



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:55 am BST

PDB ID : 3HHZ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

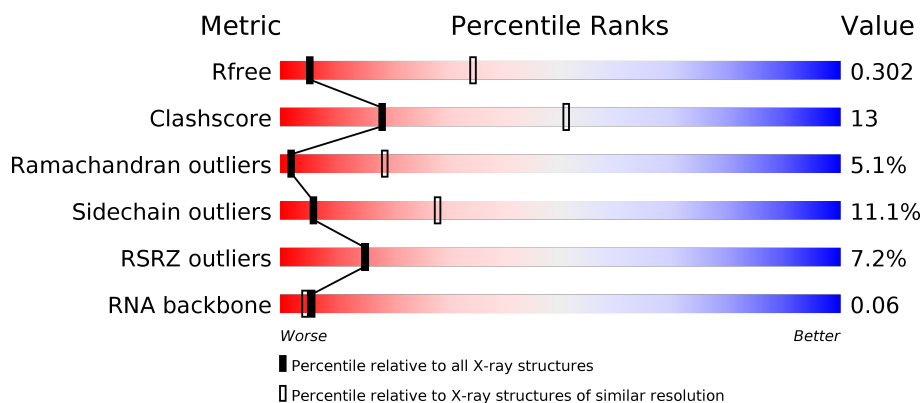
1 Overall quality at a glance i

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 on 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	<div> <div>9%</div> <div> <div>47%</div> <div>31%</div> <div>6%</div> <div>16%</div> </div> </div>
1	B	87	<div> <div>31%</div> <div>62%</div> <div>20%</div> <div>•</div> <div>16%</div> </div>
1	C	87	<div> <div>7%</div> <div>57%</div> <div>23%</div> <div>••</div> <div>16%</div> </div>
1	D	87	<div> <div>31%</div> <div>71%</div> <div>9%</div> <div>•</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	87	<div><div></div><div>16%</div><div>60%</div><div>21%</div><div>16%</div></div>
2	K	421	<div><div></div><div>3%</div><div>62%</div><div>30%</div><div>7%</div></div>
2	L	421	<div><div></div><div>%</div><div>61%</div><div>33%</div><div>5%</div></div>
2	M	421	<div><div></div><div>3%</div><div>61%</div><div>32%</div><div>7%</div></div>
2	N	421	<div><div></div><div>5%</div><div>68%</div><div>28%</div><div></div></div>
2	O	421	<div><div></div><div>3%</div><div>62%</div><div>32%</div><div>6%</div></div>
3	R	45	<div><div></div><div>7%</div><div>31%</div><div>80%</div><div>49%</div><div>13%</div></div>

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			

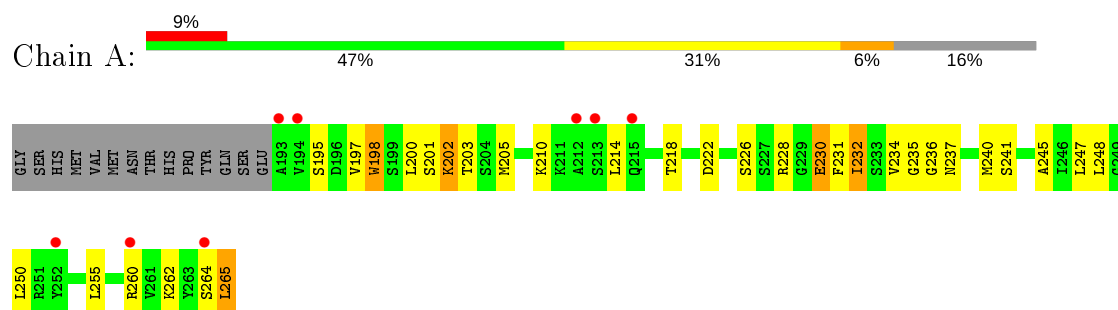
- Molecule 3 is a RNA chain called RNA (45-MER).

