 17% .




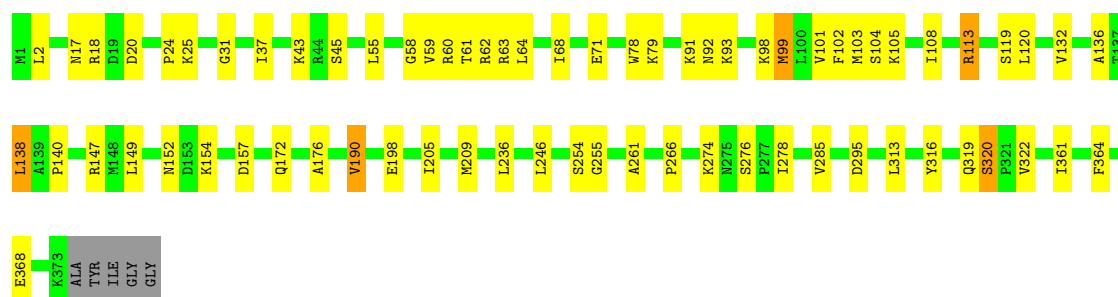
- Molecule 4: CRISPR system Cascade subunit CasC

Chain H:  80% 18% ..



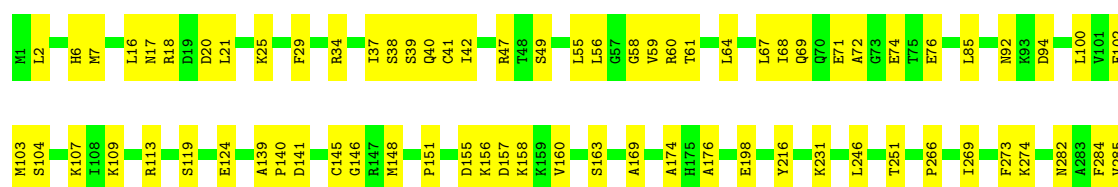
- Molecule 4: CRISPR system Cascade subunit CasC

Chain I:  80% 17% ..



- Molecule 4: CRISPR system Cascade subunit CasC

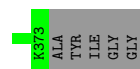
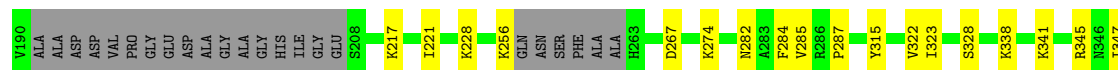
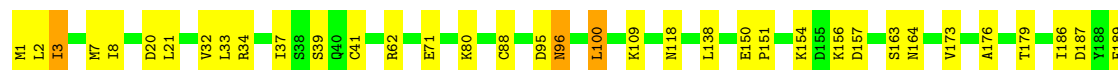
Chain J:  76% 23% .





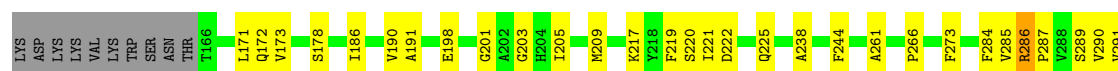
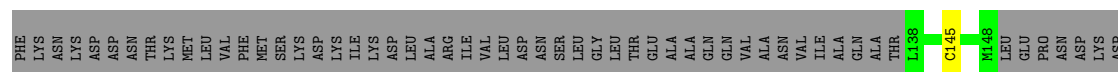
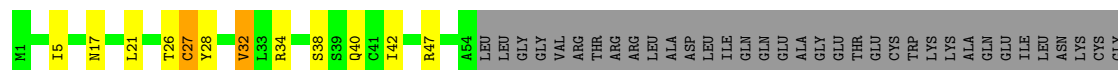
• Molecule 4: CRISPR system Cascade subunit CasC

Chain K: 78% 13% 7%



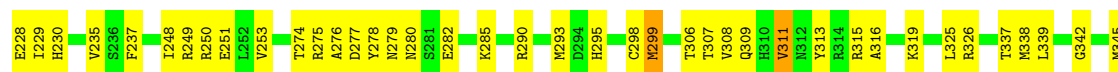
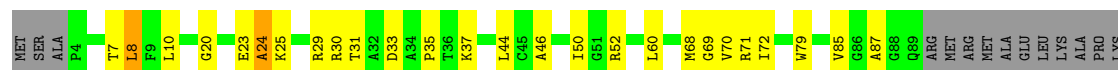
• Molecule 4: CRISPR system Cascade subunit CasC

Chain G: 52% 15% 33%



• Molecule 5: CRISPR system Cascade subunit CasD

Chain B: 63% 24% 11%



• Molecule 6: CRISPR-associated endoribonuclease Cse3

LYS	L103	M1
VAL	A104	I2
GLU	A105	L7
GLN	K110	I8
GLY	E111	I9
GLN	Y112	D10
GLY	N113	
TYR	P114	P15
W217		P20
L225	L122	
L231	R125	K23
V235	L126	W24
L236	R127	L25
E237	V128	L28
	N129	
	A130	R34
D240	S131	
	V132	M37
L245	R133	
	R134	S41
G253	H135	
K254	M139	R44
A255		
K256	Q142	F51
S257		
F258		S56
	T146	P57
G261	I147	
L262	E148	Q61
L263	H154	K62
S264	K155	T63
V265	R156	
L266		L66
P267	L159	F67
I268		R68
ARG	D162	V69
ASN	A163	D70
ASP	S164	
GLY	S165	I73
	T166	
	D168	N76
		D77
	Q187	I81
		I82
	L191	Q85
	Q193	
	L194	D91
	G195	W92
	W196	D93
	V197	Y94
		C95
		F96
LVS	P204	Q97
ASN		
ASN		F102

