



Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 01:38 PM JST

PDB ID : 9JT2 / pdb_00009jt2
EMDB ID : EMD-61790
Title : substrate-bound NbaSPARDA complexes
Authors : Zhuang, L.
Deposited on : 2024-10-01
Resolution : 3.19 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) : 2.44

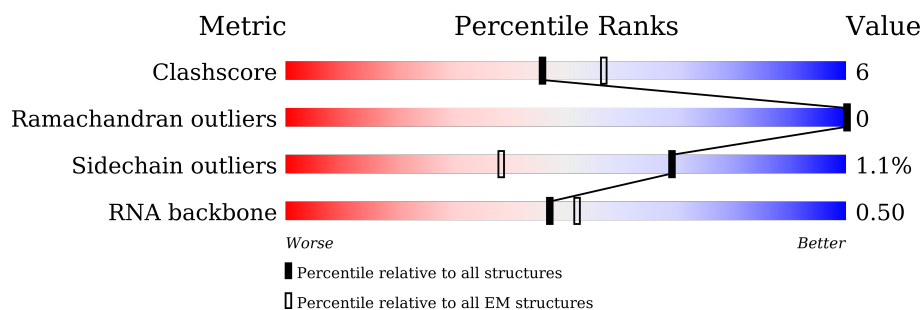
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.19 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.






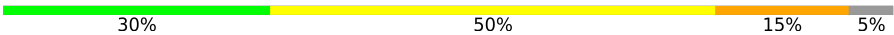





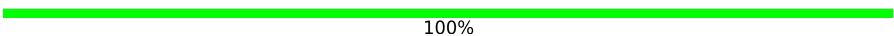
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	485	86% 10% .
1	E	485	88% 8% .
1	I	485	86% 10% .
1	M	485	84% 12% .
2	B	442	74% 18% . 7%
2	F	442	78% 14% 7%
2	J	442	73% 14% . 12%
2	N	442	66% 21% . 12%

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Mol	Chain	Length	Quality of chain
3	C	20	
3	G	20	
3	K	20	
3	O	20	
4	D	21	
4	H	21	
4	L	21	
4	P	21	
5	Q	8	
5	R	8	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 31178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ago.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	468	Total	C	N	O	S	0	0
			3715	2356	655	690	14		
1	E	468	Total	C	N	O	S	0	0
			3715	2356	655	690	14		
1	I	465	Total	C	N	O	S	0	0
			3696	2344	651	687	14		
1	M	465	Total	C	N	O	S	0	0
			3696	2344	651	687	14		

- Molecule 2 is a protein called DREN-APAZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3304	2106	575	614	9		
2	F	409	Total	C	N	O	S	0	0
			3297	2101	574	613	9		
2	J	389	Total	C	N	O	S	0	0
			3149	2001	551	588	9		
2	N	389	Total	C	N	O	S	0	0
			3149	2001	551	588	9		

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*CP*GP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	19	Total	C	N	O	P	0	0
			405	181	73	132	19		
3	G	20	Total	C	N	O	P	0	0
			427	191	78	138	20		
3	K	18	Total	C	N	O	P	0	0
			385	172	71	124	18		
3	O	19	Total	C	N	O	P	0	0
			405	181	73	132	19		

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	18	Total	C	N	O	P	0	0
			370	176	67	109	18		
4	H	19	Total	C	N	O	P	0	0
			391	186	69	117	19		
4	L	18	Total	C	N	O	P	0	0
			370	176	67	109	18		
4	P	18	Total	C	N	O	P	0	0
			370	176	67	109	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	8	Total	C	N	O	P	0	0
			164	78	30	48	8		
5	R	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

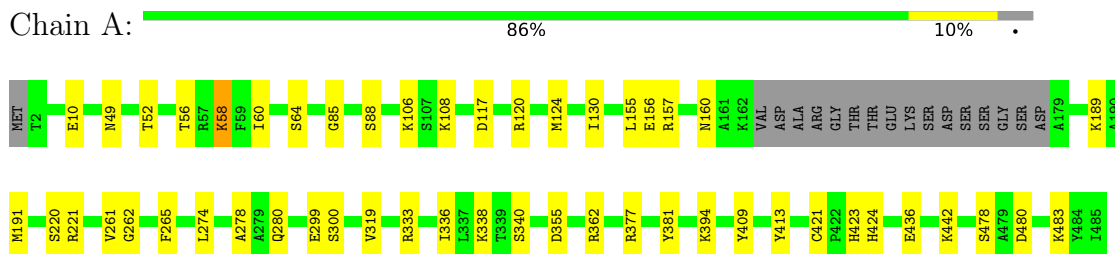
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	I	1	Total	Mg	0
			1	1	
6	M	1	Total	Mg	0
			1	1	

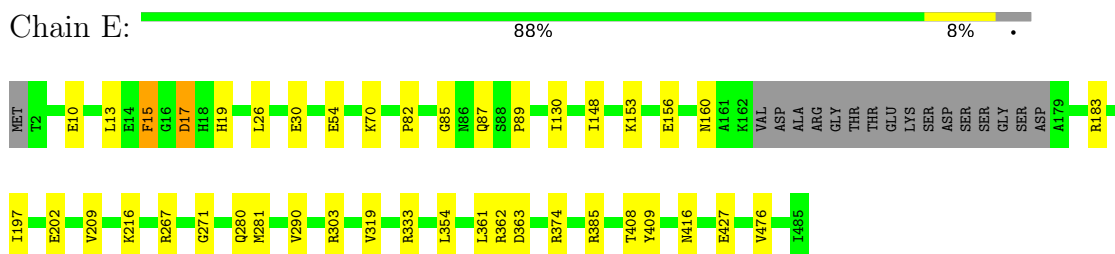
3 Residue-property plots [i](#)