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

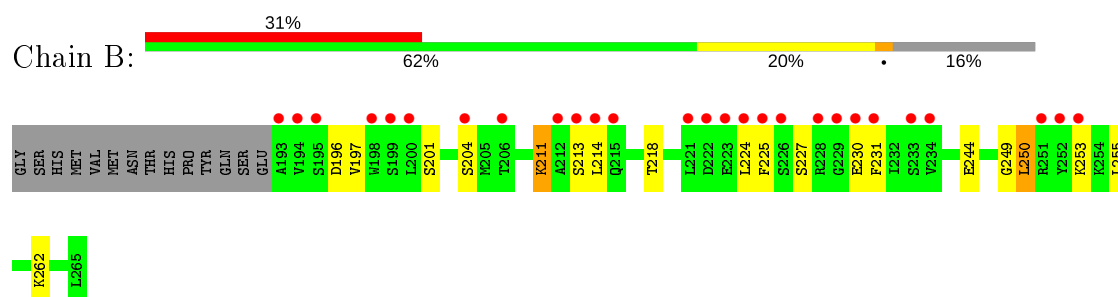
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

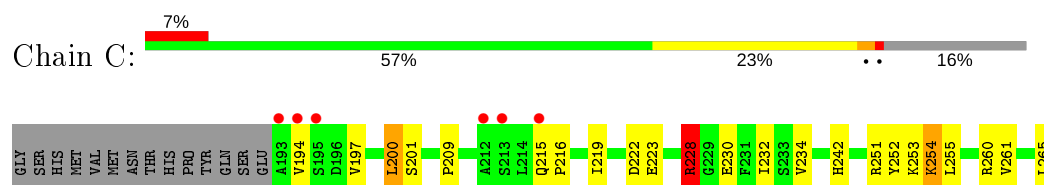
• Molecule 1: Phosphoprotein



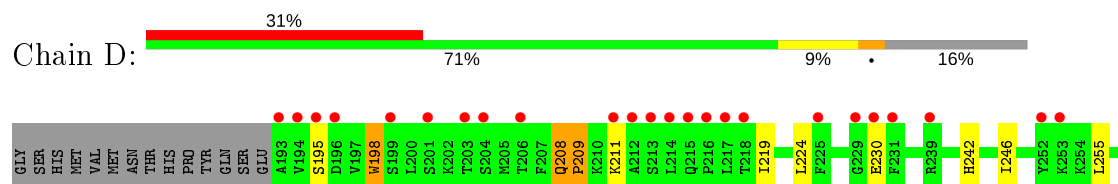
• Molecule 1: Phosphoprotein

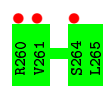


• Molecule 1: Phosphoprotein

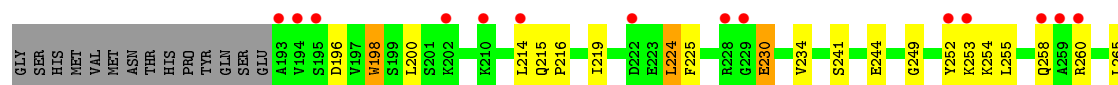


• Molecule 1: Phosphoprotein

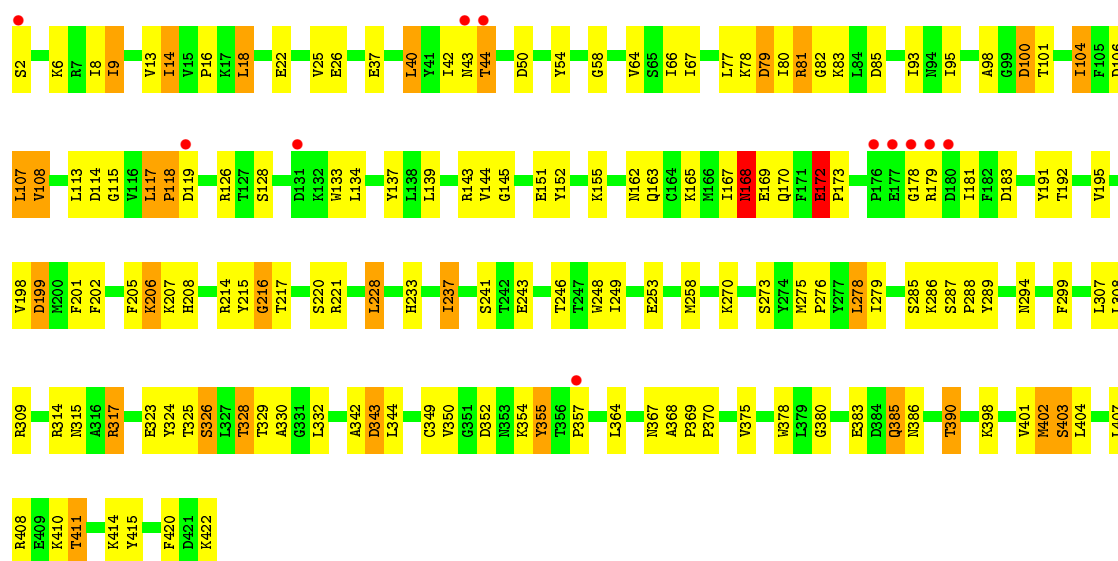




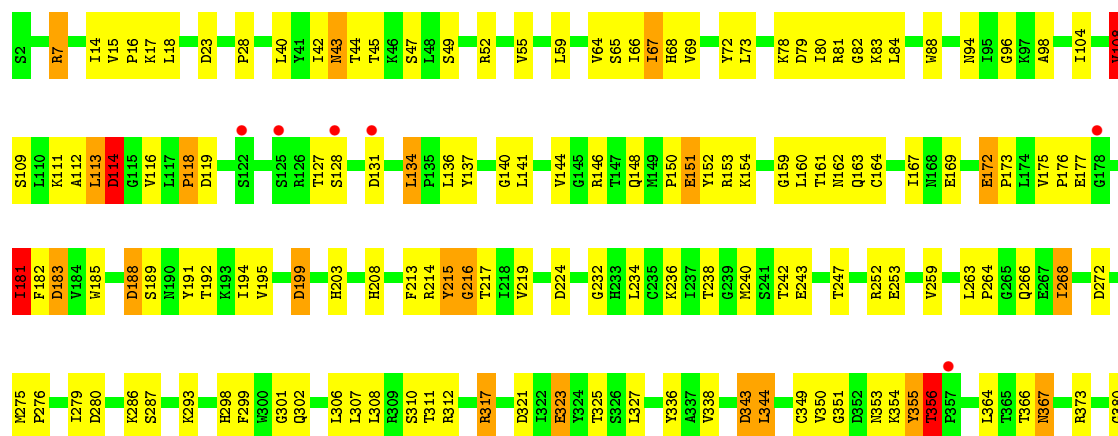
• Molecule 1: Phosphoprotein

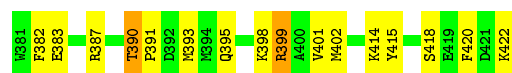


• Molecule 2: Nucleoprotein

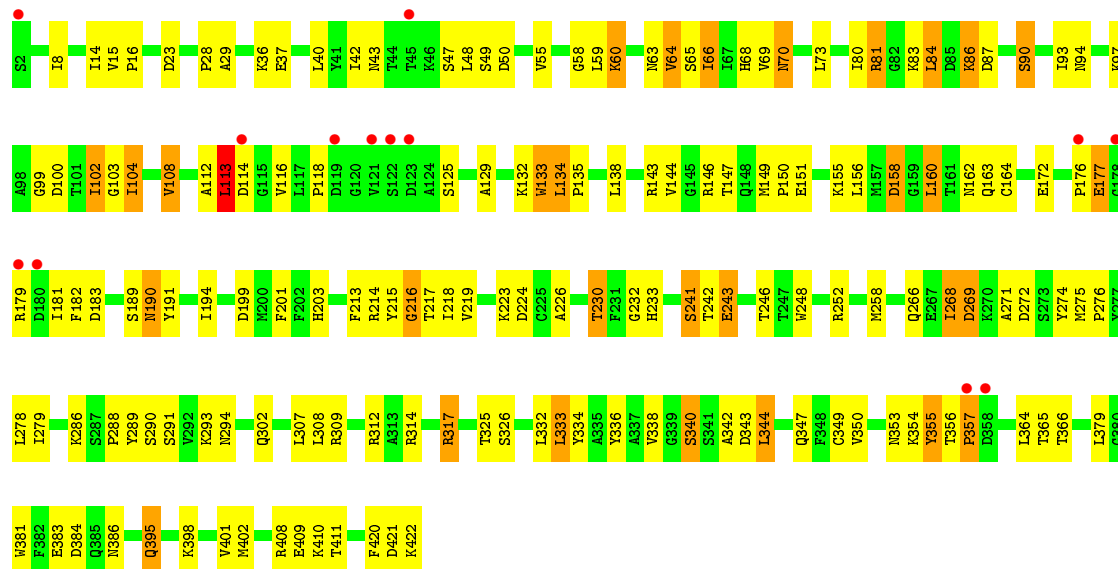


• Molecule 2: Nucleoprotein

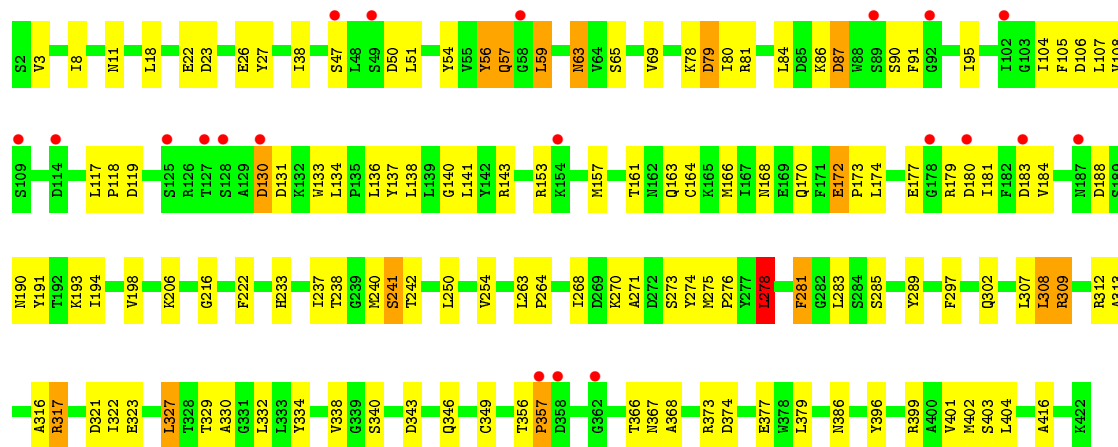




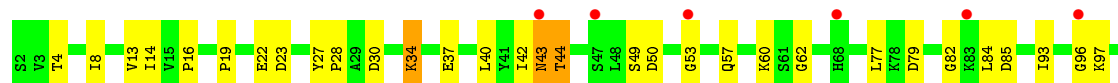
• Molecule 2: Nucleoprotein

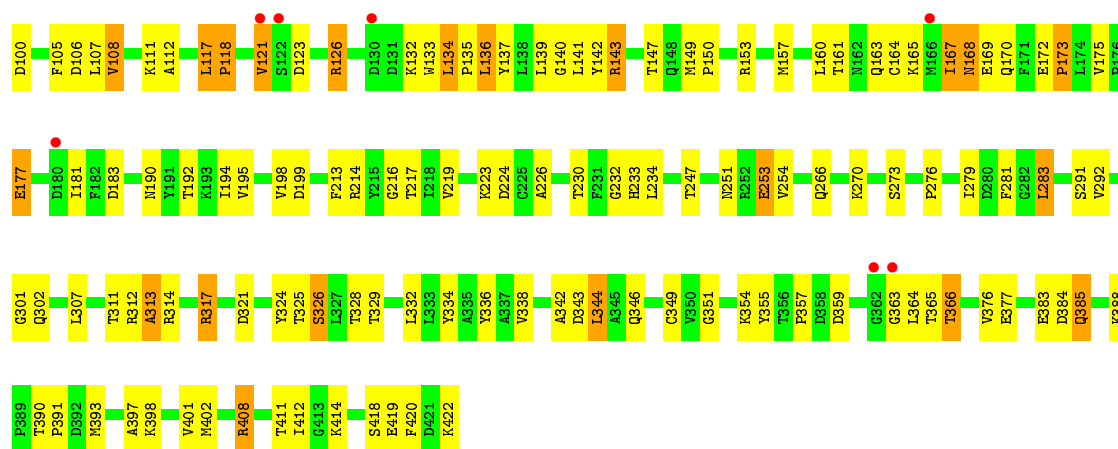


• Molecule 2: Nucleoprotein

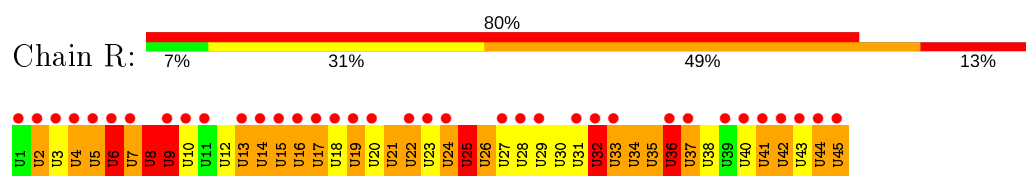


• Molecule 2: Nucleoprotein





• 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 29.91 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.50) 98.5 (29.91-3.50)	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 (5.12%)	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)	0.28 , 110.6	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	0.87	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	0.37	0/586	0.57	0/784