Chain M: 38% 17% 45%

DC	DG	DG	DA	DA	DA	DG	DG	DT	DT	DG	DA	DC	DA	DG	DT	DT	DG	DT	DT	G20	A24	C31	T32	A33	A34	T35	C38	A42	C43	G44	G45	C46	A47	T49	T52	DT	DA	DC	DC	DA	DG	DC	DT
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	----	----	----	----	----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57434	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN 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	0.15	0/1405	0.37	0/2187
2	C	0.22	0/3596	0.57	1/4901 (0.0%)
3	E	0.26	0/1382	0.68	2/1862 (0.1%)
4	F	0.20	0/2875	0.46	1/3900 (0.0%)
4	G	0.22	0/1967	0.54	0/2670
4	H	0.19	0/2934	0.46	2/3977 (0.1%)
4	I	0.19	0/2911	0.47	2/3949 (0.1%)
4	J	0.20	0/2901	0.51	1/3937 (0.0%)
4	K	0.19	0/2752	0.49	1/3726 (0.0%)
5	B	0.20	0/2769	0.51	1/3759 (0.0%)
6	D	0.20	0/2095	0.58	1/2845 (0.0%)
7	M	0.26	0/748	0.48	0/1150
All	All	0.20	0/28335	0.51	12/38863 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	B	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	57	LYS	CA-CB-CG	6.47	127.03	114.10
4	I	99	MET	CB-CG-SD	5.66	129.67	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	145	PRO	CA-N-CD	-5.59	104.17	112.00
4	H	321	PRO	CA-N-CD	-5.42	104.41	112.00
4	H	292	LYS	CB-CG-CD	5.41	123.75	111.30
2	C	276	LEU	CA-CB-CG	5.37	135.10	116.30
4	K	228	LYS	CA-CB-CG	5.32	124.73	114.10
4	J	158	LYS	CB-CG-CD	5.26	123.39	111.30
4	F	341	LYS	CB-CG-CD	5.22	123.30	111.30
3	E	116	MET	CA-CB-CG	5.18	124.46	114.10
4	I	198	GLU	CA-CB-CG	5.09	124.28	114.10
6	D	37	MET	CB-CG-SD	5.07	127.90	112.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	24	ALA	Peptide
2	C	305	VAL	Peptide

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	32	0
2	C	3495	0	3405	65	0
3	E	1352	0	1387	31	0
4	F	2819	0	2745	46	0
4	G	1927	0	1854	40	0
4	H	2878	0	2805	47	0
4	I	2854	0	2766	47	0
4	J	2845	0	2746	53	0
4	K	2701	0	2651	35	0
5	B	2701	0	2679	69	0
6	D	2039	0	1995	61	0
7	M	669	0	372	11	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
All	All	27540	0	26043	460	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 9.