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

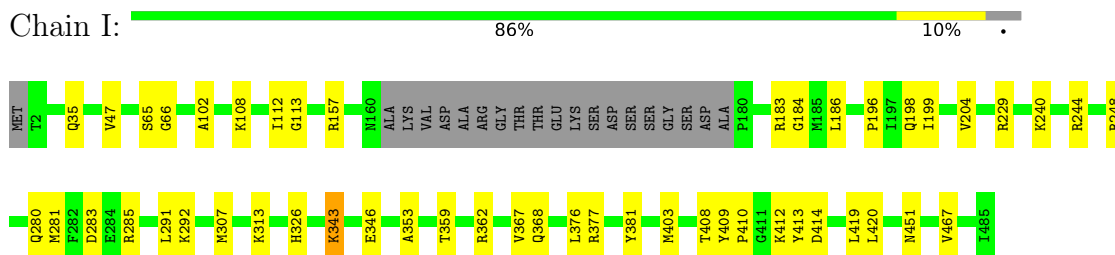
- Molecule 1: Ago



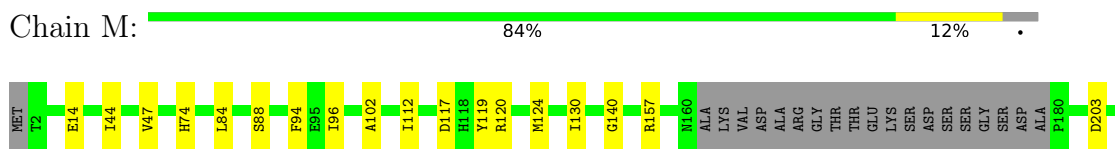
- Molecule 1: Ago



- Molecule 1: Ago

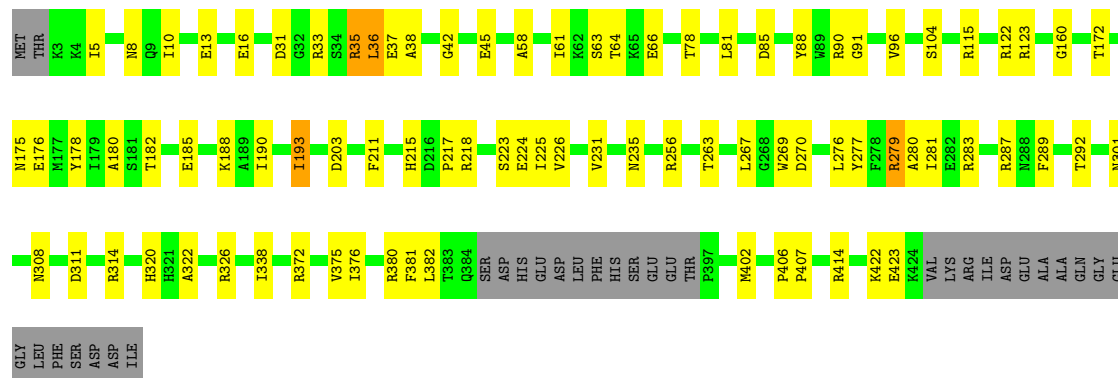


- Molecule 1: Ago



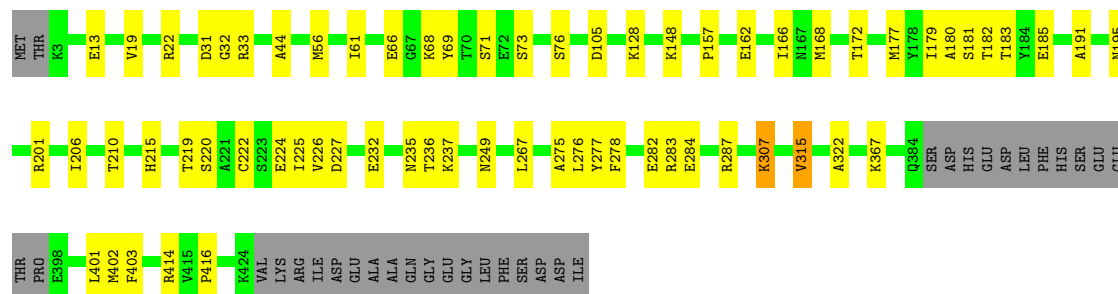
- Molecule 2: DREN-APAZ

Chain B: 74% 18% 7%



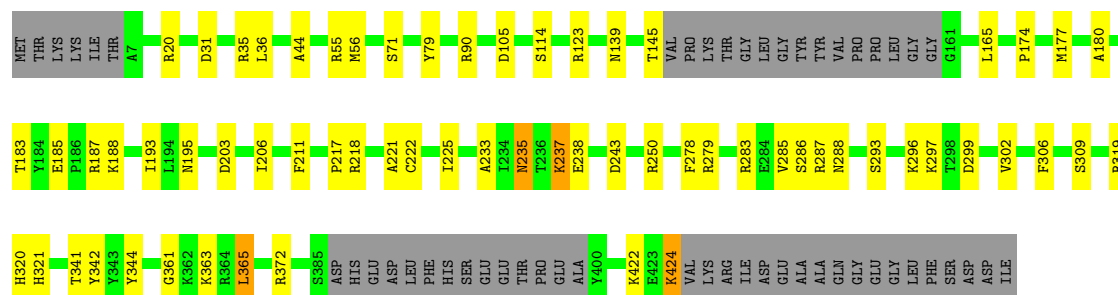
- Molecule 2: DREN-APAZ

Chain F: 78% 14% 7%



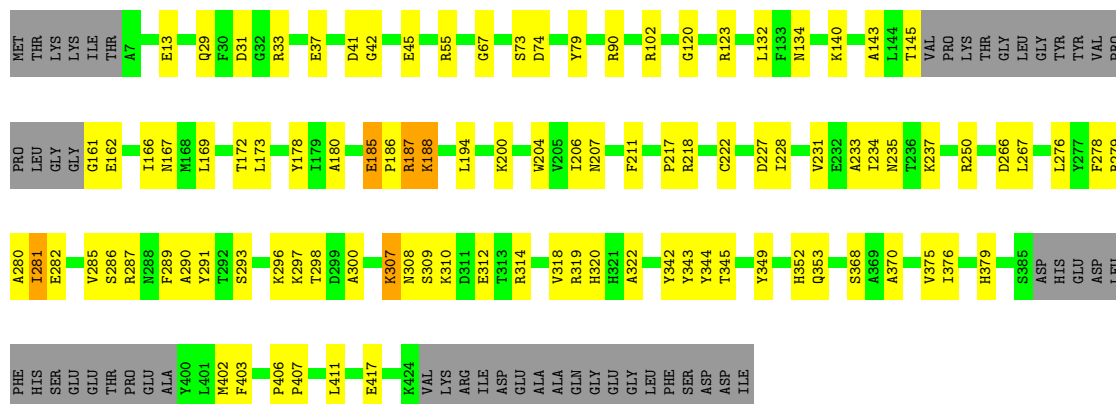
- Molecule 2: DREN-APAZ

Chain J: 73% 14% 1% 12%



- Molecule 2: DREN-APAZ

Chain N: 



• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C
P*GP*AP*UP*A)-3')

Chain C: 



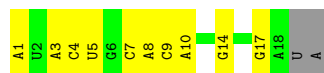
• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C
P*GP*AP*UP*A)-3')

Chain G: 

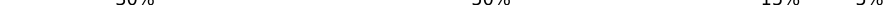


• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C
P*GP*AP*UP*A)-3')

Chain K: 




• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C
P*GP*AP*UP*A)-3')

Chain O: 



• Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP
*GP*TP*AP*TP*T)-3')

Chain D:  81% 5% 14%



- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain H:  62% 29% 10%




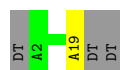
- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain L:  62% 24% 14%




- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain P:  81% 5% 14%



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

Chain Q:  75% 25%



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

Chain R:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/3800	0.38	0/5131
1	E	0.14	0/3800	0.35	0/5131
1	I	0.14	0/3781	0.36	0/5105
1	M	0.14	0/3781	0.35	0/5105
2	B	0.16	0/3386	0.41	0/4588
2	F	0.18	0/3378	0.48	0/4577
2	J	0.18	0/3224	0.47	0/4365
2	N	0.19	0/3224	0.50	0/4365
3	C	0.15	0/452	0.33	0/700
3	G	0.11	0/477	0.25	0/739
3	K	0.12	0/430	0.30	0/666
3	O	0.15	0/452	0.37	0/700
4	D	0.22	0/414	0.45	0/637
4	H	0.18	0/437	0.42	0/671
4	L	0.21	0/414	0.41	0/637
4	P	0.20	0/414	0.41	0/637
5	Q	0.20	0/183	0.48	0/278
5	R	0.20	0/183	0.45	0/278
All	All	0.16	0/32230	0.41	0/44310

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3715	0	3695	30	0
1	E	3715	0	3695	25	0
1	I	3696	0	3673	31	0
1	M	3696	0	3673	39	0
2	B	3304	0	3243	59	0
2	F	3297	0	3235	44	0
2	J	3149	0	3073	45	0
2	N	3149	0	3073	74	0
3	C	405	0	206	6	0
3	G	427	0	217	6	0
3	K	385	0	196	6	0
3	O	405	0	206	9	0
4	D	370	0	204	1	0
4	H	391	0	216	5	0
4	L	370	0	204	8	0
4	P	370	0	204	1	0
5	Q	164	0	91	2	0
5	R	164	0	91	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
All	All	31178	0	29195	362	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 6.