1	B	0.39	0/586	0.52	0/784
1	C	0.38	0/586	0.56	0/784
1	D	0.37	0/586	0.55	0/784
1	E	0.39	0/586	0.55	0/784
2	K	0.44	0/3403	0.59	0/4607
2	L	0.43	0/3403	0.64	4/4607 (0.1%)
2	M	0.42	0/3403	0.58	0/4607
2	N	0.43	0/3403	0.65	4/4607 (0.1%)
2	O	0.42	0/3403	0.59	0/4607
3	R	1.01	0/989	1.63	12/1526 (0.8%)
All	All	0.47	0/20934	0.70	20/28481 (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 (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	130	ASP	N-CA-C	13.65	147.86	111.00
2	N	131	ASP	N-CA-CB	-8.63	95.06	110.60
2	L	367	ASN	CB-CA-C	-7.90	94.61	110.40
3	R	36	U	O4'-C1'-N1	7.88	114.51	108.20
3	R	9	U	O4'-C1'-N1	7.56	114.25	108.20
2	N	91	PHE	CB-CA-C	-7.55	95.29	110.40
3	R	34	U	O4'-C1'-N1	6.99	113.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	34	U	C1'-O4'-C4'	-6.64	104.59	109.90
3	R	25	U	C4'-C3'-C2'	-6.35	96.25	102.60
3	R	36	U	C1'-O4'-C4'	-6.18	104.95	109.90
2	N	130	ASP	CB-CA-C	-5.88	98.64	110.40
3	R	32	U	C3'-C2'-C1'	5.86	106.19	101.50
2	L	356	THR	CB-CA-C	-5.70	96.22	111.60
2	L	119	ASP	N-CA-C	-5.38	96.48	111.00
3	R	24	U	O4'-C1'-N1	5.32	112.45	108.20
3	R	19	U	C1'-O4'-C4'	-5.31	105.65	109.90
3	R	6	U	C3'-C2'-C1'	5.31	105.75	101.50
3	R	8	U	C3'-C2'-C1'	-5.25	97.30	101.50
3	R	36	U	O4'-C4'-C3'	-5.13	98.87	104.00
2	L	356	THR	N-CA-C	5.12	124.83	111.00