All (460) 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)
5:B:358:ARG:HH12	6:D:97:GLN:HE22	1.29	0.78
4:F:2:LEU:HB2	4:F:274:LYS:O	1.87	0.74
4:I:2:LEU:HB2	4:I:274:LYS:O	1.89	0.72
5:B:212:MET:HE1	5:B:250:ARG:HG2	1.70	0.72
2:C:305:VAL:HG22	2:C:306:PRO:HD2	1.73	0.70
4:K:189:PHE:O	6:D:110:LYS:NZ	2.24	0.70
2:C:202:CYS:SG	5:B:121:ARG:NH2	2.65	0.70
5:B:207:ILE:HD11	5:B:251:GLU:HB3	1.75	0.69
2:C:246:PRO:HB3	2:C:351:SER:HB3	1.75	0.69
2:C:222:GLY:HA2	2:C:225:ARG:HD2	1.75	0.68
5:B:315:ARG:HB2	5:B:319:LYS:HG3	1.77	0.67
6:D:7:LEU:HB2	6:D:82:ILE:HB	1.77	0.67
4:G:34:ARG:NH2	4:G:284:PHE:O	2.28	0.66
6:D:253:GLY:O	6:D:256:LYS:NZ	2.28	0.66
5:B:8:LEU:HD22	5:B:151:LEU:HD13	1.79	0.65
1:A:-4:A:H2'	1:A:-3:A:H8	1.62	0.64
4:J:69:GLN:HE22	4:J:76:GLU:HA	1.63	0.64
4:J:2:LEU:HB2	4:J:274:LYS:O	1.98	0.64
4:F:29:PHE:HB3	4:F:34:ARG:HG3	1.81	0.63
5:B:20:GLY:HA2	5:B:31:THR:HA	1.81	0.63
2:C:122:MET:HG2	2:C:405:ILE:HG12	1.79	0.63
2:C:272:ILE:H	2:C:290:ALA:HB2	1.64	0.62
5:B:345:MET:HB3	5:B:349:ARG:HH11	1.64	0.62
4:G:26:THR:O	5:B:79:TRP:NE1	2.32	0.62
4:G:27:CYS:SG	4:G:28:TYR:N	2.73	0.62
1:A:33:G:N2	6:D:165:SER:O	2.33	0.62
2:C:110:ASP:O	2:C:112:HIS:ND1	2.31	0.61
5:B:72:ILE:HB	5:B:209:PRO:HG2	1.83	0.61
4:K:32:VAL:HG21	4:K:287:PRO:HG3	1.82	0.61
6:D:66:LEU:HD22	6:D:85:GLN:HE22	1.64	0.61
6:D:166:THR:HG23	6:D:168:ASP:H	1.65	0.61
4:I:295:ASP:HB3	4:J:286:ARG:HB3	1.83	0.61
1:A:24:C:H5'	4:J:40:GLN:HB2	1.82	0.61
4:K:96:ASN:C	4:K:96:ASN:HD22	2.08	0.61
2:C:333:PRO:HG2	2:C:336:LEU:HD11	1.81	0.61
1:A:49:U:OP2	6:D:254:LYS:NZ	2.34	0.61
4:J:155:ASP:OD1	4:J:156:LYS:N	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:8:LEU:HD23	5:B:141:LEU:HB2	1.83	0.60
4:J:17:ASN:HB3	4:J:25:LYS:HD2	1.82	0.60
4:K:95:ASP:OD1	4:K:95:ASP:N	2.35	0.60
4:I:20:ASP:N	4:I:20:ASP:OD1	2.34	0.60
5:B:358:ARG:NH2	6:D:97:GLN:OE1	2.30	0.60
1:A:8:G:O2'	4:F:18:ARG:NH2	2.34	0.60
4:H:94:ASP:N	4:H:94:ASP:OD1	2.35	0.60
1:A:21:G:H2'	4:J:148:MET:HG2	1.83	0.60
4:H:195:VAL:HG21	4:I:63:ARG:HB2	1.84	0.60
4:G:191:ALA:HB3	4:G:203:GLY:HA3	1.84	0.59
5:B:37:LYS:HA	5:B:68:MET:HE1	1.84	0.59
4:H:29:PHE:HB3	4:H:34:ARG:HG3	1.84	0.59
4:I:64:LEU:HD11	4:I:103:MET:HE2	1.84	0.59
4:F:37:ILE:HB	4:F:176:ALA:HB3	1.84	0.59
4:H:74:GLU:N	4:H:74:GLU:OE1	2.35	0.59
7:M:46:DC:N3	7:M:47:DA:N6	2.50	0.59
3:E:57:LYS:HD2	3:E:58:ARG:N	2.17	0.59
1:A:52:G:OP1	6:D:62:LYS:NZ	2.35	0.59
6:D:66:LEU:HD21	6:D:261:GLY:H	1.68	0.59
2:C:520:ILE:HD13	2:C:522:PRO:HD2	1.85	0.58
1:A:-6:U:H3	5:B:52:ARG:HH21	1.52	0.58
2:C:147:GLU:N	2:C:147:GLU:OE2	2.37	0.58
4:I:274:LYS:HE3	4:I:278:ILE:HG12	1.85	0.58
2:C:118:TYR:HB2	2:C:124:ARG:HG3	1.86	0.58
4:J:60:ARG:HG2	4:J:100:LEU:HD22	1.86	0.58
4:J:293:GLU:N	4:J:293:GLU:OE2	2.35	0.58
4:K:345:ARG:HH21	4:K:347:ILE:HG21	1.69	0.58
4:F:31:GLY:HA3	4:G:290:VAL:HG21	1.85	0.58
4:H:187:ASP:OD1	4:I:25:LYS:NZ	2.37	0.57
2:C:120:ASN:HB3	2:C:123:ASP:HB2	1.86	0.57
6:D:23:LYS:H	6:D:23:LYS:HD2	1.70	0.57
5:B:37:LYS:NZ	5:B:213:ASP:OD2	2.37	0.57
5:B:229:ILE:O	5:B:230:HIS:ND1	2.37	0.57
5:B:248:ILE:HD12	5:B:250:ARG:HH12	1.69	0.57
6:D:111:GLU:OE2	6:D:113:ASN:ND2	2.37	0.57
3:E:17:GLU:OE1	3:E:17:GLU:N	2.38	0.57
3:E:50:GLN:HG2	5:B:278:TYR:HB2	1.86	0.57
4:F:187:ASP:OD1	4:H:25:LYS:NZ	2.33	0.57
4:J:94:ASP:OD1	4:J:94:ASP:N	2.38	0.57
4:K:7:MET:HG2	4:K:217:LYS:HB2	1.87	0.57
4:K:34:ARG:NH2	4:K:284:PHE:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:93:LYS:NZ	7:M:33:DA:OP2	2.37	0.56
4:J:323:ILE:HG12	4:J:360:TYR:HE2	1.70	0.56
3:E:50:GLN:O	5:B:279:ASN:ND2	2.38	0.56
4:J:273:PHE:HD1	4:J:323:ILE:HD11	1.69	0.56
4:K:154:LYS:NZ	7:M:24:DA:OP2	2.38	0.56
4:G:47:ARG:HD3	4:G:145:CYS:HB2	1.87	0.56
5:B:10:LEU:HD11	5:B:44:LEU:HD21	1.88	0.56
5:B:295:HIS:HE1	6:D:56:SER:HA	1.70	0.56
1:A:17:U:OP1	4:I:43:LYS:NZ	2.37	0.56
4:G:34:ARG:NH1	4:G:178:SER:O	2.38	0.56
6:D:41:SER:OG	6:D:44:ARG:NH1	2.39	0.56
4:F:106:ASP:OD1	4:F:106:ASP:N	2.37	0.56
4:H:96:ASN:OD1	4:H:96:ASN:N	2.39	0.56
5:B:35:PRO:HD2	5:B:70:VAL:HG11	1.88	0.56
5:B:276:ALA:HB2	5:B:316:ALA:HB1	1.86	0.56
6:D:122:LEU:HB3	6:D:236:LEU:HB3	1.88	0.56
4:J:103:MET:O	4:J:107:LYS:NZ	2.40	0.55
4:K:39:SER:HB2	4:K:173:VAL:HG13	1.88	0.55
2:C:123:ASP:OD2	2:C:221:LYS:NZ	2.34	0.55
4:F:297:VAL:HG23	4:H:285:VAL:HG11	1.88	0.55