All (362) 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:N:308:ASN:HB3	2:N:314:ARG:HG2	1.47	0.94
3:C:13:U:H2'	3:C:14:G:H8	1.38	0.89
2:N:79:TYR:O	2:N:123:ARG:HA	1.75	0.86
3:C:13:U:H2'	3:C:14:G:C8	2.11	0.85
2:N:161:GLY:HA3	2:N:411:LEU:O	1.79	0.82
2:B:280:ALA:HA	2:B:287:ARG:HE	1.45	0.80
1:M:291:LEU:HD21	1:M:456:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:456:ILE:HG23	1:M:457:PRO:HD3	1.68	0.76
1:M:455:PRO:HB2	1:M:457:PRO:HD2	1.73	0.70
2:F:166:ILE:HG23	2:F:168:MET:H	1.58	0.68
2:N:307:LYS:HE2	2:N:309:SER:HA	1.76	0.66
1:M:280:GLN:HG2	1:M:319:VAL:HG22	1.78	0.65
2:N:308:ASN:CB	2:N:314:ARG:HG2	2.25	0.64
2:N:180:ALA:HB3	2:N:211:PHE:HB3	1.78	0.63
2:J:187:ARG:HH21	3:K:17:G:H21	1.46	0.63
2:J:221:ALA:O	2:J:225:ILE:N	2.32	0.63
2:N:29:GLN:HB2	2:N:45:GLU:HB3	1.80	0.62
2:N:169:LEU:HD12	2:N:403:PHE:HB3	1.80	0.62
1:I:47:VAL:HG22	1:I:102:ALA:HB3	1.81	0.62
2:F:201:ARG:NH2	2:F:220:SER:OG	2.33	0.62
2:J:293:SER:HB3	2:J:296:LYS:HB2	1.82	0.60
2:F:249:ASN:HB2	4:H:7:DC:H4'	1.82	0.60
2:B:280:ALA:HB2	2:B:287:ARG:HG2	1.83	0.60
2:B:36:LEU:HD13	2:N:29:GLN:HG2	1.83	0.60
1:E:156:GLU:HA	1:E:160:ASN:HB2	1.84	0.60
2:B:31:ASP:O	2:B:42:GLY:HA3	2.02	0.59
2:B:33:ARG:NH2	2:N:45:GLU:OE1	2.35	0.59
1:E:374:ARG:NH2	1:E:416:ASN:OD1	2.36	0.59
2:F:162:GLU:HG2	2:F:414:ARG:HG3	1.84	0.59
2:J:235:ASN:CG	2:J:237:LYS:H	2.10	0.59
1:A:130:ILE:HG13	1:A:189:LYS:HB3	1.85	0.59
1:E:280:GLN:HG2	1:E:319:VAL:HG22	1.85	0.59
2:F:185:GLU:H	2:F:206:ILE:HG21	1.67	0.59
2:B:292:THR:O	2:B:380:ARG:NH1	2.34	0.59
2:N:90:ARG:HH21	2:N:120:GLY:HA2	1.67	0.59
2:B:91:GLY:O	2:N:55:ARG:NH1	2.36	0.59
2:F:179:ILE:HG23	2:F:232:GLU:HB2	1.86	0.58
1:I:368:GLN:HE21	1:I:419:LEU:HD23	1.69	0.58
2:J:55:ARG:HD3	2:J:145:THR:HB	1.86	0.58
4:L:17:DG:H2"	4:L:18:DT:C6	2.38	0.58
1:M:377:ARG:NH1	2:N:417:GLU:OE2	2.35	0.57
2:F:267:LEU:HB3	2:F:276:LEU:HB3	1.86	0.57
1:M:338:LYS:NZ	1:M:346:GLU:OE2	2.37	0.57
2:B:203:ASP:OD1	2:B:203:ASP:N	2.38	0.57
2:F:73:SER:O	2:F:128:LYS:NZ	2.37	0.57
2:N:319:ARG:HH21	2:N:342:TYR:HB3	1.69	0.57
1:A:333:ARG:NH2	1:A:436:GLU:OE1	2.37	0.57
2:N:307:LYS:HE3	2:N:312:GLU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NH2	3:C:2:U:OP1	2.39	0.56
1:E:267:ARG:NH1	1:E:271:GLY:O	2.38	0.56
1:E:333:ARG:HB3	1:E:361:LEU:HB2	1.87	0.56
2:F:224:GLU:CD	2:F:224:GLU:H	2.12	0.56
1:I:65:SER:OG	1:I:66:GLY:N	2.39	0.56
2:J:44:ALA:O	2:J:56:MET:HA	2.06	0.56
2:B:276:LEU:H	2:B:322:ALA:HB1	1.70	0.56
2:B:311:ASP:OD2	2:B:311:ASP:N	2.37	0.55
4:H:4:DC:N4	4:H:5:DG:O6	2.39	0.55
1:A:117:ASP:O	1:A:157:ARG:NH2	2.39	0.55
2:N:278:PHE:HE2	2:N:287:ARG:HG2	1.70	0.55
2:F:191:ALA:O	2:F:195:ASN:ND2	2.39	0.55
2:N:320:HIS:HB2	2:N:343:TYR:O	2.06	0.55
1:M:74:HIS:O	1:M:74:HIS:ND1	2.34	0.55
2:N:289:PHE:H	2:N:300:ALA:HB3	1.72	0.55
1:I:367:VAL:HG12	1:I:420:LEU:HD23	1.89	0.55
2:B:185:GLU:HG2	2:B:225:ILE:HD12	1.89	0.55
2:N:73:SER:OG	2:N:74:ASP:N	2.39	0.55
1:M:207:ASP:OD1	1:M:207:ASP:N	2.38	0.55
2:B:270:ASP:OD1	2:B:270:ASP:N	2.38	0.54
2:N:55:ARG:HB3	2:N:145:THR:HG21	1.89	0.54
2:N:375:VAL:O	2:N:379:HIS:ND1	2.40	0.54
2:B:281:ILE:HG13	2:B:283:ARG:H	1.71	0.54
2:F:105:ASP:OD1	2:F:105:ASP:N	2.40	0.54
2:N:31:ASP:O	2:N:42:GLY:HA2	2.07	0.54
2:N:280:ALA:HB2	2:N:287:ARG:HB2	1.90	0.54
2:J:183:THR:HG23	2:J:185:GLU:H	1.72	0.54
1:E:10:GLU:OE2	1:E:385:ARG:NH1	2.39	0.54
2:F:180:ALA:H	2:F:210:THR:HG23	1.72	0.54
2:N:178:TYR:HA	2:N:233:ALA:HA	1.90	0.54
2:N:290:ALA:HA	2:N:298:THR:HB	1.90	0.54
2:J:279:ARG:O	2:J:287:ARG:NH2	2.39	0.54
2:N:344:TYR:HD1	2:N:353:GLN:HE21	1.55	0.54
2:B:160:GLY:HA2	2:B:414:ARG:HB2	1.89	0.54
2:F:181:SER:OG	2:F:182:THR:N	2.41	0.54
1:I:204:VAL:HG13	1:I:229:ARG:HD2	1.90	0.53
2:N:204:TRP:HZ2	2:N:207:ASN:HB2	1.72	0.53
2:J:319:ARG:NH1	2:J:344:TYR:OH	2.36	0.53
2:F:284:GLU:OE2	2:F:287:ARG:NH1	2.41	0.53
1:M:47:VAL:HG22	1:M:102:ALA:HB3	1.89	0.53
2:N:169:LEU:HD21	2:N:379:HIS:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:SER:HA	2:B:226:VAL:HB	1.90	0.53
2:J:90:ARG:NH1	2:J:114:SER:O	2.42	0.53
1:E:183:ARG:NH1	3:G:1:A:OP3	2.41	0.53
1:A:85:GLY:N	1:A:88:SER:OG	2.42	0.53
2:J:180:ALA:HB3	2:J:233:ALA:HB2	1.90	0.52
