



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:03 PM UTC

PDB ID : 3HHZ / pdb_00003hhz
Title : Complex of the vesicular stomatitis virus nucleocapsid and the nucleocapsid-binding domain of the phosphoprotein
Authors : Green, T.J.; Luo, M.
Deposited on : 2009-05-18
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

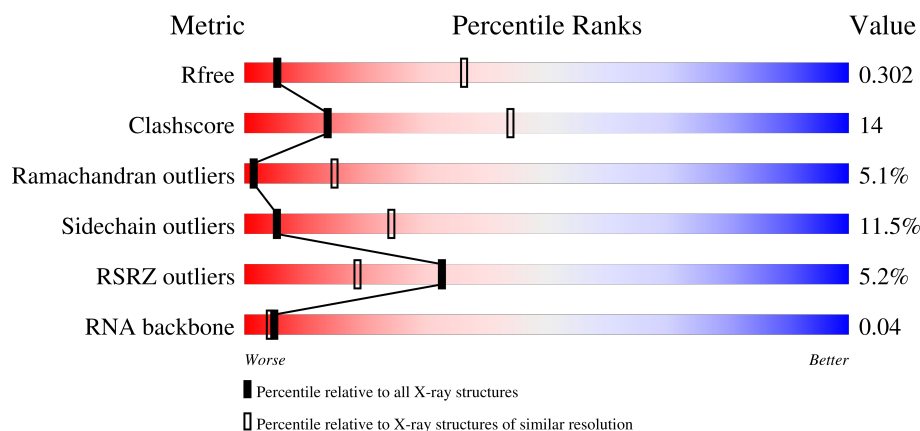
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	87	3% 45% 32% 7% 16%
1	B	87	9% 60% 22% • 16%
1	C	87	• 56% 23% 5% 16%
1	D	87	5% 71% 9% • 16%

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Mol	Chain	Length	Quality of chain
1	E	87	
2	K	421	
2	L	421	
2	M	421	
2	N	421	
2	O	421	
3	R	45	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20415 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	S	0	0	0
			576	368	100	106	2			
1	B	73	Total	C	N	O	S	0	0	0
			576	368	100	106	2			
1	C	73	Total	C	N	O	S	0	0	0
			576	368	100	106	2			
1	D	73	Total	C	N	O	S	0	0	0
			576	368	100	106	2			
1	E	73	Total	C	N	O	S	0	0	0
			576	368	100	106	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	GLY	-	expression tag	UNP P04880
A	180	SER	-	expression tag	UNP P04880
A	181	HIS	-	expression tag	UNP P04880
A	182	MET	-	expression tag	UNP P04880
B	179	GLY	-	expression tag	UNP P04880
B	180	SER	-	expression tag	UNP P04880
B	181	HIS	-	expression tag	UNP P04880
B	182	MET	-	expression tag	UNP P04880
C	179	GLY	-	expression tag	UNP P04880
C	180	SER	-	expression tag	UNP P04880
C	181	HIS	-	expression tag	UNP P04880
C	182	MET	-	expression tag	UNP P04880
D	179	GLY	-	expression tag	UNP P04880
D	180	SER	-	expression tag	UNP P04880
D	181	HIS	-	expression tag	UNP P04880
D	182	MET	-	expression tag	UNP P04880
E	179	GLY	-	expression tag	UNP P04880
E	180	SER	-	expression tag	UNP P04880
E	181	HIS	-	expression tag	UNP P04880

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Chain	Residue	Modelled	Actual	Comment	Reference
E	182	MET	-	expression tag	UNP P04880

- Molecule 2 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	L	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	M	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	N	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
2	O	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			

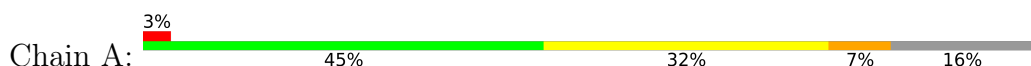
- Molecule 3 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

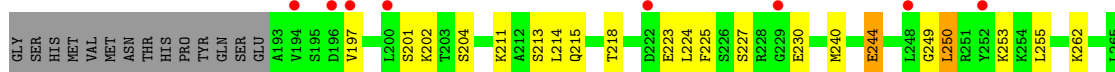
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Phosphoprotein



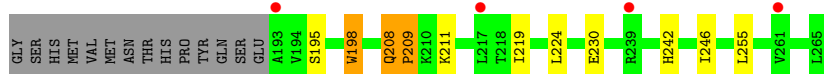
• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein

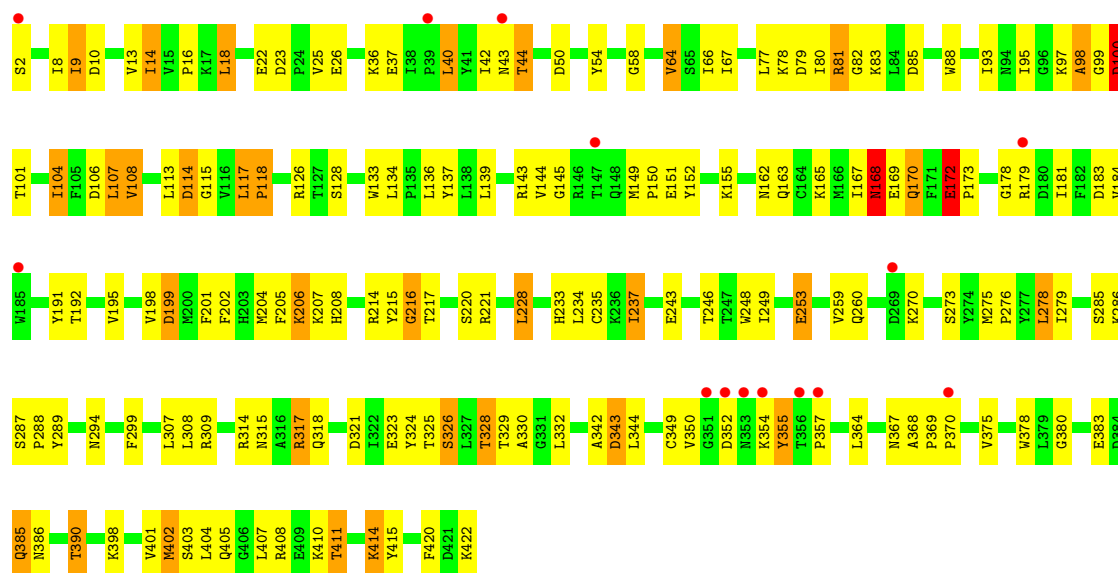


• Molecule 1: Phosphoprotein

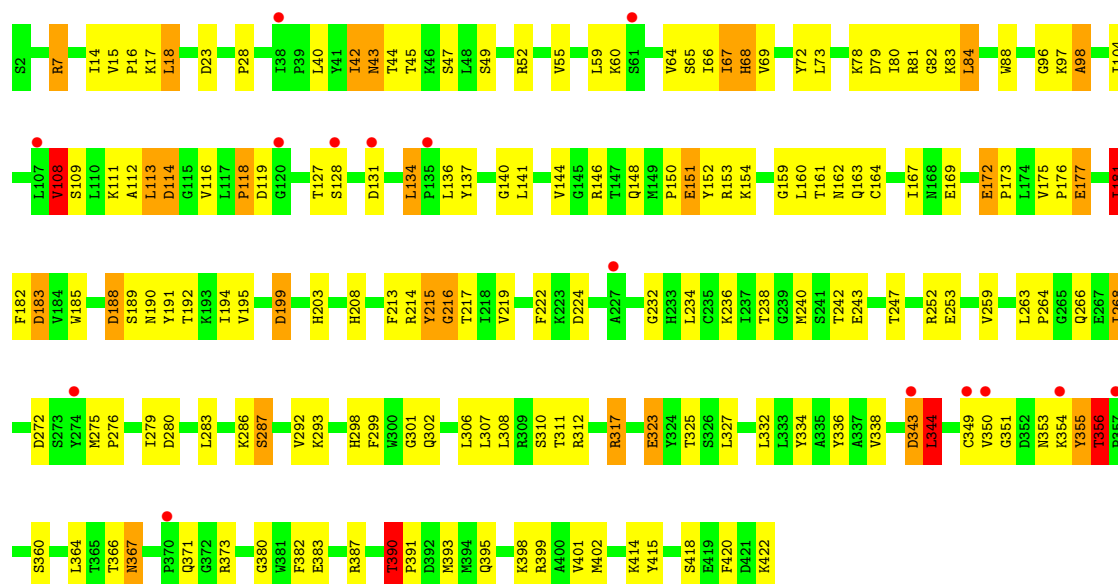




• Molecule 2: Nucleoprotein

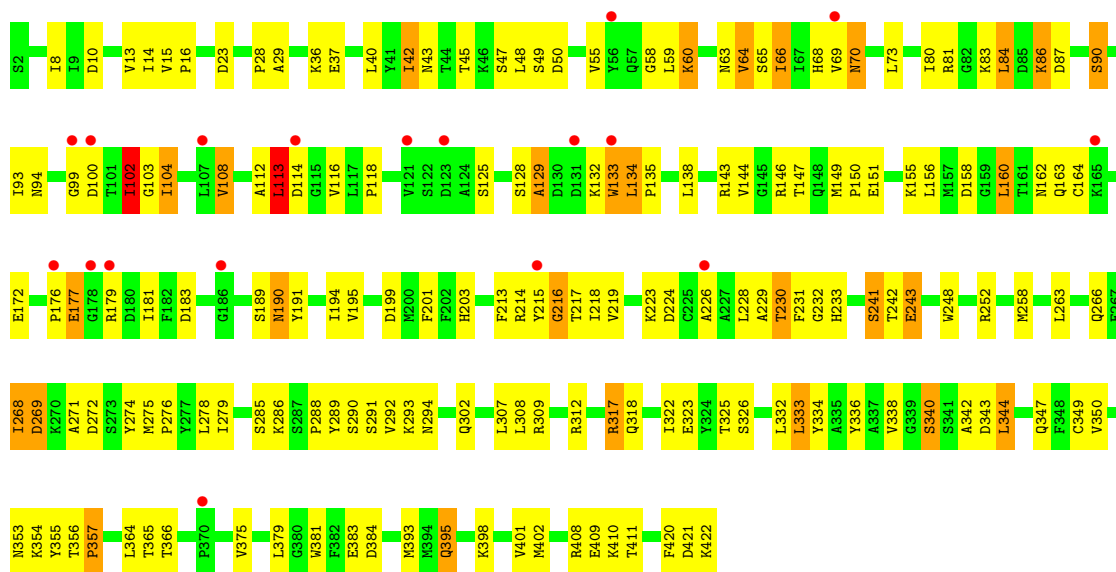


• Molecule 2: Nucleoprotein

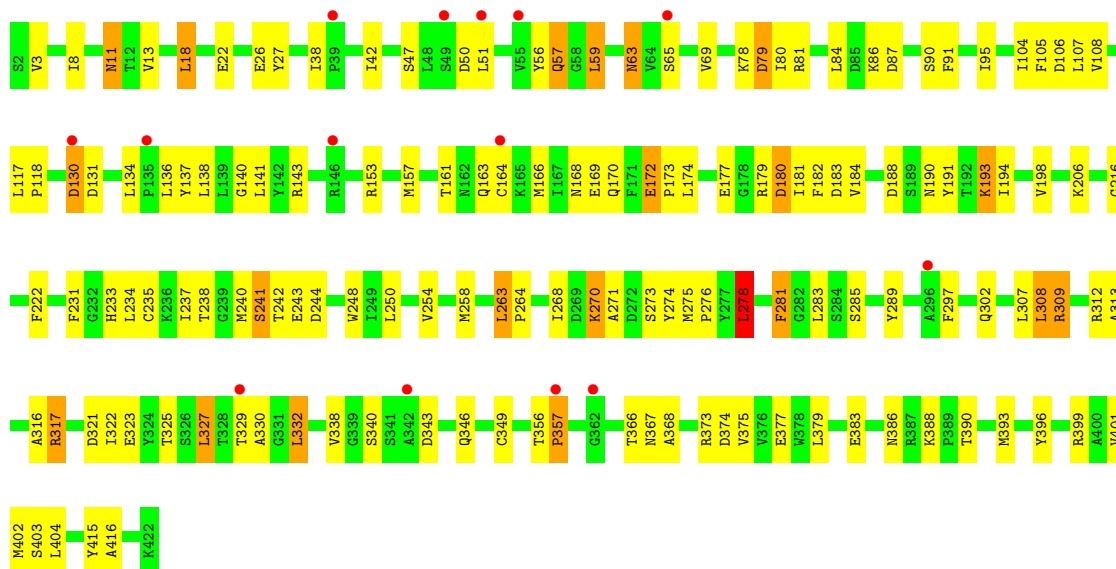


• Molecule 2: Nucleoprotein

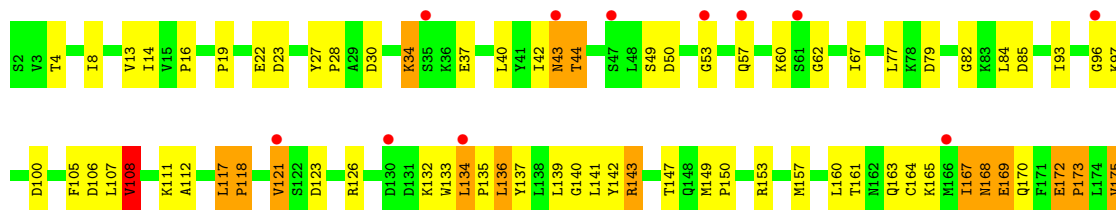


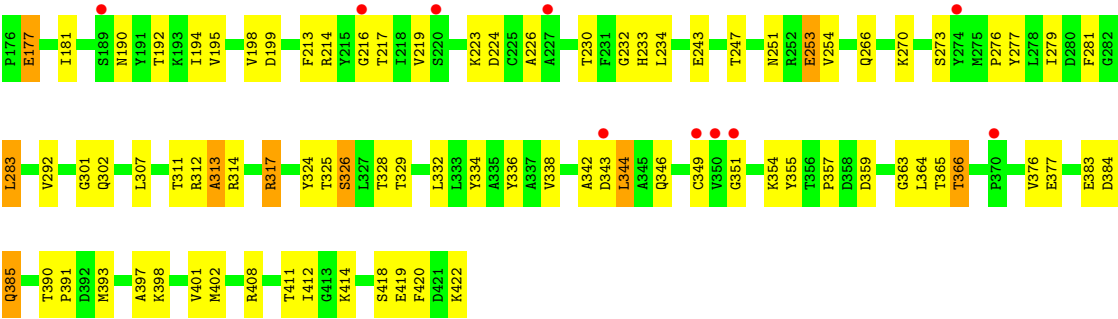


• Molecule 2: Nucleoprotein

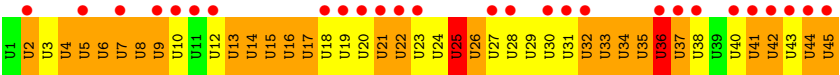


• Molecule 2: Nucleoprotein





● Molecule 3: RNA (45-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.57Å 235.25Å 96.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.50) 98.3 (30.00-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.254 , 0.323 0.248 , 0.302	Depositor DCC
R_{free} test set	2443 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	93.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	20415	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/586	0.87	0/784
1	B	0.53	0/586	0.85	2/784 (0.3%)
1	C	0.50	0/586	0.83	0/784
1	D	0.52	0/586	0.83	0/784
1	E	0.51	0/586	0.84	0/784
2	K	0.55	0/3403	0.90	4/4607 (0.1%)
2	L	0.56	0/3403	0.96	12/4607 (0.3%)
2	M	0.55	0/3403	0.90	4/4607 (0.1%)
2	N	0.54	0/3403	0.96	9/4607 (0.2%)
2	O	0.54	0/3403	0.91	2/4607 (0.0%)
3	R	0.84	0/989	1.28	3/1526 (0.2%)
All	All	0.56	0/20934	0.94	36/28481 (0.1%)

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	M	0	2

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	130	ASP	N-CA-C	17.40	147.86	110.80
2	N	131	ASP	N-CA-CB	-10.64	95.06	110.81
2	N	131	ASP	N-CA-C	-9.71	102.00	114.04
2	L	367	ASN	CB-CA-C	-7.95	94.61	110.42
2	L	119	ASP	N-CA-C	-7.78	96.48	108.31
2	N	91	PHE	CB-CA-C	-7.60	95.29	110.42
2	L	356	THR	CB-CA-C	-7.08	96.22	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	356	THR	N-CA-C	6.79	124.83	109.81
2	L	108	VAL	N-CA-C	6.56	122.99	109.34
2	L	390	THR	CA-C-N	6.41	127.85	119.84
2	L	390	THR	C-N-CA	6.41	127.85	119.84
2	O	172	GLU	CA-C-N	6.38	127.81	119.84
2	O	172	GLU	C-N-CA	6.38	127.81	119.84
2	M	322	ILE	N-CA-C	6.35	116.28	108.53
3	R	25	U	C4'-C3'-C2'	-6.35	96.25	102.60
1	B	215	GLN	CA-C-N	6.30	126.33	119.90
1	B	215	GLN	C-N-CA	6.30	126.33	119.90
2	L	283	LEU	N-CA-C	-5.97	105.83	113.23
2	K	170	GLN	N-CA-C	5.96	113.67	108.78
2	N	130	ASP	CB-CA-C	-5.92	98.64	110.42
2	M	102	ILE	CB-CA-C	5.57	120.42	111.29
2	L	68	HIS	N-CA-C	-5.45	107.89	114.75
2	L	287	SER	CA-C-N	5.35	124.86	119.19
2	L	287	SER	C-N-CA	5.35	124.86	119.19
3	R	34	U	C1'-O4'-C4'	-5.31	104.59	109.90
2	K	318	GLN	CA-C-N	5.28	126.44	119.84
2	K	318	GLN	C-N-CA	5.28	126.44	119.84
2	N	390	THR	CA-C-N	5.27	126.42	119.84
2	N	390	THR	C-N-CA	5.27	126.42	119.84
2	M	318	GLN	CA-C-N	5.24	125.00	119.76
2	M	318	GLN	C-N-CA	5.24	125.00	119.76
2	N	388	LYS	CA-C-N	5.19	125.19	119.90
2	N	388	LYS	C-N-CA	5.19	125.19	119.90
3	R	36	U	O4'-C4'-C3'	-5.13	98.87	104.00
2	L	190	ASN	N-CA-C	5.07	116.80	111.28
2	K	114	ASP	N-CA-C	5.03	117.34	110.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	112	ALA	Peptide
2	M	113	LEU	Peptide

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	576	0	597	17	0
1	B	576	0	597	10	0
1	C	576	0	597	10	0
1	D	576	0	597	5	0
1	E	576	0	597	15	0
2	K	3327	0	3287	116	0
2	L	3327	0	3287	131	0
2	M	3327	0	3287	113	0
2	N	3327	0	3287	84	0
2	O	3327	0	3287	99	0
3	R	900	0	451	48	0
All	All	20415	0	19871	583	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 14.