4:H:297:VAL:HG23	4:I:285:VAL:HG11	1.88	0.55
4:G:201:GLY:HA3	7:M:44:DG:H8	1.70	0.55
5:B:33:ASP:OD1	5:B:33:ASP:N	2.39	0.55
4:I:37:ILE:HB	4:I:176:ALA:HB3	1.89	0.55
4:K:186:ILE:HD12	4:K:186:ILE:H	1.72	0.55
4:K:154:LYS:H	4:K:154:LYS:HD2	1.72	0.55
3:E:161:ILE:HG23	3:E:165:LYS:HE3	1.88	0.55
5:B:354:ASP:OD1	5:B:354:ASP:N	2.37	0.55
4:F:68:ILE:HD13	4:F:116:LEU:HD21	1.89	0.54
4:I:295:ASP:OD1	4:I:295:ASP:N	2.39	0.54
4:G:47:ARG:HH11	4:G:145:CYS:HB2	1.72	0.54
3:E:30:ARG:HD2	5:B:342:GLY:HA3	1.89	0.54
4:J:68:ILE:O	4:J:72:ALA:HB2	2.06	0.54
4:G:171:LEU:HD11	4:G:219:PHE:HD2	1.71	0.54
6:D:129:ASN:OD1	6:D:129:ASN:N	2.40	0.54
4:I:108:ILE:HG23	4:I:132:VAL:HG22	1.89	0.54
6:D:139:MET:HE2	6:D:142:GLN:HG3	1.87	0.54
3:E:158:ASP:O	3:E:162:LYS:NZ	2.38	0.54
4:G:349:ASN:HB3	4:G:352:GLU:HG2	1.89	0.54
1:A:6:C:O2'	4:F:41:CYS:SG	2.64	0.54
2:C:459:HIS:HD2	2:C:489:LEU:HD11	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:58:GLY:H	4:I:105:LYS:HB2	1.71	0.54
4:K:187:ASP:OD1	4:K:187:ASP:N	2.40	0.54
4:G:190:VAL:HG12	4:G:205:ILE:HG23	1.89	0.54
4:J:58:GLY:HA2	4:J:104:SER:HB2	1.90	0.54
4:K:34:ARG:NH1	4:K:179:THR:O	2.41	0.54
5:B:24:ALA:HB1	5:B:29:ARG:HA	1.90	0.54
4:I:101:VAL:HG13	4:I:149:LEU:HD22	1.90	0.53
2:C:344:VAL:HG13	2:C:377:SER:HB3	1.89	0.53
4:G:285:VAL:HG21	5:B:198:ARG:HD2	1.90	0.53
4:F:295:ASP:N	4:F:295:ASP:OD1	2.41	0.53
4:H:141:ASP:OD1	4:H:141:ASP:N	2.34	0.53
2:C:214:LEU:HD13	2:C:218:CYS:HB3	1.91	0.53
4:I:266:PRO:O	4:J:315:TYR:OH	2.21	0.53
4:K:2:LEU:HB3	4:K:274:LYS:O	2.08	0.53
4:K:163:SER:OG	4:K:164:ASN:N	2.38	0.53
5:B:70:VAL:HG22	5:B:139:VAL:HG22	1.90	0.53
4:H:69:GLN:HG3	4:H:78:TRP:HB2	1.90	0.53
4:K:20:ASP:N	4:K:20:ASP:OD1	2.40	0.53
3:E:27:ARG:HA	3:E:66:LYS:HD2	1.91	0.52
4:H:185:GLU:OE2	4:H:185:GLU:N	2.42	0.52
4:I:55:LEU:HB3	4:I:140:PRO:HG2	1.92	0.52
4:J:92:ASN:ND2	4:J:94:ASP:O	2.41	0.52
4:K:8:ILE:O	4:K:267:ASP:N	2.42	0.52
4:H:203:GLY:O	4:I:62:ARG:NH1	2.42	0.52
6:D:70:ASP:OD2	6:D:125:ARG:NH2	2.41	0.52
1:A:21:G:OP2	4:I:18:ARG:NH2	2.42	0.52
4:F:282:ASN:HA	4:F:285:VAL:HG23	1.91	0.52
6:D:193:GLN:HB3	6:D:231:LEU:HB3	1.91	0.52
4:H:153:ASP:HB2	7:M:42:DA:H5''	1.91	0.52
4:I:102:PHE:HB3	4:I:147:ARG:HG2	1.91	0.52
6:D:77:ASP:N	6:D:77:ASP:OD1	2.39	0.52
2:C:104:LEU:O	2:C:108:LEU:HB2	2.10	0.52
4:I:261:ALA:HB3	4:J:174:ALA:HB2	1.92	0.52
6:D:8:LEU:HD23	6:D:105:ALA:HB3	1.91	0.52
1:A:-7:G:H4'	5:B:46:ALA:HB2	1.90	0.52
4:F:34:ARG:NH1	4:F:284:PHE:O	2.38	0.52
5:B:311:VAL:O	5:B:349:ARG:N	2.39	0.52
2:C:145:GLU:OE1	2:C:264:TRP:NE1	2.41	0.52
4:F:367:GLU:OE2	4:F:367:GLU:N	2.42	0.52
5:B:295:HIS:CE1	6:D:57:PRO:HD3	2.45	0.52
4:F:315:TYR:OH	4:G:266:PRO:O	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:104:SER:H	4:I:136:ALA:HB1	1.75	0.52
4:J:64:LEU:HD22	4:J:85:LEU:HD11	1.92	0.52
2:C:166:TYR:OH	2:C:276:LEU:HD13	2.10	0.51
6:D:73:ILE:HG13	6:D:81:ILE:HD11	1.92	0.51
2:C:182:SER:OG	2:C:326:SER:OG	2.23	0.51
3:E:57:LYS:HD2	3:E:58:ARG:H	1.74	0.51
5:B:199:TRP:CE2	5:B:202:GLU:HB3	2.46	0.51
6:D:34:ARG:HA	6:D:34:ARG:NH1	2.26	0.51
2:C:370:ASP:OD1	2:C:370:ASP:N	2.39	0.51
4:G:273:PHE:HZ	4:G:357:VAL:HG13	1.74	0.51
4:I:91:LYS:NZ	7:M:35:DT:OP1	2.44	0.51
6:D:37:MET:HE1	6:D:95:CYS:HA	1.93	0.51
4:J:146:GLY:H	4:J:169:ALA:HB2	1.75	0.51
5:B:339:LEU:HD12	5:B:364:LYS:HG3	1.91	0.51
6:D:187:GLN:NE2	6:D:237:GLU:OE2	2.42	0.51
1:A:4:U:H4'	4:F:147:ARG:HA	1.92	0.51
4:H:334:PRO:HG2	4:H:337:TYR:HE1	1.76	0.51
6:D:28:ILE:HD11	6:D:197:VAL:HG12	1.93	0.51
6:D:240:ASP:N	6:D:240:ASP:OD1	2.43	0.50
3:E:132:GLN:HA	3:E:132:GLN:NE2	2.26	0.50
1:A:1:G:OP2	4:G:40:GLN:NE2	2.45	0.50
4:G:32:VAL:HG12	4:G:34:ARG:HE	1.77	0.50
5:B:248:ILE:HB	5:B:250:ARG:HH22	1.77	0.50
4:K:37:ILE:HB	4:K:176:ALA:HB3	1.93	0.50
5:B:307:THR:OG1	5:B:308:VAL:N	2.43	0.50
1:A:-4:A:H2'	1:A:-3:A:C8	2.45	0.50
4:I:119:SER:OG	4:I:120:LEU:N	2.45	0.50
2:C:464:ILE:HG12	2:C:482:ALA:HB1	1.93	0.49
4:H:258:ASN:HA	4:I:172:GLN:HG2	1.94	0.49
4:J:55:LEU:HD22	4:J:140:PRO:HG2	1.94	0.49
4:H:2:LEU:HB3	4:H:274:LYS:O	2.11	0.49
3:E:63:LEU:HD22	3:E:117:GLU:HB3	1.94	0.49
4:G:17:ASN:HD22	4:G:38:SER:H	1.61	0.49
3:E:60:VAL:HG23	3:E:144:LEU:HD23	1.94	0.49
4:J:39:SER:HA	4:J:42:ILE:HD12	1.95	0.49
4:F:144:LEU:HD22	4:F:171:LEU:HB2	1.95	0.49