2:B:263:THR:O	2:B:267:LEU:N	2.41	0.52
1:E:281:MET:HA	1:E:290:VAL:O	2.10	0.52
2:F:68:LYS:NZ	2:F:69:TYR:O	2.43	0.52
2:F:235:ASN:OD1	2:F:235:ASN:N	2.43	0.52
2:J:283:ARG:HG3	2:J:285:VAL:HG22	1.92	0.52
2:B:256:ARG:HG2	2:B:269:TRP:HH2	1.75	0.51
1:I:183:ARG:NH1	3:K:1:A:OP1	2.43	0.51
1:I:186:LEU:HD23	1:I:199:ILE:HD11	1.93	0.51
2:N:307:LYS:HB2	2:N:314:ARG:HB3	1.92	0.51
2:B:308:ASN:HD22	2:B:314:ARG:HB2	1.76	0.51
1:M:333:ARG:NH2	1:M:436:GLU:OE1	2.43	0.51
1:I:313:LYS:HG3	1:I:353:ALA:HB2	1.92	0.51
1:I:198:GLN:OE1	1:I:240:LYS:NZ	2.44	0.51
4:L:19:DA:H2'	4:L:19:DA:N3	2.24	0.51
2:F:33:ARG:NH1	2:J:31:ASP:OD2	2.44	0.51
1:I:281:MET:HE2	1:I:291:LEU:HD13	1.93	0.51
1:I:307:MET:HB2	1:I:346:GLU:HG2	1.92	0.51
2:N:291:TYR:HD1	2:N:293:SER:H	1.59	0.51
1:A:156:GLU:OE1	1:A:160:ASN:ND2	2.43	0.50
1:E:408:THR:OG1	1:E:409:TYR:N	2.43	0.50
1:I:408:THR:OG1	1:I:409:TYR:N	2.44	0.50
2:B:90:ARG:NE	2:B:115:ARG:O	2.44	0.50
1:E:333:ARG:NH2	1:E:363:ASP:OD2	2.44	0.50
1:M:410:PRO:HA	4:P:19:DA:H5'	1.93	0.50
2:N:185:GLU:OE2	2:N:188:LYS:HB2	2.11	0.50
1:E:82:PRO:HG2	1:E:89:PRO:HD3	1.93	0.50
2:N:222:CYS:SG	2:N:227:ASP:N	2.84	0.50
1:E:148:ILE:HD11	1:E:197:ILE:HB	1.94	0.50
2:J:35:ARG:NH1	2:N:37:GLU:OE1	2.45	0.50
1:E:202:GLU:HG2	1:E:209:VAL:HG11	1.94	0.49
2:F:183:THR:HG21	2:F:226:VAL:HB	1.94	0.49
1:M:157:ARG:O	1:M:157:ARG:NH1	2.44	0.49
2:B:289:PHE:H	2:B:301:ASN:HD21	1.59	0.49
1:I:403:MET:HE1	1:I:451:ASN:HB3	1.93	0.49
2:B:280:ALA:HA	2:B:287:ARG:NE	2.21	0.49
2:B:287:ARG:HD2	2:B:289:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:SER:O	2:F:76:SER:OG	2.31	0.49
2:N:167:ASN:OD1	2:N:167:ASN:N	2.42	0.49
2:N:376:ILE:HA	2:N:379:HIS:CE1	2.48	0.49
1:I:377:ARG:NH1	1:I:381:TYR:O	2.45	0.49
3:O:13:U:H2'	3:O:14:G:C8	2.48	0.49
2:B:66:GLU:HB3	2:B:104:SER:HB3	1.94	0.48
1:I:184:GLY:HA2	1:I:467:VAL:HG23	1.94	0.48
4:L:17:DG:H2''	4:L:18:DT:H6	1.78	0.48
4:L:18:DT:H3'	4:L:19:DA:C8	2.48	0.48
1:M:463:LYS:HD3	1:M:485:ILE:HG22	1.96	0.48
2:B:277:TYR:HB2	2:B:320:HIS:HB2	1.96	0.48
2:F:201:ARG:NH2	2:F:222:CYS:SG	2.83	0.48
2:F:401:LEU:HD22	2:F:403:PHE:HE1	1.78	0.48
2:N:194:LEU:HD23	2:N:200:LYS:HZ1	1.79	0.48
1:A:262:GLY:O	1:A:278:ALA:HA	2.13	0.48
2:F:283:ARG:H	2:F:283:ARG:HD3	1.79	0.48
1:I:248:ARG:NH1	1:I:283:ASP:OD1	2.45	0.48
2:N:41:ASP:OD1	2:N:41:ASP:N	2.46	0.48
1:M:120:ARG:O	1:M:124:MET:HG3	2.13	0.48
2:N:279:ARG:NH2	2:N:349:TYR:OH	2.45	0.48
2:B:36:LEU:H	2:B:36:LEU:HG	1.53	0.48
1:I:244:ARG:NH1	1:M:140:GLY:O	2.47	0.48
2:N:345:THR:HA	2:N:353:GLN:NE2	2.28	0.48
2:B:81:LEU:O	2:B:122:ARG:NH1	2.40	0.48
3:C:9:C:H2'	3:C:10:A:H8	1.79	0.47
2:F:249:ASN:HD22	4:H:7:DC:H1'	1.79	0.47
2:J:361:GLY:O	2:J:365:LEU:HG	2.14	0.47
2:B:256:ARG:HH12	4:D:6:DT:H5''	1.78	0.47
1:I:113:GLY:HA2	1:I:157:ARG:HG2	1.95	0.47
1:M:238:TYR:O	1:M:242:SER:HB3	2.14	0.47
2:N:173:LEU:HB2	2:N:237:LYS:HG2	1.96	0.47
1:M:44:ILE:HB	1:M:96:ILE:HD13	1.95	0.47
3:O:14:G:H2'	3:O:15:A:C8	2.49	0.47
1:M:309:ARG:NH1	1:M:348:ASP:OD2	2.44	0.47
1:E:70:LYS:HE3	4:H:19:DA:H61	1.80	0.47
1:I:410:PRO:HA	4:L:19:DA:P	2.54	0.47
1:I:413:TYR:HD1	1:I:414:ASP:HB2	1.80	0.47
2:J:278:PHE:O	2:J:320:HIS:ND1	2.41	0.47
1:M:454:LEU:HD13	1:M:455:PRO:HD2	1.96	0.47
1:A:409:TYR:OH	1:A:413:TYR:O	2.29	0.47
2:B:78:THR:HG21	2:B:123:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:C:H2'	3:C:10:A:C8	2.49	0.47
2:J:309:SER:O	2:J:309:SER:OG	2.24	0.47
1:M:334:VAL:HG23	1:M:359:THR:HG21	1.97	0.47
2:J:71:SER:O	2:J:71:SER:OG	2.32	0.47
1:M:456:ILE:O	1:M:457:PRO:C	2.57	0.47
2:N:267:LEU:HD23	2:N:278:PHE:HB3	1.97	0.47
2:B:178:TYR:HD1	2:B:231:VAL:HG13	1.80	0.46
2:F:236:THR:OG1	2:F:237:LYS:NZ	2.48	0.46
2:J:286:SER:OG	2:J:288:ASN:OD1	2.32	0.46
1:A:299:GLU:HG3	1:A:300:SER:H	1.80	0.46
2:F:148:LYS:HD2	2:F:148:LYS:HA	1.75	0.46
2:J:105:ASP:OD1	2:J:105:ASP:N	2.46	0.46
1:M:84:LEU:HA	1:M:88:SER:HB3	1.97	0.46
1:E:26:LEU:O	1:E:30:GLU:HB2	2.14	0.46
1:M:264:SER:H	1:M:277:SER:HB3	1.81	0.46
3:O:4:C:H2'	3:O:5:U:C6	2.50	0.46
2:N:266:ASP:OD1	2:N:266:ASP:N	2.49	0.46
2:N:318:VAL:HB	2:N:345:THR:HG23	1.97	0.46
1:A:261:VAL:HB	1:A:336:ILE:HD13	1.98	0.46
1:I:359:THR:O	1:I:362:ARG:NH2	2.48	0.46