All (583) 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:M:113:LEU:HD22	2:M:114:ASP:N	1.62	1.14
2:M:214:ARG:HA	2:M:217:THR:HG22	1.29	1.13
2:L:317:ARG:HD2	3:R:13:U:H2'	1.21	1.11
2:O:317:ARG:H	2:O:317:ARG:HD2	1.16	1.05
2:O:214:ARG:HA	2:O:217:THR:HG22	1.40	1.03
2:O:324:TYR:O	2:O:328:THR:HG22	1.60	1.00
2:K:107:LEU:O	2:K:108:VAL:HB	1.66	0.95
2:L:268:ILE:HD13	2:L:268:ILE:H	1.27	0.95
2:N:317:ARG:H	2:N:317:ARG:HE	1.14	0.94
2:M:113:LEU:CD2	2:M:114:ASP:N	2.32	0.93
2:O:43:ASN:HB2	2:O:111:LYS:HA	1.50	0.92
2:L:338:VAL:HG13	2:L:373:ARG:HH12	1.32	0.91
2:K:317:ARG:NH1	3:R:22:U:H3'	1.86	0.90
2:K:81:ARG:HE	2:K:82:GLY:H	1.20	0.89
2:M:113:LEU:HD22	2:M:113:LEU:C	1.98	0.88
2:K:58:GLY:HA3	2:K:64:VAL:HB	1.54	0.88
2:M:80:ILE:HG13	2:M:102:ILE:O	1.73	0.88
2:M:317:ARG:H	2:M:317:ARG:HE	1.20	0.87
2:O:214:ARG:HA	2:O:217:THR:CG2	2.04	0.87
2:L:317:ARG:NH1	3:R:13:U:H3'	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:LYS:HA	2:K:101:THR:HG22	1.57	0.87
2:M:336:TYR:O	2:M:340:SER:HB2	1.76	0.86
2:M:113:LEU:CD2	2:M:114:ASP:H	1.89	0.84
2:L:356:THR:O	2:L:356:THR:HG22	1.74	0.83
2:O:317:ARG:H	2:O:317:ARG:CD	1.91	0.82
2:O:317:ARG:HD2	2:O:317:ARG:N	1.96	0.81
2:L:263:LEU:HG	2:L:264:PRO:HD2	1.63	0.80
2:O:390:THR:OG1	2:O:393:MET:HG3	1.81	0.80
2:L:79:ASP:HB3	2:L:81:ARG:HG2	1.65	0.79
2:K:354:LYS:HD3	2:K:355:TYR:H	1.49	0.78
2:M:42:ILE:HG21	2:M:194:ILE:HD11	1.67	0.77
2:K:104:ILE:HG12	2:K:104:ILE:O	1.85	0.77
2:L:317:ARG:HD2	3:R:13:U:C2'	2.10	0.77
3:R:8:U:H2'	3:R:9:U:H5''	1.67	0.77
2:K:167:ILE:O	2:K:168:ASN:HB2	1.83	0.76
2:O:177:GLU:HA	2:O:181:ILE:HD13	1.67	0.76
2:K:317:ARG:H	2:K:317:ARG:HE	1.34	0.76
2:L:367:ASN:O	2:L:367:ASN:CG	2.28	0.76
2:L:222:PHE:HE2	2:L:275:MET:HE1	1.51	0.75
2:L:137:TYR:O	2:L:141:LEU:HG	1.87	0.74
2:L:268:ILE:H	2:L:268:ILE:CD1	1.98	0.73
2:M:162:ASN:C	2:M:164:CYS:H	1.95	0.73
2:L:65:SER:HB2	2:L:68:HIS:ND1	2.04	0.72
2:N:143:ARG:HH22	3:R:44:U:H3'	1.54	0.72
2:O:251:ASN:HB3	2:O:253:GLU:HG2	1.72	0.72
2:L:222:PHE:CE2	2:L:275:MET:HE1	2.24	0.72
2:K:233:HIS:CE1	2:K:237:ILE:HD13	2.24	0.72
2:O:117:LEU:HB3	2:O:118:PRO:HD3	1.71	0.71
1:D:219:ILE:HD11	1:D:224:LEU:HD21	1.72	0.71
2:K:214:ARG:HA	2:K:217:THR:HG22	1.72	0.70
2:L:390:THR:HG23	2:L:393:MET:HG2	1.74	0.70
2:O:317:ARG:CD	2:O:317:ARG:N	2.54	0.70
3:R:35:U:H2'	3:R:36:U:H5''	1.74	0.70
2:L:81:ARG:HD3	2:L:208:HIS:CE1	2.27	0.69
1:A:214:LEU:HD11	1:A:262:LYS:HE2	1.74	0.69
2:L:268:ILE:HA	2:L:275:MET:HE2	1.73	0.69
2:N:38:ILE:HD13	2:N:281:PHE:HE2	1.57	0.69
1:B:204:SER:HB2	1:B:218:THR:HB	1.74	0.69
2:O:411:THR:HG23	2:O:414:LYS:H	1.57	0.69
2:L:398:LYS:O	2:L:402:MET:HG2	1.92	0.69
1:D:195:SER:HB2	1:D:198:TRP:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:268:ILE:HD13	2:L:268:ILE:N	2.05	0.68
2:L:338:VAL:HG13	2:L:373:ARG:NH1	2.08	0.68
2:O:408:ARG:O	2:O:411:THR:HG22	1.94	0.67
2:O:194:ILE:O	2:O:198:VAL:HG23	1.95	0.67
2:M:224:ASP:HB2	2:M:279:ILE:HG13	1.76	0.67
2:O:50:ASP:HB2	2:O:121:VAL:HA	1.77	0.67
2:L:356:THR:O	2:L:356:THR:CG2	2.43	0.66
2:K:77:LEU:C	2:K:79:ASP:H	2.03	0.66
2:K:104:ILE:HD11	2:K:198:VAL:HA	1.78	0.66
2:N:238:THR:HB	2:N:240:MET:HG3	1.78	0.66
2:N:63:ASN:HD22	2:N:63:ASN:H	1.43	0.66
2:L:238:THR:HB	2:L:240:MET:HG3	1.75	0.66
2:M:214:ARG:HA	2:M:217:THR:CG2	2.18	0.66
2:K:328:THR:HG21	2:K:415:TYR:OH	1.96	0.65
2:N:172:GLU:HB2	2:N:173:PRO:HD3	1.76	0.65
2:N:270:LYS:HE2	2:N:270:LYS:HA	1.78	0.65
2:M:381:TRP:O	2:M:384:ASP:HB2	1.97	0.65
2:L:73:LEU:HD13	2:L:194:ILE:HG21	1.79	0.65
2:M:248:TRP:HZ3	2:M:333:LEU:HD23	1.61	0.65
2:L:192:THR:O	2:L:280:ASP:HB3	1.97	0.64
2:O:14:ILE:HG23	2:O:16:PRO:HD3	1.79	0.64
2:M:214:ARG:O	2:M:216:GLY:N	2.29	0.64
1:A:195:SER:HB2	1:A:198:TRP:HB2	1.80	0.64
2:K:107:LEU:O	2:K:108:VAL:CB	2.43	0.64
2:N:317:ARG:NH1	3:R:40:U:H3'	2.12	0.64
2:L:418:SER:O	2:L:422:LYS:HE3	1.97	0.64
2:K:143:ARG:HH22	3:R:26:U:H3'	1.60	0.64
2:K:408:ARG:NH2	3:R:24:U:H2'	2.13	0.64
2:L:79:ASP:HB3	2:L:81:ARG:CG	2.28	0.64
2:K:81:ARG:HE	2:K:82:GLY:N	1.92	0.63
2:K:167:ILE:HG22	2:K:168:ASN:O	1.98	0.63
2:N:366:THR:C	2:N:368:ALA:H	2.07	0.63
2:O:136:LEU:HD13	2:O:163:GLN:HG2	1.79	0.63
2:K:324:TYR:O	2:K:328:THR:HG23	1.98	0.63
2:M:214:ARG:HH21	2:M:218:ILE:HD13	1.62	0.63
2:N:130:ASP:O	2:N:130:ASP:CG	2.40	0.63
2:K:117:LEU:H	2:K:118:PRO:HD3	1.63	0.63
2:M:199:ASP:OD1	2:M:217:THR:HG23	1.99	0.62
2:M:29:ALA:H	2:M:266:GLN:HE22	1.46	0.62
2:K:2:SER:HB3	2:L:243:GLU:HG3	1.80	0.62
2:K:191:TYR:O	2:K:195:VAL:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:28:PRO:HD2	2:L:266:GLN:HE21	1.65	0.62
2:N:188:ASP:HB3	2:N:191:TYR:HB3	1.81	0.62
2:K:167:ILE:O	2:K:168:ASN:CB	2.47	0.62
2:M:40:LEU:HD11	2:M:194:ILE:HG13	1.81	0.62
2:O:27:TYR:HB3	2:O:266:GLN:NE2	2.14	0.62
2:L:146:ARG:HD3	2:L:219:VAL:HG11	1.82	0.61
2:L:79:ASP:C	2:L:81:ARG:H	2.05	0.61
2:L:317:ARG:H	2:L:317:ARG:NE	1.98	0.61
2:M:317:ARG:HH11	3:R:4:U:H5''	1.66	0.60
2:K:199:ASP:OD1	2:K:217:THR:HG23	2.01	0.60
2:M:113:LEU:HD23	2:M:114:ASP:H	1.63	0.60
2:L:17:LYS:HG3	2:M:268:ILE:HD11	1.82	0.60
2:N:346:GLN:HE21	2:N:349:CYS:HB3	1.65	0.60
2:L:188:ASP:CG	2:L:189:SER:N	2.60	0.60
2:M:83:LYS:HD3	2:M:83:LYS:H	1.66	0.60
2:N:184:VAL:HG21	2:O:165:LYS:HG2	1.84	0.60
2:O:28:PRO:HD2	2:O:266:GLN:HE21	1.67	0.60
2:O:172:GLU:HB3	2:O:173:PRO:HD2	1.83	0.60
2:K:308:LEU:O	2:K:309:ARG:HB2	2.02	0.60
2:M:233:HIS:CE1	2:M:312:ARG:HD2	2.36	0.60
2:M:231:PHE:CZ	2:M:258:MET:HE1	2.37	0.60
2:O:334:TYR:O	2:O:338:VAL:HG23	2.02	0.60
2:K:81:ARG:NE	2:K:82:GLY:H	1.94	0.59
2:K:286:LYS:HE2	3:R:21:U:OP2	2.01	0.59
2:K:143:ARG:NH2	3:R:26:U:H3'	2.17	0.59
2:K:299:PHE:CE1	2:K:328:THR:HG22	2.37	0.59
2:M:144:VAL:HG11	2:M:156:LEU:HG	1.84	0.59
2:M:317:ARG:NH1	3:R:5:U:OP2	2.36	0.59
2:N:317:ARG:H	2:N:317:ARG:NE	1.92	0.59
2:M:14:ILE:HG23	2:M:16:PRO:HD3	1.84	0.59
2:N:273:SER:O	2:N:276:PRO:HD2	2.03	0.59
2:L:214:ARG:HA	2:L:217:THR:HG22	1.85	0.59
2:K:14:ILE:HG22	2:K:16:PRO:HD3	1.85	0.58
2:L:275:MET:HB3	2:L:276:PRO:HD3	1.85	0.58
2:L:395:GLN:HA	2:L:395:GLN:HE21	1.68	0.58
2:M:214:ARG:C	2:M:216:GLY:H	2.11	0.58
2:O:135:PRO:HB2	2:O:213:PHE:HE2	1.68	0.57
2:L:199:ASP:OD1	2:L:217:THR:HG23	2.04	0.57
2:L:336:TYR:CD1	2:L:393:MET:HE2	2.38	0.57
3:R:16:U:H2'	3:R:17:U:C6	2.38	0.57
2:N:140:GLY:HA2	2:N:216:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:374:ASP:HB3	2:N:377:GLU:HG3	1.85	0.57
2:O:346:GLN:NE2	2:O:349:CYS:HB3	2.19	0.57
2:L:136:LEU:HD13	2:L:213:PHE:HA	1.86	0.57
2:M:408:ARG:HD3	2:M:411:THR:HG23	1.87	0.56
2:K:342:ALA:O	2:K:343:ASP:C	2.49	0.56
2:M:59:LEU:HD12	2:M:64:VAL:HG11	1.87	0.56
3:R:25:U:H2'	3:R:26:U:O4'	2.05	0.56
2:L:181:ILE:HD12	2:L:182:PHE:H	1.71	0.56
1:A:260:ARG:HD2	1:A:265:LEU:HD21	1.88	0.56
1:E:219:ILE:HD11	1:E:224:LEU:HD11	1.87	0.56
2:L:23:ASP:HB3	2:L:286:LYS:HE3	1.88	0.56
2:O:169:GLU:CD	2:O:170:GLN:H	2.14	0.56
2:M:149:MET:C	2:M:151:GLU:H	2.14	0.56
2:K:172:GLU:HB2	2:K:173:PRO:HD3	1.87	0.56
2:L:390:THR:CG2	2:L:393:MET:HG2	2.36	0.55
2:N:386:ASN:HD21	2:O:365:THR:HG21	1.69	0.55
2:L:116:VAL:HG23	2:L:118:PRO:HD3	1.88	0.55
3:R:36:U:H2'	3:R:37:U:H5''	1.89	0.55
2:M:224:ASP:CG	3:R:3:U:H4'	2.31	0.55
2:N:47:SER:HB3	2:N:50:ASP:HB2	1.88	0.55
2:M:226:ALA:O	2:M:230:THR:HG23	2.06	0.55
1:A:232:ILE:HG23	1:B:202:LYS:HZ3	1.71	0.55
2:L:172:GLU:H	2:L:173:PRO:CD	2.20	0.55
2:N:401:VAL:O	2:N:404:LEU:HB2	2.06	0.55
2:M:356:THR:N	2:M:357:PRO:HD3	2.22	0.55
2:L:151:GLU:HG3	3:R:15:U:O2'	2.06	0.55
2:L:164:CYS:HB3	2:L:169:GLU:HG2	1.88	0.55
2:N:104:ILE:HG12	2:N:104:ILE:O	2.06	0.55
2:O:336:TYR:CD1	2:O:393:MET:HG2	2.42	0.55
2:K:279:ILE:HD11	2:K:287:SER:HB2	1.90	0.54
2:L:243:GLU:O	2:L:247:THR:HG23	2.07	0.54
2:L:253:GLU:OE1	2:L:323:GLU:HG3	2.07	0.54
2:L:380:GLY:HA2	2:M:354:LYS:HE3	1.89	0.54
2:M:84:LEU:HD23	2:M:102:ILE:HD12	1.88	0.54
2:M:155:LYS:O	2:M:158:ASP:HB3	2.07	0.54
2:K:137:TYR:HD1	2:K:163:GLN:HG3	1.73	0.54
2:M:179:ARG:HA	2:M:183:ASP:HB2	1.90	0.54
2:N:332:LEU:HD13	2:N:393:MET:HE2	1.89	0.54
2:K:214:ARG:O	2:K:216:GLY:N	2.41	0.54
2:M:28:PRO:HD2	2:M:266:GLN:HE21	1.71	0.54
2:L:366:THR:O	2:L:367:ASN:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:GLU:HB2	2:M:108:VAL:HG11	1.88	0.54
2:O:44:THR:OG1	2:O:112:ALA:O	2.25	0.54
3:R:35:U:C2'	3:R:36:U:H5''	2.36	0.54
1:C:219:ILE:HD11	2:M:364:LEU:HB2	1.88	0.54
2:K:214:ARG:C	2:K:216:GLY:H	2.14	0.54
2:N:323:GLU:O	2:N:327:LEU:HB2	2.07	0.54
2:O:192:THR:HA	2:O:195:VAL:HG12	1.90	0.54
2:M:317:ARG:H	2:M:317:ARG:NE	1.96	0.54
2:O:165:LYS:O	2:O:167:ILE:HG12	2.08	0.54