1:A:-1:C:H1'	5:B:85:VAL:HG13	1.94	0.49
2:C:179:ALA:HB3	2:C:298:LYS:HD2	1.95	0.49
4:J:7:MET:HG2	4:J:269:ILE:HG12	1.95	0.48
4:G:221:ILE:HD11	4:G:244:PHE:CD2	2.47	0.48
4:K:3:ILE:HG23	4:K:221:ILE:HB	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:289:SER:O	4:G:299:GLN:NE2	2.46	0.48
6:D:164:SER:O	6:D:164:SER:OG	2.31	0.48
2:C:250:LEU:HD11	2:C:391:TRP:HE3	1.79	0.48
4:F:317:ASP:OD2	4:F:320:SER:OG	2.29	0.48
4:H:309:ASN:HB2	4:H:342:LEU:HD11	1.95	0.48
4:K:274:LYS:HD3	4:K:322:VAL:HG21	1.94	0.48
2:C:92:VAL:HG11	2:C:114:LEU:HD13	1.95	0.48
6:D:10:ASP:HB3	6:D:104:ALA:HB2	1.95	0.48
4:F:285:VAL:HG11	4:G:297:VAL:HG23	1.95	0.48
4:J:16:LEU:HD13	4:J:37:ILE:HD11	1.94	0.48
4:F:155:ASP:OD1	4:F:155:ASP:N	2.47	0.48
4:H:365:LYS:N	4:H:368:GLU:OE1	2.47	0.48
4:K:256:LYS:O	6:D:166:THR:OG1	2.32	0.48
5:B:7:THR:HG22	5:B:142:GLN:HG2	1.96	0.48
2:C:147:GLU:OE1	2:C:150:LYS:HG3	2.14	0.48
4:F:108:ILE:O	4:F:112:ALA:HB3	2.13	0.48
4:F:314:GLY:O	4:G:349:ASN:ND2	2.47	0.48
2:C:262:GLN:O	2:C:386:ARG:NH2	2.47	0.48
1:A:0:G:H22	5:B:124:THR:HG23	1.79	0.48
4:J:156:LYS:NZ	4:J:160:VAL:O	2.47	0.48
5:B:326:ARG:HG3	5:B:352:PRO:HD2	1.96	0.47
6:D:2:ILE:HG13	6:D:114:PRO:HD3	1.96	0.47
6:D:9:ILE:HG21	6:D:25:LEU:HD11	1.96	0.47
2:C:408:LYS:HE2	2:C:465:ALA:HB1	1.94	0.47
4:F:141:ASP:OD1	4:F:141:ASP:N	2.46	0.47
4:H:273:PHE:HZ	4:H:357:VAL:HG13	1.80	0.47
4:K:156:LYS:NZ	4:K:157:ASP:O	2.47	0.47
2:C:92:VAL:HG12	2:C:116:LEU:HD23	1.96	0.47
2:C:456:ILE:HD13	2:C:493:VAL:HG21	1.96	0.47
4:H:62:ARG:HH22	7:M:38:DC:H4'	1.79	0.47
4:K:282:ASN:HA	4:K:285:VAL:HG23	1.96	0.47
5:B:23:GLU:HG3	5:B:30:ARG:HD2	1.96	0.47
4:F:349:ASN:HB3	4:F:352:GLU:HB3	1.96	0.47
5:B:8:LEU:HD13	5:B:151:LEU:HB3	1.96	0.47
1:A:2:A:H62	7:M:49:DT:H3	1.62	0.47
2:C:108:LEU:HD21	2:C:160:LEU:HD12	1.96	0.47
4:F:285:VAL:HG12	4:G:295:ASP:HB2	1.96	0.47
4:H:263:HIS:NE2	4:I:172:GLN:OE1	2.36	0.47
5:B:228:GLU:OE1	5:B:249:ARG:NH1	2.36	0.47
2:C:451:PRO:HB3	4:G:21:LEU:HB2	1.96	0.47
3:E:42:SER:O	3:E:46:TRP:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:133:ARG:HH21	6:D:156:ARG:HD3	1.79	0.47
1:A:32:A:C6	6:D:196:TRP:HB2	2.50	0.47
4:H:138:LEU:HD22	4:H:138:LEU:HA	1.79	0.47
5:B:374:ARG:NH1	6:D:15:PRO:O	2.38	0.47
2:C:501:GLN:O	3:E:157:SER:OG	2.29	0.47
5:B:173:ARG:HH22	5:B:196:GLN:HB3	1.79	0.47
4:H:7:MET:HE2	4:H:217:LYS:HD2	1.96	0.46
6:D:255:ALA:HB1	6:D:258:PHE:HB2	1.95	0.46
5:B:346:THR:OG1	5:B:347:THR:N	2.43	0.46
2:C:197:THR:H	2:C:199:HIS:CE1	2.33	0.46
4:F:295:ASP:OD2	4:F:333:TYR:OH	2.26	0.46
4:J:6:HIS:HB3	4:J:216:TYR:HE1	1.80	0.46
4:I:368:GLU:OE2	4:I:368:GLU:N	2.46	0.46
4:J:282:ASN:HA	4:J:285:VAL:HG23	1.97	0.46
4:I:92:ASN:OD1	4:I:92:ASN:N	2.42	0.46
5:B:134:ASP:OD1	5:B:198:ARG:NH1	2.48	0.46
3:E:76:ARG:HB3	3:E:134:CYS:HB2	1.96	0.46
1:A:-4:A:P	5:B:29:ARG:HH21	2.38	0.46
2:C:171:GLY:O	2:C:175:ARG:NH2	2.46	0.46
2:C:172:ASP:OD1	2:C:172:ASP:N	2.41	0.46
2:C:367:ALA:HB1	2:C:461:GLU:HG3	1.97	0.46
4:J:198:GLU:OE2	4:J:198:GLU:N	2.34	0.46
4:K:80:LYS:NZ	4:K:118:ASN:OD1	2.48	0.46
6:D:191:LEU:HD21	6:D:194:LEU:HD22	1.97	0.46
1:A:11:A:O2'	4:F:190:VAL:O	2.32	0.46
1:A:24:C:O2'	4:J:41:CYS:SG	2.62	0.46
2:C:194:GLU:OE1	5:B:25:LYS:HG2	2.16	0.46
3:E:27:ARG:HD3	3:E:70:GLU:HG3	1.97	0.46
3:E:148:GLU:HB3	4:G:291:VAL:HG12	1.98	0.46
1:A:20:G:H5'	4:I:255:GLY:HA2	1.98	0.46
4:I:99:MET:HE3	4:I:99:MET:HA	1.98	0.46
5:B:274:THR:OG1	5:B:275:ARG:N	2.49	0.46
2:C:87:ASP:OD1	2:C:87:ASP:N	2.49	0.45
2:C:237:ILE:HG23	2:C:329:VAL:HG11	1.98	0.45
4:J:295:ASP:OD1	4:J:295:ASP:N	2.47	0.45
4:K:109:LYS:HA	4:K:109:LYS:HD3	1.80	0.45
2:C:379:LEU:HD12	2:C:422:LEU:HD11	1.98	0.45
4:F:103:MET:SD	4:F:108:ILE:HB	2.57	0.45
4:F:174:ALA:HB2	4:G:261:ALA:HB3	1.98	0.45
4:I:157:ASP:OD1	4:I:157:ASP:N	2.49	0.45
5:B:282:GLU:OE2	5:B:285:LYS:NZ	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:68:ARG:NE	6:D:262:LEU:HB3	2.32	0.45
4:I:71:GLU:OE1	4:I:113:ARG:NE	2.45	0.45
4:J:37:ILE:HB	4:J:176:ALA:HB3	1.97	0.45
2:C:356:ILE:HA	2:C:356:ILE:HD13	1.84	0.45
3:E:105:PHE:HA	3:E:123:ILE:HD11	1.98	0.45
4:F:177:ILE:HD11	4:F:281:ALA:HB1	1.99	0.45
2:C:358:LEU:H	2:C:358:LEU:HG	1.50	0.45
2:C:427:ASN:OD1	2:C:427:ASN:N	2.50	0.45
4:H:99:MET:HE3	4:H:99:MET:HB2	1.81	0.45
4:J:21:LEU:HD22	5:B:375:GLY:HA3	1.99	0.45