2:B:182:THR:OG1	2:B:185:GLU:OE1	2.34	0.46
2:J:174:PRO:O	2:J:237:LYS:HG3	2.15	0.46
2:N:280:ALA:HA	2:N:287:ARG:HD3	1.98	0.46
2:B:45:GLU:OE1	2:N:33:ARG:NH2	2.47	0.46
1:A:280:GLN:HG2	1:A:319:VAL:HG22	1.97	0.46
2:B:58:ALA:HB3	2:B:96:VAL:HG12	1.97	0.46
1:E:216:LYS:HB2	1:E:216:LYS:HE3	1.67	0.46
2:B:279:ARG:HE	2:B:280:ALA:H	1.63	0.45
1:I:376:LEU:HD13	2:J:372:ARG:HA	1.98	0.45
2:J:177:MET:HE3	2:J:235:ASN:OD1	2.16	0.45
3:K:9:C:H2'	3:K:10:A:C8	2.50	0.45
2:N:217:PRO:HD2	2:N:218:ARG:NH1	2.31	0.45
2:B:175:ASN:OD1	2:B:235:ASN:ND2	2.49	0.45
2:B:176:GLU:OE1	2:B:215:HIS:ND1	2.48	0.45
2:B:326:ARG:HA	2:B:326:ARG:HD2	1.75	0.45
1:A:355:ASP:OD1	1:A:362:ARG:NH2	2.49	0.45
2:J:218:ARG:H	2:J:218:ARG:HG2	1.64	0.45
2:B:37:GLU:HA	2:N:29:GLN:HE22	1.82	0.45
2:J:422:LYS:HD3	2:J:422:LYS:HA	1.75	0.45
1:A:377:ARG:NH1	1:A:381:TYR:O	2.45	0.45
2:J:306:PHE:HE2	2:J:319:ARG:HE	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HB2	1:E:15:PHE:CE1	2.51	0.45
2:F:367:LYS:H	2:F:367:LYS:HG2	1.48	0.45
1:I:413:TYR:HE2	2:J:363:LYS:HD2	1.81	0.45
2:J:203:ASP:HA	2:J:211:PHE:HE2	1.82	0.45
2:J:235:ASN:OD1	2:J:237:LYS:HD2	2.17	0.45
2:N:67:GLY:O	2:N:102:ARG:NH1	2.50	0.45
2:N:188:LYS:HB3	2:N:188:LYS:HE2	1.62	0.45
2:N:368:SER:O	2:N:370:ALA:N	2.50	0.45
3:O:3:A:H2'	3:O:4:C:C6	2.52	0.45
2:B:338:ILE:HD11	2:B:375:VAL:HG13	1.99	0.45
1:E:354:LEU:HD13	1:E:362:ARG:HG2	1.99	0.45
1:I:280:GLN:HE21	1:I:292:LYS:HD3	1.81	0.45
1:M:377:ARG:NH2	2:N:162:GLU:OE1	2.42	0.44
2:N:186:PRO:O	2:N:187:ARG:HB2	2.16	0.44
2:F:227:ASP:N	2:F:227:ASP:OD2	2.47	0.44
2:F:19:VAL:HG11	2:F:61:ILE:HG12	1.99	0.44
2:N:352:HIS:N	2:N:353:GLN:OE1	2.50	0.44
1:I:108:LYS:O	1:I:112:ILE:HG12	2.17	0.44
4:L:18:DT:H5'	4:L:19:DA:C4	2.53	0.44
2:J:206:ILE:HG12	2:J:250:ARG:HG2	1.99	0.44
2:N:402:MET:SD	2:N:402:MET:N	2.90	0.44
2:B:172:THR:OG1	2:B:402:MET:O	2.34	0.44
3:C:4:C:H2'	3:C:5:U:C6	2.53	0.44
1:A:106:LYS:HE2	1:A:106:LYS:HB2	1.83	0.44
2:B:35:ARG:NH2	2:B:36:LEU:HD23	2.33	0.44
2:B:381:PHE:HD1	2:B:382:LEU:HD22	1.83	0.44
3:G:7:C:H2'	3:G:8:A:C8	2.53	0.44
2:N:267:LEU:HD22	2:N:276:LEU:HB3	1.99	0.44
2:F:267:LEU:HD23	2:F:278:PHE:H	1.82	0.44
2:N:180:ALA:HA	2:N:231:VAL:HG11	2.00	0.44
2:N:296:LYS:HE3	2:N:297:LYS:H	1.83	0.44
3:O:5:U:H2'	3:O:6:G:C8	2.52	0.44
3:O:18:A:H2'	3:O:19:U:C6	2.53	0.44
1:A:191:MET:HE1	1:A:478:SER:H	1.83	0.43
2:F:215:HIS:NE2	2:F:222:CYS:SG	2.89	0.43
1:M:337:LEU:HB3	1:M:458:ILE:HD11	1.98	0.43
1:I:285:ARG:H	1:I:326:HIS:HE1	1.66	0.43
2:J:177:MET:O	2:J:235:ASN:HB3	2.18	0.43
1:M:266:TYR:CE1	1:M:465:GLY:HA3	2.53	0.43
2:N:279:ARG:HH12	2:N:281:ILE:C	2.26	0.43
3:G:16:C:H2'	3:G:17:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:343:LYS:HE2	1:I:343:LYS:HB3	1.71	0.43
1:M:301:ARG:NH2	1:M:311:ASP:OD1	2.52	0.43
2:N:222:CYS:HB2	2:N:228:ILE:HG22	2.00	0.43
1:E:153:LYS:HD2	1:E:153:LYS:HA	1.83	0.43
2:F:307:LYS:HZ2	2:F:315:VAL:HA	1.84	0.43
1:M:130:ILE:HD13	1:M:130:ILE:HA	1.90	0.43
2:N:237:LYS:HD2	2:N:237:LYS:HA	1.79	0.43
2:N:307:LYS:HE3	2:N:312:GLU:CA	2.49	0.43
1:A:108:LYS:HE2	1:A:108:LYS:HB2	1.85	0.43
1:M:284:GLU:OE1	1:M:326:HIS:NE2	2.51	0.43
2:N:206:ILE:HD12	2:N:206:ILE:HA	1.93	0.43
1:A:220:SER:OG	1:A:221:ARG:N	2.51	0.43
2:B:13:GLU:OE1	2:J:20:ARG:NH2	2.52	0.43
1:E:85:GLY:O	1:E:87:GLN:N	2.52	0.43
2:F:157:PRO:HB3	2:F:416:PRO:HD3	1.99	0.43
2:J:341:THR:OG1	2:J:342:TYR:N	2.51	0.43
1:M:44:ILE:HD11	1:M:94:PHE:HD2	1.84	0.43
1:M:117:ASP:O	1:M:119:TYR:N	2.52	0.43
1:E:130:ILE:HD13	1:E:130:ILE:HA	1.90	0.43
2:F:73:SER:OG	2:F:76:SER:OG	2.33	0.43
3:G:4:C:H2'	3:G:5:U:C6	2.53	0.43
1:I:204:VAL:O	1:I:229:ARG:NH1	2.52	0.43
1:I:412:LYS:HA	1:I:412:LYS:HD3	1.77	0.43
1:M:291:LEU:HD21	1:M:456:ILE:CD1	2.43	0.43
1:M:373:ALA:HB1	2:N:166:ILE:HD11	2.01	0.43
2:B:422:LYS:HG3	2:B:423:GLU:HB2	2.00	0.42
2:J:177:MET:HE3	2:J:177:MET:HB3	1.76	0.42
1:M:277:SER:OG	1:M:278:ALA:N	2.51	0.42
2:N:406:PRO:HA	2:N:407:PRO:HD3	1.86	0.42
2:B:372:ARG:O	2:B:376:ILE:HG22	2.18	0.42
2:F:172:THR:HB	2:F:402:MET:HB3	2.01	0.42
3:K:4:C:H2'	3:K:5:U:C6	2.55	0.42
1:A:58:LYS:N	1:A:58:LYS:HD2	2.33	0.42
2:B:38:ALA:HB3	2:B:88:TYR:OH	2.19	0.42