2:K:169:GLU:HG2	2:K:170:GLN:N	2.23	0.53
1:B:240:MET:HE2	1:B:244:GLU:HB2	1.91	0.53
2:M:401:VAL:HG21	2:M:420:PHE:HB2	1.89	0.53
1:B:211:LYS:HB2	1:B:214:LEU:HD12	1.89	0.53
2:L:14:ILE:HG23	2:L:16:PRO:HD3	1.90	0.53
1:E:255:LEU:HA	2:O:384:ASP:CG	2.34	0.53
2:K:205:PHE:O	2:K:207:LYS:N	2.40	0.53
2:K:407:LEU:HD13	2:K:414:LYS:HA	1.90	0.53
2:N:402:MET:O	2:N:403:SER:HB2	2.07	0.53
2:L:343:ASP:O	2:L:344:LEU:C	2.52	0.53
3:R:34:U:H2'	3:R:35:U:C6	2.44	0.53
2:K:54:TYR:CE2	2:K:118:PRO:HA	2.43	0.53
2:K:117:LEU:N	2:K:118:PRO:CD	2.71	0.53
2:M:241:SER:OG	2:M:243:GLU:HG2	2.09	0.53
2:M:290:SER:O	2:M:294:ASN:ND2	2.41	0.53
2:K:169:GLU:HG2	2:K:170:GLN:H	1.74	0.52
2:N:263:LEU:HD12	2:N:264:PRO:HD2	1.90	0.52
2:M:342:ALA:O	2:M:343:ASP:C	2.52	0.52
2:L:66:ILE:HG23	2:L:67:ILE:HG12	1.92	0.52
2:O:140:GLY:HA2	2:O:216:GLY:HA3	1.90	0.52
1:D:198:TRP:HE3	1:D:198:TRP:O	1.92	0.52
1:E:215:GLN:HG3	1:E:216:PRO:HD2	1.92	0.52
2:M:42:ILE:HD12	2:M:43:ASN:N	2.24	0.52
2:M:132:LYS:HB3	2:M:133:TRP:HD1	1.74	0.52
2:O:251:ASN:O	2:O:254:VAL:N	2.34	0.52
2:L:350:VAL:HG23	2:L:351:GLY:H	1.75	0.52
2:M:203:HIS:CD2	2:M:272:ASP:OD2	2.63	0.52
2:M:354:LYS:HG2	2:M:355:TYR:H	1.75	0.52
2:N:143:ARG:NH2	3:R:45:U:OP2	2.43	0.52
1:A:230:GLU:O	1:A:234:VAL:HG22	2.08	0.52
2:K:144:VAL:HG22	2:K:155:LYS:HB3	1.92	0.52
2:K:370:PRO:HG2	2:K:378:TRP:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:268:ILE:HG22	2:N:275:MET:HG3	1.91	0.52
2:O:139:LEU:O	2:O:142:TYR:HB3	2.09	0.52
2:K:58:GLY:CA	2:K:64:VAL:HB	2.34	0.52
2:K:202:PHE:HE2	2:K:208:HIS:HD1	1.58	0.52
1:C:230:GLU:O	1:C:234:VAL:HG22	2.10	0.52
2:O:199:ASP:OD2	2:O:277:TYR:OH	2.27	0.52
2:O:214:ARG:CA	2:O:217:THR:HG22	2.29	0.52
1:A:235:GLY:HA2	2:L:364:LEU:HB2	1.93	0.51
2:K:117:LEU:N	2:K:118:PRO:HD3	2.23	0.51
2:K:149:MET:HE3	2:K:150:PRO:HD2	1.92	0.51
2:N:137:TYR:HD1	2:N:163:GLN:HE22	1.58	0.51
2:L:79:ASP:C	2:L:81:ARG:N	2.68	0.51
1:B:253:LYS:HB3	2:L:367:ASN:HB2	1.91	0.51
2:K:422:LYS:HD3	2:L:399:ARG:HD2	1.91	0.51
2:N:322:ILE:HD12	2:N:327:LEU:HD23	1.91	0.51
2:O:281:PHE:HB3	2:O:283:LEU:HD21	1.90	0.51
2:L:43:ASN:CG	2:L:44:THR:N	2.66	0.51
2:O:342:ALA:HB1	2:O:344:LEU:HD23	1.93	0.51
2:L:43:ASN:O	2:L:44:THR:HG23	2.11	0.51
2:L:234:LEU:HD22	2:L:301:GLY:HA2	1.92	0.51
2:M:47:SER:O	2:M:49:SER:N	2.43	0.51
2:K:248:TRP:CD1	2:K:375:VAL:HG22	2.45	0.51
2:M:408:ARG:HD3	2:M:411:THR:CG2	2.40	0.51
1:A:198:TRP:HA	1:A:198:TRP:CE3	2.45	0.51
2:K:43:ASN:O	2:K:44:THR:C	2.54	0.51
2:L:317:ARG:CZ	3:R:13:U:H3'	2.41	0.51
2:M:317:ARG:HH11	3:R:4:U:C5'	2.24	0.51
2:K:18:LEU:HD13	2:L:232:GLY:HA2	1.93	0.51
2:O:97:LYS:O	2:O:100:ASP:HB2	2.10	0.51
1:A:200:LEU:HB3	1:A:203:THR:OG1	2.11	0.51
2:M:66:ILE:HA	2:M:69:VAL:HG22	1.93	0.51
2:N:254:VAL:HG13	2:N:297:PHE:HA	1.92	0.51
2:K:37:GLU:HB2	2:K:108:VAL:HG11	1.93	0.50
2:K:113:LEU:HD23	2:K:113:LEU:H	1.75	0.50
2:N:79:ASP:C	2:N:81:ARG:H	2.19	0.50
2:O:195:VAL:O	2:O:217:THR:OG1	2.28	0.50
2:N:275:MET:O	2:N:278:LEU:HG	2.11	0.50
2:O:401:VAL:HG21	2:O:420:PHE:HB2	1.93	0.50
2:L:355:TYR:O	2:L:356:THR:CB	2.59	0.50
2:L:299:PHE:HZ	2:L:415:TYR:CE1	2.30	0.50
2:M:55:VAL:HA	2:M:64:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:263:LEU:CG	2:L:264:PRO:HD2	2.38	0.50
2:N:136:LEU:HD22	2:N:163:GLN:HG2	1.93	0.50
2:O:224:ASP:HB2	2:O:279:ILE:HG13	1.94	0.50
2:M:66:ILE:HD11	2:M:191:TYR:HB2	1.94	0.50
1:E:225:PHE:HD1	1:E:230:GLU:HG3	1.77	0.50
2:L:298:HIS:CE1	2:L:317:ARG:HH22	2.30	0.50
2:K:228:LEU:HD11	2:O:19:PRO:HD3	1.93	0.49
2:N:399:ARG:HA	2:N:402:MET:HE3	1.94	0.49
2:O:312:ARG:O	2:O:313:ALA:C	2.55	0.49
2:K:299:PHE:CZ	2:K:328:THR:HG22	2.47	0.49
2:N:184:VAL:CG2	2:O:165:LYS:HG2	2.42	0.49
2:L:185:TRP:HB3	2:L:191:TYR:CE1	2.48	0.49
2:M:334:TYR:O	2:M:338:VAL:HG23	2.12	0.49
2:O:42:ILE:CG2	2:O:190:ASN:HB3	2.42	0.49
1:A:231:PHE:HD2	1:A:232:ILE:HD13	1.78	0.49
1:C:253:LYS:O	1:C:254:LYS:HB2	2.11	0.49
2:N:233:HIS:HB2	2:N:312:ARG:NH2	2.27	0.49
2:O:43:ASN:HD22	2:O:111:LYS:HD3	1.77	0.49
2:O:336:TYR:CG	2:O:393:MET:HG2	2.48	0.49
1:B:214:LEU:HD13	1:B:262:LYS:HE3	1.95	0.49
2:K:43:ASN:HB3	2:K:67:ILE:HG23	1.95	0.49
2:K:330:ALA:HA	2:L:344:LEU:HD21	1.94	0.49
2:O:137:TYR:O	2:O:141:LEU:HG	2.12	0.49
1:E:253:LYS:HE3	2:O:364:LEU:HD22	1.94	0.49
2:K:324:TYR:C	2:K:326:SER:H	2.21	0.49
2:O:117:LEU:CB	2:O:118:PRO:HD3	2.42	0.48
2:O:134:LEU:N	2:O:135:PRO:CD	2.76	0.48
1:A:237:ASN:HD21	2:L:364:LEU:HD21	1.77	0.48
2:N:338:VAL:HG13	2:N:373:ARG:CZ	2.43	0.48
2:K:402:MET:O	2:K:403:SER:C	2.56	0.48
2:L:306:LEU:HA	2:L:310:SER:HB3	1.95	0.48
2:M:288:PRO:HG2	2:M:289:TYR:CE2	2.49	0.48
3:R:41:U:H2'	3:R:43:U:O5'	2.13	0.48
2:M:135:PRO:HB2	2:M:213:PHE:CE2	2.48	0.48
2:O:397:ALA:O	2:O:398:LYS:C	2.57	0.48
2:K:288:PRO:HG2	2:K:289:TYR:CE2	2.48	0.48
1:C:205:MET:HE1	1:C:243:LYS:HB2	1.94	0.48
2:K:8:ILE:HG22	2:M:349:CYS:SG	2.53	0.48
2:K:398:LYS:O	2:K:402:MET:HG2	2.13	0.48
2:L:214:ARG:C	2:L:216:GLY:H	2.22	0.48
2:N:275:MET:HB3	2:N:276:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:302:GLN:HG2	2:N:316:ALA:CB	2.44	0.48
2:O:419:GLU:O	2:O:422:LYS:HE2	2.13	0.48
2:L:7:ARG:HG2	2:L:7:ARG:NH1	2.28	0.48
2:M:134:LEU:O	2:M:138:LEU:HG	2.14	0.48
2:M:354:LYS:HG2	2:M:355:TYR:N	2.29	0.48
2:K:317:ARG:HD3	3:R:22:U:H2'	1.96	0.48
2:L:140:GLY:HA2	2:L:216:GLY:HA3	1.96	0.48
2:L:232:GLY:O	2:L:236:LYS:HG2	2.14	0.48
2:K:253:GLU:OE1	2:K:323:GLU:HG2	2.13	0.48
2:K:317:ARG:HE	2:K:317:ARG:N	2.06	0.48
2:M:224:ASP:OD2	3:R:3:U:H4'	2.13	0.48
2:M:317:ARG:NH2	3:R:5:U:H5''	2.29	0.48
2:M:395:GLN:HE21	2:M:395:GLN:HA	1.79	0.48
2:N:308:LEU:O	2:N:309:ARG:HB2	2.14	0.48
1:E:198:TRP:C	1:E:200:LEU:H	2.22	0.47
2:K:26:GLU:OE1	2:K:285:SER:HB2	2.14	0.47
2:K:108:VAL:O	2:K:108:VAL:HG12	2.14	0.47
2:L:49:SER:HB2	2:L:52:ARG:HH12	1.78	0.47
2:M:230:THR:HB	2:M:302:GLN:OE1	2.13	0.47
2:L:84:LEU:HD21	2:L:96:GLY:HA3	1.96	0.47
2:L:240:MET:HE2	2:L:334:TYR:OH	2.13	0.47
2:N:86:LYS:HG2	2:N:87:ASP:H	1.79	0.47
2:O:93:ILE:N	2:O:93:ILE:HD12	2.29	0.47
2:K:350:VAL:C	2:K:352:ASP:H	2.22	0.47
2:M:398:LYS:HD2	2:M:421:ASP:HA	1.96	0.47
2:O:317:ARG:NH1	3:R:32:U:H5''	2.29	0.47
2:K:77:LEU:O	2:K:79:ASP:N	2.46	0.47
2:K:133:TRP:HE3	2:K:163:GLN:HE21	1.62	0.47
2:L:183:ASP:C	2:L:185:TRP:H	2.21	0.47
2:L:172:GLU:H	2:L:173:PRO:HD2	1.79	0.47
2:K:167:ILE:HG22	2:K:168:ASN:C	2.40	0.47
2:M:58:GLY:C	2:M:60:LYS:H	2.22	0.47
2:O:50:ASP:CB	2:O:121:VAL:HA	2.44	0.47
2:K:25:VAL:HG11	2:K:288:PRO:HA	1.96	0.47
2:K:286:LYS:HD2	3:R:20:U:H5''	1.96	0.47
3:R:8:U:H6	3:R:8:U:OP2	1.98	0.47
1:A:198:TRP:NE1	1:A:228:ARG:HA	2.30	0.47
2:N:137:TYR:O	2:N:141:LEU:HG	2.15	0.47
2:N:330:ALA:HB2	2:O:344:LEU:HD21	1.97	0.47
1:E:260:ARG:HA	1:E:265:LEU:HB2	1.96	0.47
2:K:270:LYS:HD3	2:K:273:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:GLU:HA	2:L:154:LYS:HD3	1.97	0.47
2:L:336:TYR:CD1	2:L:393:MET:CE	2.98	0.47
2:L:353:ASN:N	2:L:353:ASN:OD1	2.48	0.47
2:M:144:VAL:HG22	2:M:155:LYS:HB3	1.97	0.47
2:M:90:SER:OG	2:M:274:TYR:HD1	1.98	0.47
3:R:44:U:H2'	3:R:45:U:H5''	1.97	0.47
2:M:64:VAL:O	2:M:64:VAL:HG13	2.15	0.46
2:M:160:LEU:O	2:M:164:CYS:HB3	2.15	0.46
2:N:346:GLN:NE2	2:N:349:CYS:HB3	2.30	0.46
2:L:238:THR:C	2:L:240:MET:H	2.22	0.46
2:M:66:ILE:HD13	2:M:66:ILE:O	2.14	0.46
2:O:273:SER:O	2:O:276:PRO:HD2	2.15	0.46
2:K:9:ILE:HG13	2:L:252:ARG:HH22	1.79	0.46
2:K:162:ASN:OD1	2:K:165:LYS:HD2	2.15	0.46
1:E:234:VAL:O	2:K:364:LEU:HB2	2.14	0.46
2:O:22:GLU:HA	2:O:22:GLU:OE1	2.16	0.46
2:O:37:GLU:HB2	2:O:108:VAL:HG11	1.97	0.46
2:M:176:PRO:O	2:M:177:GLU:C	2.58	0.46
2:N:241:SER:OG	2:N:242:THR:N	2.49	0.46
2:N:401:VAL:HG11	2:N:416:ALA:HB1	1.98	0.46
2:K:14:ILE:HD11	2:L:259:VAL:HG13	1.97	0.46
2:K:43:ASN:HD22	2:K:67:ILE:HG23	1.81	0.46
2:K:380:GLY:HA2	2:L:354:LYS:NZ	2.30	0.46
2:N:65:SER:HB3	2:N:118:PRO:HG3	1.97	0.46
2:L:367:ASN:O	2:L:367:ASN:ND2	2.48	0.46
2:M:275:MET:HB3	2:M:276:PRO:HD3	1.98	0.46
2:N:18:LEU:HD22	2:O:232:GLY:HA2	1.97	0.46
2:K:14:ILE:HD13	2:K:14:ILE:HA	1.83	0.46
2:K:23:ASP:OD2	2:K:286:LYS:NZ	2.47	0.46
2:N:57:GLN:HB2	2:N:63:ASN:HD21	1.81	0.46
2:N:177:GLU:HG2	2:N:179:ARG:H	1.80	0.46
2:O:34:LYS:HD2	2:O:34:LYS:HA	1.83	0.46
2:N:396:TYR:O	2:N:399:ARG:HB3	2.16	0.46
3:R:34:U:H2'	3:R:35:U:O4'	2.16	0.46
2:K:385:GLN:HG2	2:K:390:THR:HG23	1.98	0.46
2:K:401:VAL:HG21	2:K:420:PHE:HB2	1.97	0.46
2:L:382:PHE:CE2	2:L:387:ARG:HA	2.51	0.46
2:O:398:LYS:O	2:O:402:MET:HG2	2.16	0.46
2:O:312:ARG:O	2:O:314:ARG:N	2.49	0.45
2:K:202:PHE:O	2:K:206:LYS:N	2.49	0.45
2:N:27:TYR:CE2	2:N:263:LEU:HD23	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:190:ASN:O	2:N:194:ILE:HG12	2.16	0.45