2:C:445:LYS:HE2	2:C:446:LYS:HZ1	1.80	0.45
3:E:38:PHE:CG	5:B:338:MET:HG3	2.51	0.45
4:J:157:ASP:OD1	4:J:157:ASP:N	2.50	0.45
5:B:298:CYS:SG	5:B:299:MET:N	2.89	0.45
4:I:152:ASN:OD1	4:I:154:LYS:N	2.44	0.45
4:J:47:ARG:HH12	4:J:60:ARG:HH21	1.64	0.45
6:D:93:ASP:O	6:D:97:GLN:HB3	2.17	0.45
6:D:130:ALA:HB1	6:D:159:LEU:HB3	1.99	0.45
2:C:209:ASP:OD1	2:C:209:ASP:N	2.49	0.44
4:H:294:SER:OG	4:H:295:ASP:N	2.50	0.44
4:G:222:ASP:OD1	4:G:225:GLN:HB3	2.17	0.44
4:G:304:LEU:O	4:G:308:VAL:HG23	2.16	0.44
5:B:309:GLN:HE22	5:B:337:THR:HG23	1.81	0.44
1:A:-6:U:H1'	1:A:-4:A:H1'	2.00	0.44
4:H:230:LEU:HD22	4:H:236:LEU:HD23	1.99	0.44
4:H:335:LEU:HD23	4:H:335:LEU:HA	1.85	0.44
4:G:172:GLN:HE22	4:G:220:SER:HB3	1.81	0.44
4:I:361:ILE:HG22	4:I:364:PHE:HE2	1.83	0.44
4:J:124:GLU:CD	4:J:124:GLU:H	2.26	0.44
6:D:146:THR:OG1	6:D:148:GLU:OE2	2.29	0.44
2:C:375:LEU:HD12	2:C:425:LEU:HD12	1.99	0.44
4:H:20:ASP:OD1	4:H:20:ASP:N	2.44	0.44
4:I:64:LEU:O	4:I:68:ILE:HG12	2.18	0.44
4:G:198:GLU:OE2	4:G:198:GLU:N	2.35	0.44
6:D:62:LYS:HA	6:D:62:LYS:HD2	1.78	0.44
6:D:131:SER:HB2	6:D:156:ARG:HG2	2.00	0.44
2:C:251:TRP:HA	2:C:389:LYS:O	2.17	0.44
3:E:3:ARG:HD3	3:E:3:ARG:HA	1.77	0.44
4:H:174:ALA:HB3	4:H:218:TYR:HB3	1.98	0.44
4:J:141:ASP:OD1	4:J:141:ASP:N	2.49	0.44
4:F:295:ASP:HB2	4:H:285:VAL:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:231:LYS:HB2	4:J:231:LYS:HE2	1.74	0.44
3:E:80:THR:HG23	3:E:82:PRO:HD2	2.00	0.44
4:F:270:LEU:HG	4:F:326:TRP:HE3	1.83	0.44
4:I:254:SER:O	4:I:254:SER:OG	2.34	0.44
4:J:109:LYS:O	4:J:113:ARG:HG3	2.17	0.44
4:K:21:LEU:HD22	6:D:25:LEU:HD12	1.99	0.44
4:G:5:ILE:HB	4:G:219:PHE:HB2	2.00	0.44
1:A:30:G:O2'	4:K:41:CYS:SG	2.70	0.44
4:F:32:VAL:HG23	4:F:34:ARG:HE	1.83	0.44
4:J:38:SER:HB3	4:J:40:GLN:HG2	2.00	0.44
4:J:266:PRO:O	4:K:315:TYR:OH	2.31	0.44
2:C:445:LYS:HE2	2:C:445:LYS:HB2	1.68	0.44
4:J:40:GLN:HG2	4:J:40:GLN:H	1.58	0.44
5:B:248:ILE:HB	5:B:250:ARG:NH2	2.33	0.43
1:A:37:U:H6	1:A:38:C:H5	1.65	0.43
4:G:310:ASP:O	4:G:312:ARG:N	2.50	0.43
2:C:308:GLN:HB2	2:C:320:ALA:HA	1.99	0.43
4:F:194:ASP:OD2	4:H:47:ARG:NH2	2.45	0.43
4:H:297:VAL:O	4:H:301:ILE:HG13	2.19	0.43
4:K:71:GLU:N	4:K:71:GLU:OE1	2.51	0.43
5:B:71:ARG:HB2	5:B:190:LEU:HD22	1.99	0.43
5:B:184:ASN:OD1	5:B:184:ASN:N	2.47	0.43
5:B:293:MET:SD	5:B:293:MET:N	2.78	0.43
1:A:20:G:H22	7:M:31:DC:H5	1.66	0.43
4:F:174:ALA:HB3	4:F:218:TYR:HB3	2.00	0.43
4:J:59:VAL:H	4:J:104:SER:HA	1.82	0.43
2:C:262:GLN:OE1	2:C:386:ARG:NE	2.52	0.43
4:H:222:ASP:HB3	4:H:225:GLN:HB3	2.00	0.43
4:J:67:LEU:O	4:J:71:GLU:HG3	2.19	0.43
4:K:96:ASN:C	4:K:96:ASN:ND2	2.76	0.43
2:C:286:VAL:HB	2:C:290:ALA:HB3	2.01	0.43
4:G:209:MET:HE2	4:G:209:MET:HB3	1.90	0.43
1:A:12:G:O2'	1:A:14:A:OP1	2.36	0.43
2:C:498:GLU:O	2:C:509:ARG:NH1	2.51	0.43
4:K:150:GLU:HA	4:K:151:PRO:HD3	1.81	0.43
5:B:362:LEU:HA	5:B:365:ARG:HG2	2.00	0.43
2:C:90:VAL:HB	2:C:102:ILE:HD12	2.00	0.43
4:H:83:GLU:HG2	4:H:122:LEU:HD11	2.00	0.43
4:J:289:SER:O	4:J:299:GLN:NE2	2.39	0.43
4:J:311:ILE:HD13	4:J:311:ILE:HA	1.91	0.43
6:D:91:ASP:N	6:D:91:ASP:OD1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-5:G:H3'	5:B:20:GLY:HA3	2.01	0.42
2:C:107:THR:HA	2:C:114:LEU:HD21	2.00	0.42
4:F:289:SER:O	4:F:299:GLN:NE2	2.44	0.42
4:H:282:ASN:HA	4:H:285:VAL:HG23	2.00	0.42
4:I:24:PRO:HD2	4:I:209:MET:HE2	2.01	0.42
4:G:338:LYS:HA	4:G:338:LYS:HD3	1.85	0.42
6:D:61:GLN:NE2	6:D:63:THR:OG1	2.52	0.42
6:D:162:ASP:OD1	6:D:162:ASP:N	2.44	0.42
1:A:16:A:O2'	4:I:60:ARG:NH1	2.42	0.42
2:C:446:LYS:HE2	2:C:446:LYS:N	2.34	0.42
3:E:82:PRO:HG3	3:E:156:TRP:CD1	2.54	0.42
4:F:113:ARG:HD2	4:F:113:ARG:HA	1.76	0.42
4:H:311:ILE:O	4:H:315:TYR:HB2	2.18	0.42
4:I:93:LYS:HB2	4:I:98:LYS:HE2	2.02	0.42
6:D:122:LEU:N	6:D:236:LEU:O	2.46	0.42
6:D:139:MET:HE1	6:D:147:ILE:H	1.83	0.42
2:C:500:ALA:HB1	2:C:502:THR:HG23	2.00	0.42
3:E:57:LYS:HE3	3:E:59:GLU:HB2	2.01	0.42
4:F:274:LYS:HD2	4:F:278:ILE:HG12	2.01	0.42
4:I:190:VAL:HG22	4:I:205:ILE:HG12	2.00	0.42
2:C:380:HIS:NE2	2:C:419:ASP:OD1	2.46	0.42
3:E:131:GLN:N	3:E:131:GLN:OE1	2.52	0.42
4:K:138:LEU:HD12	4:K:138:LEU:HA	1.87	0.42
4:G:286:ARG:HD2	4:G:286:ARG:HA	1.46	0.42
5:B:125:LEU:HD22	5:B:125:LEU:HA	1.90	0.42
2:C:116:LEU:HD23	2:C:116:LEU:HA	1.92	0.42
4:F:165:THR:O	4:F:165:THR:OG1	2.37	0.42