2:F:275:ALA:HB1	2:F:322:ALA:HB1	2.00	0.42
1:I:196:PRO:HB2	1:I:240:LYS:HD3	2.01	0.42
3:O:7:C:H2'	3:O:8:A:C8	2.54	0.42
2:B:5:ILE:HD12	2:B:5:ILE:HA	1.86	0.42
1:M:441:THR:HG22	1:M:452:GLN:HB2	2.02	0.42
1:A:423:HIS:O	1:A:424:HIS:ND1	2.53	0.42
3:G:10:A:H2'	3:G:11:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:165:LEU:HD21	2:J:372:ARG:HE	1.85	0.42
4:L:4:DC:H2'	4:L:5:DG:H8	1.85	0.42
1:A:60:ILE:O	1:A:64:SER:OG	2.31	0.42
2:J:36:LEU:HD23	2:N:13:GLU:HG3	2.01	0.42
1:E:303:ARG:NH1	3:G:13:U:OP1	2.52	0.42
2:J:188:LYS:HB3	2:J:188:LYS:HE3	1.64	0.42
2:N:172:THR:OG1	2:N:173:LEU:N	2.52	0.42
1:A:394:LYS:HD2	1:A:421:CYS:HB3	2.02	0.42
2:B:281:ILE:HG13	2:B:283:ARG:N	2.35	0.42
2:F:22:ARG:HA	2:F:22:ARG:HD3	1.88	0.42
2:F:219:THR:OG1	2:F:220:SER:N	2.52	0.42
2:F:177:MET:HG3	2:F:236:THR:HG22	2.02	0.41
1:A:10:GLU:OE2	1:A:442:LYS:NZ	2.47	0.41
1:A:56:THR:O	1:A:60:ILE:HG22	2.21	0.41
2:B:406:PRO:HA	2:B:407:PRO:HD3	1.84	0.41
1:E:15:PHE:CD2	1:E:15:PHE:N	2.87	0.41
2:J:79:TYR:O	2:J:123:ARG:HA	2.19	0.41
2:N:234:ILE:HG23	2:N:235:ASN:HB2	2.00	0.41
2:N:250:ARG:NH2	3:O:17:G:OP1	2.52	0.41
2:B:188:LYS:H	2:B:188:LYS:HG2	1.65	0.41
2:F:235:ASN:HB2	2:F:237:LYS:HG2	2.02	0.41
2:J:217:PRO:O	2:J:222:CYS:N	2.46	0.41
1:M:212:PRO:HA	1:M:219:SER:HA	2.02	0.41
1:A:49:ASN:O	1:A:52:THR:OG1	2.31	0.41
1:A:338:LYS:HG2	1:A:340:SER:H	1.85	0.41
1:E:54:GLU:CD	1:E:54:GLU:H	2.27	0.41
2:N:55:ARG:HD2	2:N:55:ARG:HA	1.93	0.41
1:A:157:ARG:HD2	1:A:157:ARG:HA	1.84	0.41
2:B:217:PRO:HG2	2:B:218:ARG:HD2	2.02	0.41
2:B:224:GLU:HG2	2:B:225:ILE:HG12	2.02	0.41
2:N:132:LEU:HB3	2:N:134:ASN:HD22	1.85	0.41
3:O:13:U:H2'	3:O:14:G:H8	1.84	0.41
1:A:480:ASP:HB3	1:A:483:LYS:HG3	2.02	0.41
1:E:17:ASP:C	1:E:19:HIS:H	2.28	0.41
2:F:31:ASP:OD1	2:F:32:GLY:N	2.54	0.41
2:J:193:ILE:HG22	2:J:195:ASN:H	1.85	0.41
1:M:442:LYS:HB2	1:M:442:LYS:HE2	1.85	0.41
2:B:63:SER:OG	2:B:64:THR:N	2.53	0.41
1:I:35:GLN:HB2	1:I:244:ARG:HB3	2.03	0.41
2:J:302:VAL:HG13	2:J:321:HIS:HB2	2.02	0.41
4:L:17:DG:C2	4:L:18:DT:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:HB3	1:A:274:LEU:HD12	2.03	0.41
2:B:8:ASN:ND2	5:Q:6:DT:O2	2.54	0.41
2:B:190:ILE:HA	2:B:193:ILE:HG22	2.02	0.41
2:F:277:TYR:HA	2:F:322:ALA:HB2	2.03	0.41
2:F:282:GLU:OE1	2:F:284:GLU:HG2	2.21	0.41
4:H:17:DG:H2'	4:H:18:DT:H5'	2.03	0.41
2:J:139:ASN:OD1	2:J:139:ASN:N	2.53	0.41
2:J:177:MET:HE3	2:J:235:ASN:CG	2.46	0.41
2:J:424:LYS:HB3	2:J:424:LYS:HE3	1.73	0.41
3:K:7:C:H2'	3:K:8:A:C8	2.56	0.41
2:N:285:VAL:HG23	2:N:286:SER:H	1.86	0.41
5:Q:5:DC:H2'	5:Q:6:DT:C6	2.56	0.41
2:B:280:ALA:CB	2:B:287:ARG:HG2	2.49	0.41
2:F:44:ALA:O	2:F:56:MET:HA	2.21	0.41
1:M:203:ASP:HB3	1:M:223:ILE:HD13	2.03	0.41
2:N:276:LEU:O	2:N:322:ALA:HA	2.21	0.40
1:M:369:GLU:N	1:M:369:GLU:OE1	2.54	0.40
2:B:10:ILE:HD13	2:B:10:ILE:HA	1.96	0.40
2:B:35:ARG:HE	2:F:13:GLU:HB2	1.87	0.40
2:B:180:ALA:HB3	2:B:211:PHE:HB2	2.03	0.40
2:J:297:LYS:HZ1	2:J:299:ASP:HB3	1.87	0.40
2:N:279:ARG:NH1	2:N:282:GLU:O	2.54	0.40
1:A:58:LYS:NZ	1:A:58:LYS:HA	2.36	0.40
3:K:3:A:H2'	3:K:4:C:C6	2.57	0.40
1:A:120:ARG:O	1:A:124:MET:HG3	2.21	0.40
2:B:16:GLU:HG2	2:B:61:ILE:HD12	2.03	0.40
2:N:140:LYS:O	2:N:143:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/485 (96%)	439 (95%)	25 (5%)	0	100	100
1	E	464/485 (96%)	429 (92%)	35 (8%)	0	100	100
1	I	461/485 (95%)	428 (93%)	33 (7%)	0	100	100
1	M	461/485 (95%)	427 (93%)	34 (7%)	0	100	100
2	B	406/442 (92%)	360 (89%)	46 (11%)	0	100	100
2	F	405/442 (92%)	352 (87%)	53 (13%)	0	100	100
2	J	383/442 (87%)	340 (89%)	43 (11%)	0	100	100
2	N	383/442 (87%)	313 (82%)	70 (18%)	0	100	100
All	All	3427/3708 (92%)	3088 (90%)	339 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/408 (97%)	392 (100%)	2 (0%)	86	93
1	E	394/408 (97%)	390 (99%)	4 (1%)	73	87
1	I	393/408 (96%)	392 (100%)	1 (0%)	91	96
1	M	393/408 (96%)	388 (99%)	5 (1%)	65	83
2	B	352/380 (93%)	347 (99%)	5 (1%)	62	82
2	F	351/380 (92%)	347 (99%)	4 (1%)	70	86
2	J	336/380 (88%)	330 (98%)	6 (2%)	54	77
2	N	336/380 (88%)	330 (98%)	6 (2%)	54	77
All	All	2949/3152 (94%)	2916 (99%)	33 (1%)	69	86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	155	LEU