2:M:104:ILE:HD13	2:M:201:PHE:CD1	2.50	0.45
2:M:104:ILE:H	2:M:104:ILE:HG12	1.58	0.45
2:O:153:ARG:O	2:O:157:MET:HG3	2.16	0.45
3:R:6:U:H5''	3:R:7:U:H5''	1.99	0.45
2:K:81:ARG:O	2:K:201:PHE:HZ	1.99	0.45
2:M:65:SER:O	2:M:68:HIS:HB2	2.16	0.45
2:N:302:GLN:HG2	2:N:316:ALA:HB3	1.99	0.45
2:N:104:ILE:HD11	2:N:198:VAL:HA	1.98	0.45
1:D:242:HIS:O	1:D:246:ILE:HG12	2.17	0.45
2:O:226:ALA:O	2:O:230:THR:HG23	2.16	0.45
2:K:199:ASP:CG	2:K:214:ARG:HD2	2.42	0.45
2:L:108:VAL:HG12	2:L:109:SER:H	1.81	0.45
2:L:164:CYS:HA	2:L:167:ILE:HB	1.99	0.45
2:N:105:PHE:O	2:N:107:LEU:N	2.49	0.45
1:E:254:LYS:O	2:O:384:ASP:HB3	2.17	0.45
2:K:415:TYR:CD1	2:K:415:TYR:C	2.95	0.45
2:L:81:ARG:HD3	2:L:208:HIS:NE2	2.32	0.45
2:L:97:LYS:O	2:L:98:ALA:C	2.59	0.45
2:L:113:LEU:O	2:L:114:ASP:HB2	2.16	0.45
2:M:143:ARG:HG3	2:M:219:VAL:HG11	1.99	0.45
2:N:153:ARG:O	2:N:157:MET:HG2	2.17	0.45
1:B:225:PHE:HD1	1:B:230:GLU:HB3	1.83	0.45
1:D:208:GLN:HA	1:D:209:PRO:HD3	1.78	0.45
2:K:349:CYS:HB3	2:N:8:ILE:HD11	1.97	0.45
2:L:18:LEU:HD22	2:M:232:GLY:HA2	1.99	0.45
1:E:255:LEU:HA	2:O:384:ASP:OD1	2.17	0.44
2:L:136:LEU:HG	2:L:163:GLN:HG3	1.98	0.44
2:L:175:VAL:HG13	2:L:181:ILE:HG23	1.99	0.44
2:N:281:PHE:HB3	2:N:283:LEU:HD13	1.99	0.44
1:A:210:LYS:HE3	1:A:264:SER:HB3	1.99	0.44
1:B:197:VAL:HG23	1:B:201:SER:HB3	1.99	0.44
1:C:200:LEU:HD12	1:C:242:HIS:ND1	2.32	0.44
2:K:88:TRP:CD2	2:K:204:MET:HE3	2.53	0.44
2:K:299:PHE:HE1	2:K:328:THR:HG22	1.80	0.44
2:N:415:TYR:CD1	2:N:415:TYR:C	2.95	0.44
2:L:7:ARG:HG2	2:L:7:ARG:HH11	1.81	0.44
2:L:181:ILE:H	2:L:181:ILE:HG13	1.62	0.44
2:M:286:LYS:HZ3	3:R:2:U:H5'	1.83	0.44
2:M:347:GLN:HA	2:M:347:GLN:NE2	2.32	0.44
2:N:78:LYS:O	2:N:80:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:143:ARG:HG2	2:O:216:GLY:HA2	1.99	0.44
2:K:97:LYS:O	2:K:98:ALA:C	2.59	0.44
2:K:202:PHE:HE2	2:K:208:HIS:ND1	2.16	0.44
2:M:248:TRP:CZ3	2:M:333:LEU:HD23	2.46	0.44
2:N:180:ASP:C	2:N:182:PHE:H	2.26	0.44
2:O:160:LEU:HD12	2:O:172:GLU:HG2	1.99	0.44
2:K:422:LYS:CD	2:L:399:ARG:HD2	2.47	0.44
2:L:224:ASP:HB2	2:L:279:ILE:HG13	2.00	0.44
2:N:317:ARG:HE	2:N:317:ARG:N	1.97	0.44
2:N:379:LEU:HB3	2:O:354:LYS:HD3	2.00	0.44
2:M:80:ILE:HG13	2:M:102:ILE:C	2.40	0.43
2:N:117:LEU:H	2:N:118:PRO:HD3	1.81	0.43
2:O:117:LEU:HB3	2:O:118:PRO:CD	2.43	0.43
2:L:153:ARG:HH12	2:L:177:GLU:HG3	1.83	0.43
2:L:298:HIS:O	2:L:302:GLN:HB2	2.18	0.43
2:M:228:LEU:O	2:M:229:ALA:C	2.61	0.43
2:O:324:TYR:O	2:O:326:SER:N	2.47	0.43
2:M:146:ARG:HH12	2:M:223:LYS:HE3	1.83	0.43
2:O:385:GLN:HG2	2:O:390:THR:HG22	1.99	0.43
2:K:139:LEU:HD23	2:K:195:VAL:HG12	1.99	0.43
2:K:317:ARG:HH11	3:R:22:U:H3'	1.78	0.43
2:K:368:ALA:HB1	2:K:369:PRO:CD	2.48	0.43
2:L:64:VAL:HG22	2:L:65:SER:N	2.34	0.43
2:L:312:ARG:HD2	3:R:14:U:C2	2.54	0.43
2:M:269:ASP:OD2	2:M:269:ASP:N	2.52	0.43
2:O:199:ASP:OD1	2:O:217:THR:HG23	2.18	0.43
1:A:205:MET:O	1:A:218:THR:HA	2.19	0.43
2:K:234:LEU:O	2:K:235:CYS:C	2.60	0.43
2:L:42:ILE:O	2:L:43:ASN:C	2.61	0.43
2:L:360:SER:C	2:L:371:GLN:HE22	2.26	0.43
2:M:66:ILE:O	2:M:70:ASN:HB2	2.19	0.43
2:N:191:TYR:C	2:N:193:LYS:N	2.77	0.43
2:O:140:GLY:C	2:O:142:TYR:H	2.27	0.43
2:O:57:GLN:HG2	2:O:60:LYS:HD2	2.00	0.43
3:R:7:U:H2'	3:R:8:U:C6	2.54	0.43
2:K:99:GLY:O	2:K:100:ASP:C	2.62	0.43
3:R:4:U:H5'	3:R:5:U:OP2	2.18	0.43
1:A:251:ARG:C	1:A:253:LYS:H	2.27	0.42
2:L:72:TYR:CE1	2:L:134:LEU:HD12	2.54	0.42
2:M:10:ASP:OD2	2:M:10:ASP:C	2.61	0.42
2:N:302:GLN:HE21	2:N:313:ALA:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:53:GLY:HA3	2:O:123:ASP:HB3	2.01	0.42
2:O:84:LEU:HD11	2:O:96:GLY:HA3	2.00	0.42
2:L:127:THR:O	2:L:128:SER:HB3	2.19	0.42
2:N:59:LEU:O	2:N:173:PRO:HA	2.19	0.42
1:C:209:PRO:HD3	1:C:216:PRO:HA	2.00	0.42
2:K:40:LEU:HD13	2:K:42:ILE:HG13	2.01	0.42
2:O:408:ARG:HH21	3:R:33:U:H2'	1.83	0.42
3:R:8:U:H2'	3:R:9:U:C5'	2.44	0.42
3:R:42:U:H5''	3:R:43:U:H5''	2.00	0.42
2:L:40:LEU:HB3	2:L:109:SER:HA	2.01	0.42
2:L:279:ILE:HD11	2:L:287:SER:HB2	2.01	0.42
2:L:366:THR:OG1	2:L:367:ASN:N	2.48	0.42
2:L:401:VAL:HG21	2:L:420:PHE:HB2	2.02	0.42
2:M:162:ASN:C	2:M:164:CYS:N	2.67	0.42
1:C:201:SER:O	1:C:222:ASP:HB2	2.19	0.42
1:E:224:LEU:O	1:E:252:TYR:HB2	2.19	0.42
2:M:70:ASN:OD1	2:M:190:ASN:HB3	2.20	0.42
2:M:84:LEU:O	2:M:99:GLY:HA2	2.18	0.42
2:N:240:MET:HE2	2:N:244:ASP:HB3	2.00	0.42
2:O:126:ARG:HD2	2:O:132:LYS:HE2	2.00	0.42
2:K:199:ASP:OD2	2:K:214:ARG:NH1	2.49	0.42
2:K:315:ASN:HA	2:K:411:THR:HG21	2.01	0.42
2:K:324:TYR:O	2:K:326:SER:N	2.40	0.42
2:N:321:ASP:OD1	2:O:233:HIS:ND1	2.53	0.42
1:B:250:LEU:HD12	1:B:255:LEU:O	2.19	0.42
2:L:159:GLY:O	2:L:163:GLN:HB2	2.20	0.42
2:L:192:THR:HA	2:L:195:VAL:HG22	2.01	0.42
2:L:380:GLY:HA2	2:M:354:LYS:CE	2.49	0.42
2:O:77:LEU:HB2	2:O:105:PHE:HE1	1.85	0.42
2:M:63:ASN:O	2:M:64:VAL:HG12	2.20	0.42
2:K:10:ASP:OD2	2:K:10:ASP:C	2.62	0.42
2:L:203:HIS:HD2	2:L:272:ASP:OD1	2.03	0.42
2:M:379:LEU:HD23	2:M:379:LEU:HA	1.95	0.42
2:N:26:GLU:OE2	2:N:285:SER:N	2.42	0.42
2:O:234:LEU:HD22	2:O:301:GLY:HA2	2.01	0.42
2:L:7:ARG:HH11	2:L:7:ARG:CG	2.33	0.41
2:M:422:LYS:HE3	2:M:422:LYS:HB2	1.91	0.41
1:E:255:LEU:HB2	1:E:258:GLN:HB3	2.01	0.41
2:M:14:ILE:HD12	2:M:14:ILE:HA	1.97	0.41
2:M:73:LEU:HD21	2:M:135:PRO:HA	2.02	0.41
2:M:86:LYS:HB3	2:M:87:ASP:H	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:179:ARG:HA	2:K:183:ASP:HB2	2.02	0.41
2:K:246:THR:O	2:K:249:ILE:HB	2.19	0.41
2:K:259:VAL:O	2:K:260:GLN:C	2.63	0.41
2:L:162:ASN:HB3	2:L:215:TYR:CD1	2.56	0.41
2:K:195:VAL:HB	2:K:217:THR:OG1	2.19	0.41
2:M:149:MET:C	2:M:151:GLU:N	2.77	0.41
2:M:252:ARG:HB3	2:M:252:ARG:NH1	2.35	0.41
2:O:161:THR:O	2:O:165:LYS:HG3	2.19	0.41
1:C:228:ARG:NH1	1:C:232:ILE:HD11	2.36	0.41
1:C:260:ARG:HA	1:C:265:LEU:HD22	2.02	0.41
2:K:354:LYS:HG2	2:O:376:VAL:HG13	2.03	0.41
2:L:44:THR:HG22	2:L:111:LYS:HD2	2.02	0.41
2:L:383:GLU:O	2:L:383:GLU:HG3	2.20	0.41
2:M:36:LYS:HE2	2:M:93:ILE:HD13	2.03	0.41
2:M:102:ILE:HG22	2:M:103:GLY:N	2.36	0.41
1:E:205:MET:HE1	1:E:243:LYS:HG3	2.02	0.41
2:K:79:ASP:O	2:K:79:ASP:CG	2.63	0.41
2:M:333:LEU:HD12	2:M:393:MET:HE1	2.01	0.41
2:N:90:SER:HB3	2:N:274:TYR:CE1	2.55	0.41
2:N:356:THR:N	2:N:357:PRO:HD3	2.35	0.41
2:O:143:ARG:HB2	2:O:219:VAL:HG21	2.02	0.41
2:K:398:LYS:HG2	2:K:402:MET:HE3	2.02	0.41
2:L:43:ASN:HA	2:L:112:ALA:HB3	2.02	0.41
2:N:11:ASN:HD22	2:N:11:ASN:C	2.28	0.41
2:N:263:LEU:HA	2:N:264:PRO:HD3	1.86	0.41
2:O:390:THR:OG1	2:O:393:MET:CG	2.63	0.41
1:E:225:PHE:CZ	1:E:249:GLY:HA2	2.56	0.41
2:L:28:PRO:HD2	2:L:266:GLN:NE2	2.34	0.41
2:L:349:CYS:SG	2:O:8:ILE:HG22	2.61	0.41
2:M:317:ARG:NH2	3:R:5:U:C5'	2.84	0.41
2:M:347:GLN:HA	2:M:347:GLN:HE21	1.86	0.41
2:N:237:ILE:HD13	2:N:237:ILE:HA	1.98	0.41
2:L:136:LEU:HG	2:L:163:GLN:CG	2.51	0.41
2:L:214:ARG:O	2:L:216:GLY:N	2.54	0.41
2:M:128:SER:O	2:M:129:ALA:C	2.64	0.41
2:M:278:LEU:HG	2:M:279:ILE:N	2.35	0.41
2:N:161:THR:HA	2:N:164:CYS:SG	2.61	0.41
2:N:231:PHE:CE2	2:N:258:MET:HE1	2.54	0.41
2:O:385:GLN:HE21	2:O:385:GLN:HB2	1.68	0.41
1:A:201:SER:O	1:A:222:ASP:HB2	2.21	0.41
2:L:65:SER:HB2	2:L:68:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:317:ARG:CD	3:R:4:U:H3'	2.51	0.41
1:A:247:LEU:HA	1:A:250:LEU:HD23	2.02	0.40
1:B:224:LEU:HB3	1:B:249:GLY:O	2.21	0.40
2:L:84:LEU:HD11	2:L:88:TRP:HB2	2.03	0.40
2:L:395:GLN:HA	2:L:395:GLN:NE2	2.34	0.40
2:M:81:ARG:HD2	2:M:81:ARG:N	2.36	0.40
2:M:242:THR:HG23	2:M:243:GLU:OE1	2.21	0.40
2:N:240:MET:HE1	2:N:248:TRP:CD1	2.56	0.40
2:O:173:PRO:O	2:O:175:VAL:HG12	2.21	0.40
1:E:241:SER:HB2	1:E:244:GLU:HB2	2.02	0.40
2:K:221:ARG:HD2	2:K:276:PRO:HB2	2.02	0.40
2:K:324:TYR:C	2:K:326:SER:N	2.79	0.40
2:N:222:PHE:HE2	2:N:275:MET:SD	2.45	0.40
2:N:234:LEU:O	2:N:235:CYS:C	2.64	0.40
2:K:275:MET:O	2:K:278:LEU:HB3	2.20	0.40
2:N:63:ASN:H	2:N:63:ASN:ND2	2.14	0.40
2:O:149:MET:HG2	3:R:33:U:C6	2.56	0.40
1:A:240:MET:HG2	1:A:245:ALA:HB2	2.03	0.40
2:M:317:ARG:NH1	3:R:4:U:C5'	2.85	0.40
2:N:27:TYR:CZ	2:N:263:LEU:HD23	2.57	0.40
2:N:143:ARG:NH2	3:R:44:U:H3'	2.30	0.40
2:O:57:GLN:NE2	2:O:123:ASP:HB2	2.37	0.40
2:O:132:LYS:HB3	2:O:133:TRP:H	1.59	0.40
2:O:223:LYS:O	2:O:224:ASP:HB2	2.22	0.40
2:O:302:GLN:OE1	2:O:302:GLN:HA	2.21	0.40
1:C:197:VAL:O	1:C:200:LEU:HG	2.22	0.40
2:L:55:VAL:HG22	2:L:69:VAL:HG12	2.02	0.40
2:L:79:ASP:O	2:L:81:ARG:N	2.55	0.40
2:O:143:ARG:HB2	2:O:219:VAL:CG2	2.51	0.40
3:R:34:U:H2'	3:R:35:U:H6	1.83	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 X-ray entries followed by that with respect to entries of similar resolution.