4:I:136:ALA:O	4:I:138:LEU:N	2.52	0.42
4:F:17:ASN:HB3	4:F:25:LYS:HG3	2.02	0.42
4:F:191:ALA:O	4:F:203:GLY:N	2.44	0.42
4:I:78:TRP:CD1	4:I:79:LYS:HG3	2.55	0.42
4:K:1:MET:HE3	4:K:1:MET:N	2.35	0.42
4:G:286:ARG:HA	4:G:287:PRO:HD2	1.97	0.42
5:B:277:ASP:OD1	5:B:280:ASN:ND2	2.29	0.42
4:H:55:LEU:HD13	4:H:240:THR:HA	2.02	0.42
3:E:18:GLY:O	3:E:22:ILE:HG23	2.19	0.42
4:K:33:LEU:HB2	6:D:76:ASN:HA	2.02	0.42
5:B:290:ARG:NE	5:B:325:LEU:O	2.41	0.42
4:H:290:VAL:HG21	4:I:31:GLY:HA3	2.02	0.42
4:H:349:ASN:ND2	4:I:313:LEU:O	2.53	0.42
4:F:64:LEU:HB3	4:F:85:LEU:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:64:LEU:HD12	4:F:64:LEU:HA	1.79	0.41
4:F:100:LEU:HD23	4:F:100:LEU:HA	1.84	0.41
4:H:168:GLU:O	4:H:229:ASN:ND2	2.53	0.41
4:H:272:GLU:OE1	4:H:280:TYR:OH	2.33	0.41
4:H:358:LEU:HD23	4:H:361:ILE:HD12	2.02	0.41
6:D:68:ARG:HH22	6:D:127:ARG:N	2.17	0.41
2:C:193:HIS:H	2:C:225:ARG:NH1	2.18	0.41
3:E:108:LEU:HD22	3:E:116:MET:HE1	2.02	0.41
4:J:56:LEU:HD12	4:J:56:LEU:HA	1.93	0.41
4:H:245:LEU:HD23	4:H:354:VAL:HG22	2.01	0.41
2:C:112:HIS:CE1	2:C:151:PRO:HG3	2.56	0.41
4:H:195:VAL:HG13	4:I:61:THR:HG21	2.02	0.41
5:B:358:ARG:HH22	6:D:97:GLN:CD	2.25	0.41
7:M:46:DC:H2'	7:M:47:DA:C8	2.55	0.41
7:M:49:DT:H6	7:M:49:DT:H2'	1.69	0.41
4:F:107:LYS:HD2	4:F:107:LYS:HA	1.84	0.41
4:I:319:GLN:HB3	4:I:320:SER:H	1.64	0.41
4:J:34:ARG:NH1	4:J:284:PHE:O	2.54	0.41
4:G:326:TRP:CD2	4:G:335:LEU:HB2	2.55	0.41
1:A:33:G:C2	6:D:167:PRO:HD3	2.56	0.41
4:J:55:LEU:HB3	4:J:140:PRO:HG2	2.01	0.41
6:D:51:PHE:HB3	6:D:97:GLN:HE21	1.85	0.41
3:E:120:LEU:O	3:E:124:MET:HG3	2.21	0.41
4:G:42:ILE:HG21	4:G:217:LYS:HZ3	1.86	0.41
2:C:157:ILE:HG23	2:C:158:PRO:HD3	2.03	0.41
4:J:29:PHE:HB3	4:J:34:ARG:HG3	2.03	0.41
4:J:246:LEU:HD23	4:J:246:LEU:HA	1.91	0.41
4:K:62:ARG:HG3	4:K:100:LEU:HG	2.03	0.41
5:B:290:ARG:HH21	5:B:326:ARG:HE	1.68	0.41
4:J:61:THR:HG21	4:J:67:LEU:HD11	2.02	0.41
4:G:341:LYS:HA	4:G:341:LYS:HD2	1.76	0.41
5:B:313:TYR:HE1	5:B:349:ARG:HG2	1.86	0.41
3:E:86:GLY:HA2	3:E:89:CYS:HB2	2.02	0.40
3:E:120:LEU:HD23	3:E:120:LEU:HA	1.87	0.40
4:H:224:GLU:OE2	4:H:224:GLU:N	2.36	0.40
4:J:361:ILE:HD13	4:J:361:ILE:HA	1.91	0.40
5:B:229:ILE:HD12	5:B:229:ILE:HA	1.86	0.40
6:D:139:MET:SD	6:D:146:THR:OG1	2.79	0.40
6:D:266:LEU:HD13	6:D:266:LEU:HA	1.91	0.40
2:C:108:LEU:HD12	2:C:108:LEU:HA	1.85	0.40
3:E:63:LEU:HA	3:E:66:LYS:HZ3	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:6:HIS:HB3	4:H:216:TYR:HE1	1.87	0.40
4:F:87:LYS:HE3	4:F:122:LEU:HG	2.02	0.40
1:A:6:C:C5	1:A:8:G:H5''	2.55	0.40
2:C:174:LYS:HE2	2:C:174:LYS:HB2	1.98	0.40
2:C:256:LEU:HA	2:C:259:MET:HB2	2.04	0.40
4:I:246:LEU:HD23	4:I:246:LEU:HA	1.97	0.40
6:D:20:PRO:HB2	6:D:102:PHE:HE1	1.86	0.40
6:D:194:LEU:HD12	6:D:194:LEU:HA	1.87	0.40
3:E:22:ILE:HD12	3:E:36:PRO:HB2	2.03	0.40
4:J:68:ILE:O	4:J:72:ALA:CB	2.70	0.40
4:G:238:ALA:HB1	4:G:358:LEU:HD22	2.04	0.40
5:B:69:GLY:HA3	5:B:190:LEU:HD11	2.03	0.40
6:D:51:PHE:HB2	6:D:94:TYR:HE1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	441/546 (81%)	395 (90%)	44 (10%)	2 (0%)	25	61
3	E	163/174 (94%)	156 (96%)	7 (4%)	0	100	100
4	F	364/378 (96%)	343 (94%)	21 (6%)	0	100	100
4	G	247/378 (65%)	234 (95%)	13 (5%)	0	100	100
4	H	373/378 (99%)	350 (94%)	23 (6%)	0	100	100
4	I	371/378 (98%)	341 (92%)	29 (8%)	1 (0%)	37	70
4	J	372/378 (98%)	337 (91%)	33 (9%)	2 (0%)	25	61
4	K	344/378 (91%)	318 (92%)	26 (8%)	0	100	100
5	B	339/388 (87%)	315 (93%)	23 (7%)	1 (0%)	37	70
6	D	252/272 (93%)	232 (92%)	19 (8%)	1 (0%)	30	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3266/3648 (90%)	3021 (92%)	238 (7%)	7 (0%)	45 77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	306	PRO
4	J	151	PRO
2	C	301	LEU
5	B	87	ALA
4	I	322	VAL
6	D	235	VAL
4	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	C	370/470 (79%)	354 (96%)	16 (4%)	25 58
3	E	143/153 (94%)	137 (96%)	6 (4%)	25 59
4	F	295/313 (94%)	286 (97%)	9 (3%)	35 68
4	G	199/313 (64%)	191 (96%)	8 (4%)	27 61
4	H	302/313 (96%)	292 (97%)	10 (3%)	33 67
4	I	297/313 (95%)	287 (97%)	10 (3%)	32 66
4	J	293/313 (94%)	278 (95%)	15 (5%)	20 53
4	K	285/313 (91%)	277 (97%)	8 (3%)	38 70
5	B	282/322 (88%)	269 (95%)	13 (5%)	23 56
6	D	213/238 (90%)	204 (96%)	9 (4%)	25 59
All	All	2679/3061 (88%)	2575 (96%)	104 (4%)	30 61