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Mol	Chain	Res	Type
2	B	35	ARG
2	B	36	LEU
2	B	85	ASP
2	B	193	ILE
2	B	279	ARG
1	E	15	PHE
1	E	17	ASP
1	E	427	GLU
1	E	476	VAL
2	F	66	GLU
2	F	225	ILE
2	F	307	LYS
2	F	315	VAL
1	I	343	LYS
2	J	235	ASN
2	J	237	LYS
2	J	238	GLU
2	J	243	ASP
2	J	365	LEU
2	J	424	LYS
1	M	14	GLU
1	M	112	ILE
1	M	376	LEU
1	M	454	LEU
1	M	456	ILE
2	N	185	GLU
2	N	187	ARG
2	N	188	LYS
2	N	281	ILE
2	N	307	LYS
2	N	310	LYS

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

Mol	Chain	Res	Type
1	A	181	ASN
1	A	224	GLN
2	B	333	GLN
1	E	118	HIS
1	E	273	GLN
2	F	60	GLN
2	F	195	ASN

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Mol	Chain	Res	Type
2	F	249	ASN
2	F	352	HIS
2	F	384	GLN
1	I	213	GLN
1	I	424	HIS
2	J	273	HIS
2	J	410	HIS
1	M	21	HIS
1	M	198	GLN
1	M	424	HIS
1	M	444	ASN
2	N	17	ASN
2	N	29	GLN
2	N	249	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	18/20 (90%)	3 (16%)	0
3	G	19/20 (95%)	3 (15%)	0
3	K	17/20 (85%)	1 (5%)	0
3	O	18/20 (90%)	3 (16%)	1 (5%)
All	All	72/80 (90%)	10 (13%)	1 (1%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	12	C
3	C	13	U
3	C	19	U
3	G	4	C
3	G	15	A
3	G	18	A
3	K	14	G
3	O	16	C
3	O	17	G
3	O	19	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	O	18	A

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 6 ligands modelled in this entry, 6 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.