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	71/87 (82%)	51 (72%)	15 (21%)	5 (7%)	1	10
1	B	71/87 (82%)	55 (78%)	14 (20%)	2 (3%)	4	26
1	C	71/87 (82%)	60 (84%)	9 (13%)	2 (3%)	4	26
1	D	71/87 (82%)	52 (73%)	17 (24%)	2 (3%)	4	26
1	E	71/87 (82%)	57 (80%)	13 (18%)	1 (1%)	9	38
2	K	419/421 (100%)	338 (81%)	54 (13%)	27 (6%)	1	11
2	L	419/421 (100%)	326 (78%)	72 (17%)	21 (5%)	1	15
2	M	419/421 (100%)	330 (79%)	65 (16%)	24 (6%)	1	13
2	N	419/421 (100%)	333 (80%)	68 (16%)	18 (4%)	2	18
2	O	419/421 (100%)	315 (75%)	82 (20%)	22 (5%)	1	14
All	All	2450/2540 (96%)	1917 (78%)	409 (17%)	124 (5%)	1	15

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	118	PRO
2	K	206	LYS
2	K	215	TYR
2	K	357	PRO
2	L	43	ASN
2	L	98	ALA
2	L	108	VAL
2	L	176	PRO
2	L	344	LEU
2	L	356	THR
2	M	48	LEU
2	M	102	ILE
2	M	118	PRO
2	M	177	GLU
2	M	215	TYR
2	M	344	LEU
2	N	79	ASP
2	N	106	ASP
2	N	174	LEU
2	N	343	ASP
2	O	43	ASN
2	O	118	PRO