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	96	SER
2	C	98	LYS
2	C	109	LYS
2	C	144	VAL
2	C	200	ASN
2	C	203	HIS
2	C	259	MET
2	C	260	LEU
2	C	286	VAL
2	C	338	TRP
2	C	358	LEU
2	C	380	HIS
2	C	392	LEU
2	C	419	ASP
2	C	477	TYR
2	C	496	SER
3	E	35	LEU
3	E	91	LYS
3	E	111	LEU
3	E	114	MET
3	E	132	GLN
3	E	144	LEU
4	F	38	SER
4	F	44	ARG
4	F	97	THR
4	F	123	THR
4	F	138	LEU
4	F	157	ASP
4	F	165	THR
4	F	245	LEU
4	F	251	THR
4	H	17	ASN
4	H	94	ASP
4	H	96	ASN
4	H	122	LEU
4	H	138	LEU
4	H	141	ASP
4	H	157	ASP
4	H	234	THR
4	H	328	SER
4	H	344	SER
4	I	17	ASN
4	I	45	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	59	VAL
4	I	113	ARG
4	I	138	LEU
4	I	190	VAL
4	I	236	LEU
4	I	276	SER
4	I	316	TYR
4	I	320	SER
4	J	18	ARG
4	J	20	ASP
4	J	49	SER
4	J	74	GLU
4	J	102	PHE
4	J	119	SER
4	J	145	CYS
4	J	163	SER
4	J	251	THR
4	J	289	SER
4	J	290	VAL
4	J	294	SER
4	J	328	SER
4	J	340	SER
4	J	369	VAL
4	K	3	ILE
4	K	88	CYS
4	K	96	ASN
4	K	100	LEU
4	K	323	ILE
4	K	328	SER
4	K	338	LYS
4	K	341	LYS
4	G	27	CYS
4	G	32	VAL
4	G	173	VAL
4	G	186	ILE
4	G	286	ARG
4	G	294	SER
4	G	297	VAL
4	G	323	ILE
5	B	8	LEU
5	B	50	ILE
5	B	60	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	125	LEU
5	B	136	SER
5	B	159	VAL
5	B	235	VAL
5	B	237	PHE
5	B	253	VAL
5	B	299	MET
5	B	306	THR
5	B	311	VAL
5	B	347	THR
6	D	41	SER
6	D	63	THR
6	D	135	HIS
6	D	154	HIS
6	D	166	THR
6	D	225	LEU
6	D	245	LEU
6	D	264	SER
6	D	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	120	ASN
2	C	178	GLN
2	C	384	ASN
2	C	459	HIS
2	C	474	ASN
4	F	252	ASN
4	F	257	GLN
4	F	339	HIS
4	H	257	GLN
4	H	309	ASN
4	I	69	GLN
4	I	225	GLN
4	J	50	ASN
4	J	69	GLN
4	J	92	ASN
4	J	135	GLN
4	J	152	ASN
4	J	263	HIS
4	J	309	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	15	ASN
4	K	82	GLN
4	K	92	ASN
4	K	135	GLN
4	G	17	ASN
4	G	172	GLN
4	G	252	ASN
4	G	258	ASN
5	B	206	GLN
5	B	222	HIS
6	D	30	ASN
6	D	61	GLN
6	D	220	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/61 (93%)	30 (52%)	0

All (30) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-6	U
1	A	-5	G
1	A	-3	A
1	A	1	G
1	A	2	A
1	A	6	C
1	A	7	C
1	A	8	G
1	A	9	U
1	A	11	A
1	A	12	G
1	A	13	G
1	A	14	A
1	A	18	U
1	A	19	A
1	A	20	G
1	A	24	C
1	A	25	G
1	A	26	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	27	U
1	A	31	C
1	A	32	A
1	A	33	G
1	A	39	C
1	A	42	A
1	A	43	C
1	A	44	G
1	A	45	C
1	A	51	G
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 ⓘ

There are no chain breaks in this entry.