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Mol	Chain	Res	Type
2	O	173	PRO
2	O	366	THR
1	A	197	VAL
1	A	202	LYS
1	A	236	GLY
1	A	241	SER
1	C	254	LYS
2	K	44	THR
2	K	78	LYS
2	K	93	ILE
2	K	98	ALA
2	K	108	VAL
2	K	128	SER
2	K	325	THR
2	K	343	ASP
2	K	344	LEU
2	L	114	ASP
2	L	150	PRO
2	L	172	GLU
2	L	215	TYR
2	L	343	ASP
2	M	129	ALA
2	M	133	TRP
2	M	326	SER
2	N	95	ILE
2	N	271	ALA
2	O	62	GLY
2	O	79	ASP
2	O	313	ALA
2	O	344	LEU
1	A	226	SER
1	B	213	SER
2	K	100	ASP
2	K	115	GLY
2	K	145	GLY
2	K	168	ASN
2	K	178	GLY
2	K	216	GLY
2	K	314	ARG
2	L	80	ILE
2	L	118	PRO
2	M	150	PRO

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Mol	Chain	Res	Type
2	M	160	LEU
2	M	163	GLN
2	M	216	GLY
2	M	271	ALA
2	M	366	THR
2	N	108	VAL
2	N	166	MET
2	N	168	ASN
2	N	180	ASP
2	N	278	LEU
2	N	357	PRO
2	O	49	SER
2	O	168	ASN
2	O	326	SER
1	B	227	SER
1	D	209	PRO
2	K	22	GLU
2	K	386	ASN
2	L	151	GLU
2	L	391	PRO
2	M	100	ASP
2	M	125	SER
2	N	56	TYR
2	N	170	GLN
2	N	172	GLU
2	O	325	THR
2	O	357	PRO
1	C	228	ARG
1	E	230	GLU
2	K	80	ILE
2	K	172	GLU
2	K	326	SER
2	K	402	MET
2	L	131	ASP
2	L	161	THR
2	L	216	GLY
2	M	108	VAL
2	M	172	GLU
2	M	189	SER
2	M	190	ASN
2	N	367	ASN
2	O	23	ASP

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Mol	Chain	Res	Type
2	O	44	THR
2	O	121	VAL
2	O	363	GLY
1	D	230	GLU
2	L	47	SER
2	M	357	PRO
2	N	181	ILE
2	M	64	VAL
2	N	3	VAL
2	O	82	GLY
2	O	150	PRO
2	L	82	GLY
2	M	116	VAL
2	K	117	LEU
2	L	181	ILE
2	O	351	GLY
2	O	391	PRO
2	O	108	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 X-ray entries followed by that with respect to entries of similar resolution.

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	64/77 (83%)	56 (88%)	8 (12%)	4	22
1	B	64/77 (83%)	61 (95%)	3 (5%)	23	49
1	C	64/77 (83%)	56 (88%)	8 (12%)	4	22
1	D	64/77 (83%)	60 (94%)	4 (6%)	16	42
1	E	64/77 (83%)	58 (91%)	6 (9%)	8	31
2	K	362/362 (100%)	311 (86%)	51 (14%)	3	18
2	L	362/362 (100%)	322 (89%)	40 (11%)	6	26
2	M	362/362 (100%)	313 (86%)	49 (14%)	4	20
2	N	362/362 (100%)	326 (90%)	36 (10%)	7	29
2	O	362/362 (100%)	321 (89%)	41 (11%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2130/2195 (97%)	1884 (88%)	246 (12%)	5 24

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	TRP
1	A	202	LYS
1	A	230	GLU
1	A	232	ILE
1	A	248	LEU
1	A	250	LEU
1	A	255	LEU
1	A	265	LEU
1	B	223	GLU
1	B	244	GLU
1	B	250	LEU
1	C	194	VAL
1	C	200	LEU
1	C	215	GLN
1	C	223	GLU
1	C	232	ILE
1	C	252	TYR
1	C	255	LEU
1	C	261	VAL
1	D	198	TRP
1	D	208	GLN
1	D	211	LYS
1	D	255	LEU
1	E	196	ASP
1	E	214	LEU
1	E	223	GLU
1	E	224	LEU
1	E	250	LEU
1	E	255	LEU
2	K	9	ILE
2	K	13	VAL
2	K	14	ILE
2	K	18	LEU
2	K	36	LYS
2	K	40	LEU
2	K	50	ASP
2	K	64	VAL

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Mol	Chain	Res	Type
2	K	66	ILE
2	K	81	ARG
2	K	85	ASP
2	K	95	ILE
2	K	100	ASP
2	K	104	ILE
2	K	106	ASP
2	K	107	LEU
2	K	114	ASP
2	K	126	ARG
2	K	134	LEU
2	K	136	LEU
2	K	151	GLU
2	K	152	TYR
2	K	168	ASN
2	K	172	GLU
2	K	181	ILE
2	K	184	VAL
2	K	192	THR
2	K	199	ASP
2	K	220	SER
2	K	228	LEU
2	K	237	ILE
2	K	243	GLU
2	K	253	GLU
2	K	278	LEU
2	K	294	ASN
2	K	307	LEU
2	K	317	ARG
2	K	321	ASP
2	K	328	THR
2	K	329	THR
2	K	332	LEU
2	K	355	TYR
2	K	367	ASN
2	K	383	GLU
2	K	385	GLN
2	K	390	THR
2	K	404	LEU
2	K	405	GLN
2	K	410	LYS
2	K	411	THR

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Mol	Chain	Res	Type
2	K	414	LYS
2	L	7	ARG
2	L	15	VAL
2	L	18	LEU
2	L	42	ILE
2	L	45	THR
2	L	59	LEU
2	L	60	LYS
2	L	67	ILE
2	L	78	LYS
2	L	83	LYS
2	L	84	LEU
2	L	104	ILE
2	L	108	VAL
2	L	113	LEU
2	L	134	LEU
2	L	144	VAL
2	L	148	GLN
2	L	152	TYR
2	L	160	LEU
2	L	177	GLU
2	L	181	ILE
2	L	183	ASP
2	L	188	ASP
2	L	199	ASP
2	L	242	THR
2	L	268	ILE
2	L	292	VAL
2	L	293	LYS
2	L	307	LEU
2	L	308	LEU
2	L	311	THR
2	L	317	ARG
2	L	323	GLU
2	L	325	THR
2	L	327	LEU
2	L	332	LEU
2	L	344	LEU
2	L	355	TYR
2	L	390	THR
2	L	414	LYS
2	M	8	ILE

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Mol	Chain	Res	Type
2	M	13	VAL
2	M	15	VAL
2	M	23	ASP
2	M	42	ILE
2	M	45	THR
2	M	50	ASP
2	M	60	LYS
2	M	66	ILE
2	M	70	ASN
2	M	84	LEU
2	M	86	LYS
2	M	90	SER
2	M	94	ASN
2	M	104	ILE
2	M	113	LEU
2	M	134	LEU
2	M	147	THR
2	M	181	ILE
2	M	195	VAL
2	M	230	THR
2	M	241	SER
2	M	243	GLU
2	M	263	LEU
2	M	268	ILE
2	M	269	ASP
2	M	285	SER
2	M	291	SER
2	M	292	VAL
2	M	293	LYS
2	M	307	LEU
2	M	308	LEU
2	M	309	ARG
2	M	317	ARG
2	M	323	GLU
2	M	325	THR
2	M	332	LEU
2	M	333	LEU
2	M	340	SER
2	M	344	LEU
2	M	350	VAL
2	M	353	ASN
2	M	365	THR

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Mol	Chain	Res	Type
2	M	375	VAL
2	M	383	GLU
2	M	395	GLN
2	M	402	MET
2	M	409	GLU
2	M	410	LYS
2	N	11	ASN
2	N	13	VAL
2	N	18	LEU
2	N	22	GLU
2	N	42	ILE
2	N	51	LEU
2	N	57	GLN
2	N	59	LEU
2	N	63	ASN
2	N	69	VAL
2	N	84	LEU
2	N	134	LEU
2	N	138	LEU
2	N	169	GLU
2	N	183	ASP
2	N	193	LYS
2	N	206	LYS
2	N	241	SER
2	N	243	GLU
2	N	250	LEU
2	N	263	LEU
2	N	270	LYS
2	N	278	LEU
2	N	281	PHE
2	N	289	TYR
2	N	307	LEU
2	N	308	LEU
2	N	309	ARG
2	N	317	ARG
2	N	325	THR
2	N	327	LEU
2	N	329	THR
2	N	332	LEU
2	N	340	SER
2	N	375	VAL
2	N	383	GLU

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Mol	Chain	Res	Type
2	O	4	THR
2	O	13	VAL
2	O	30	ASP
2	O	34	LYS
2	O	40	LEU
2	O	67	ILE
2	O	85	ASP
2	O	106	ASP
2	O	107	LEU
2	O	108	VAL
2	O	117	LEU
2	O	134	LEU
2	O	136	LEU
2	O	143	ARG
2	O	147	THR
2	O	164	CYS
2	O	167	ILE
2	O	168	ASN
2	O	169	GLU
2	O	175	VAL
2	O	177	GLU
2	O	243	GLU
2	O	247	THR
2	O	253	GLU
2	O	270	LYS
2	O	283	LEU
2	O	292	VAL
2	O	307	LEU
2	O	311	THR
2	O	317	ARG
2	O	329	THR
2	O	332	LEU
2	O	343	ASP
2	O	355	TYR
2	O	359	ASP
2	O	366	THR
2	O	377	GLU
2	O	383	GLU
2	O	385	GLN
2	O	412	ILE
2	O	418	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	242	HIS
1	A	258	GLN
1	D	208	GLN
1	D	215	GLN
1	E	215	GLN
1	E	242	HIS
2	K	43	ASN
2	K	94	ASN
2	K	148	GLN
2	K	187	ASN
2	K	260	GLN
2	K	266	GLN
2	K	347	GLN
2	K	367	ASN
2	K	405	GLN
2	L	21	ASN
2	L	94	ASN
2	L	203	HIS
2	L	251	ASN
2	L	266	GLN
2	L	347	GLN
2	L	367	ASN
2	L	395	GLN
2	M	63	ASN
2	M	233	HIS
2	M	266	GLN
2	M	347	GLN
2	M	353	ASN
2	M	367	ASN
2	M	385	GLN
2	M	386	ASN
2	M	395	GLN
2	N	63	ASN
2	N	70	ASN
2	N	163	GLN
2	N	190	ASN
2	N	266	GLN
2	N	294	ASN
2	N	298	HIS
2	N	302	GLN
2	N	315	ASN

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Mol	Chain	Res	Type
2	N	346	GLN
2	N	347	GLN
2	N	371	GLN
2	N	386	ASN
2	O	11	ASN
2	O	43	ASN
2	O	63	ASN
2	O	190	ASN
2	O	266	GLN
2	O	318	GLN
2	O	347	GLN
2	O	385	GLN
2	O	395	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	44/45 (97%)	36 (81%)	8 (18%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	U
3	R	4	U
3	R	5	U
3	R	6	U
3	R	7	U
3	R	8	U
3	R	9	U
3	R	10	U
3	R	12	U
3	R	13	U
3	R	14	U
3	R	15	U
3	R	16	U
3	R	17	U
3	R	18	U
3	R	19	U
3	R	21	U
3	R	22	U
3	R	23	U

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Mol	Chain	Res	Type
3	R	25	U
3	R	26	U
3	R	27	U
3	R	28	U
3	R	29	U
3	R	30	U
3	R	31	U
3	R	32	U
3	R	33	U
3	R	35	U
3	R	36	U
3	R	37	U
3	R	38	U
3	R	41	U
3	R	42	U
3	R	44	U
3	R	45	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	4	U
3	R	5	U
3	R	6	U
3	R	15	U
3	R	25	U
3	R	32	U
3	R	36	U
3	R	41	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	73/87 (83%)	0.47	3 (4%) 41 22	58, 60, 61, 62	0
1	B	73/87 (83%)	0.80	8 (10%) 10 7	57, 62, 64, 65	0
1	C	73/87 (83%)	0.27	1 (1%) 73 48	58, 60, 63, 65	0
1	D	73/87 (83%)	0.74	4 (5%) 30 18	59, 62, 64, 64	0
1	E	73/87 (83%)	0.53	5 (6%) 23 14	55, 61, 64, 65	0
2	K	421/421 (100%)	0.20	14 (3%) 49 28	53, 63, 69, 73	0
2	L	421/421 (100%)	0.34	15 (3%) 46 25	57, 65, 69, 72	0
2	M	421/421 (100%)	0.29	18 (4%) 40 21	55, 64, 67, 69	0
2	N	421/421 (100%)	0.42	14 (3%) 49 28	57, 63, 67, 71	0
2	O	421/421 (100%)	0.37	21 (4%) 34 19	57, 64, 67, 72	0
3	R	45/45 (100%)	2.09	27 (60%) 0 0	99, 108, 127, 139	0
All	All	2515/2585 (97%)	0.39	130 (5%) 33 19	53, 63, 69, 139	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	349	CYS	4.8
2	L	357	PRO	4.7
2	N	130	ASP	4.6
1	A	193	ALA	4.5
2	O	43	ASN	4.3
2	M	123	ASP	3.9
2	K	43	ASN	3.9
2	O	61	SER	3.8
1	E	197	VAL	3.8
2	K	351	GLY	3.7
2	K	354	LYS	3.5
2	L	38	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	O	350	VAL	3.4
2	M	178	GLY	3.4
2	L	227	ALA	3.4
2	L	128	SER	3.3
3	R	45	U	3.0
1	E	253	LYS	3.0
3	R	7	U	3.0
2	K	2	SER	3.0
1	E	252	TYR	3.0
1	B	194	VAL	2.9
1	D	261	VAL	2.9
3	R	27	U	2.9
2	N	164	CYS	2.9
2	O	227	ALA	2.9
2	K	353	ASN	2.9
2	K	370	PRO	2.9
2	L	131	ASP	2.8
2	N	342	ALA	2.8
2	M	179	ARG	2.8
2	M	133	TRP	2.8
3	R	20	U	2.8
2	O	96	GLY	2.7
2	L	107	LEU	2.7
3	R	10	U	2.7
2	M	176	PRO	2.7
2	N	135	PRO	2.7
2	O	370	PRO	2.7
2	O	216	GLY	2.7
2	L	354	LYS	2.7
2	O	121	VAL	2.7
2	O	134	LEU	2.7
1	E	254	LYS	2.7
3	R	21	U	2.7
3	R	30	U	2.7
2	L	61	SER	2.7
1	B	197	VAL	2.6
2	M	370	PRO	2.6
3	R	22	U	2.6
2	M	186	GLY	2.6
2	O	53	GLY	2.6
1	B	252	TYR	2.6
1	B	222	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	189	SER	2.5
3	R	23	U	2.5
2	O	274	TYR	2.5
3	R	18	U	2.5
3	R	2	U	2.5
2	K	269	ASP	2.5
2	M	99	GLY	2.5
2	N	329	THR	2.5
3	R	28	U	2.4
2	N	146	ARG	2.4
2	L	343	ASP	2.4
3	R	19	U	2.4
3	R	44	U	2.4
2	N	49	SER	2.4
2	L	274	TYR	2.4
3	R	5	U	2.4
2	M	100	ASP	2.4
2	O	351	GLY	2.4
3	R	41	U	2.3
2	N	357	PRO	2.3
2	K	147	THR	2.3
2	K	356	THR	2.3
1	B	229	GLY	2.3
2	L	349	CYS	2.3
1	A	260	ARG	2.3
2	O	220	SER	2.3
3	R	11	U	2.3
3	R	36	U	2.3
2	O	166	MET	2.3
3	R	9	U	2.3
3	R	31	U	2.3
2	L	120	GLY	2.3
1	B	196	ASP	2.3
2	N	65	SER	2.2
3	R	32	U	2.2
3	R	40	U	2.2
1	E	264	SER	2.2
2	O	130	ASP	2.2
1	D	217	LEU	2.2
2	N	55	VAL	2.2
1	D	193	ALA	2.2
2	O	57	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	121	VAL	2.2
3	R	12	U	2.2
3	R	38	U	2.2
2	O	343	ASP	2.2
2	L	350	VAL	2.2
2	K	352	ASP	2.1
2	M	56	TYR	2.1
1	A	253	LYS	2.1
2	K	39	PRO	2.1
1	B	248	LEU	2.1
2	N	51	LEU	2.1
2	M	114	ASP	2.1
2	K	357	PRO	2.1
1	D	239	ARG	2.1
2	N	296	ALA	2.1
2	M	107	LEU	2.1
2	K	179	ARG	2.1
2	M	226	ALA	2.1
2	O	35	SER	2.1
2	M	69	VAL	2.1
1	C	213	SER	2.1
2	O	47	SER	2.1
2	K	185	TRP	2.1
2	M	165	LYS	2.1
3	R	42	U	2.1
3	R	43	U	2.1
1	B	200	LEU	2.1
2	L	135	PRO	2.0
2	L	370	PRO	2.0
2	N	362	GLY	2.0
2	M	215	TYR	2.0
2	N	39	PRO	2.0
2	M	131	ASP	2.0
3	R	37	U	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.