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

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	15	0
1	B	576	0	597	8	0
1	C	576	0	597	9	0
1	D	576	0	597	5	0
1	E	576	0	597	14	0
2	K	3327	0	3287	104	0
2	L	3327	0	3287	124	0
2	M	3327	0	3287	107	0
2	N	3327	0	3287	74	0
2	O	3327	0	3287	97	0
3	R	900	0	451	48	0
All	All	20415	0	19871	541	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 13.

All (541) 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:HD2	2:O:317:ARG:H	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:HE	2:N:317:ARG:H	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: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:HE	2:M:317:ARG:H	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
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:M:113:LEU:C	2:M:113:LEU:HD22	1.98	0.83
2:L:356:THR:HG22	2:L:356:THR:O	1.74	0.83
2:O:317:ARG:CD	2:O:317:ARG:H	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:O	2:K:104:ILE:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:L:367:ASN:O	2:L:367:ASN:CG	2.28	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:N	2:O:317:ARG:CD	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: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
2:M:162:ASN:C	2:M:164:CYS:H	1.95	0.69
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:CG2	2:L:356:THR:O	2.43	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:H	2:N:63:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:ILE:HG22	2:K:168:ASN:O	1.98	0.63
2:K:81:ARG:HE	2:K:82:GLY:N	1.92	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: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
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:K:77:LEU:C	2:K:79:ASP:H	2.03	0.61
2:L:146:ARG:HD3	2:L:219:VAL:HG11	1.82	0.61
2:L:317:ARG:NE	2:L:317:ARG:H	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: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:172:GLU:HB3	2:O:173:PRO:HD2	1.83	0.60
2:O:28:PRO:HD2	2:O:266:GLN:HE21	1.67	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: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:299:PHE:CE1	2:K:328:THR:HG22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:144:VAL:HG11	2:M:156:LEU:HG	1.84	0.59
2:K:143:ARG:NH2	3:R:26:U:H3'	2.17	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:N:366:THR:C	2:N:368:ALA:H	2.07	0.58
2:L:395:GLN:HE21	2:L:395:GLN:HA	1.68	0.58
2:N:130:ASP:O	2:N:130:ASP:CG	2.40	0.58
2:L:79:ASP:C	2:L:81:ARG:H	2.05	0.57
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
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
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: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:K:172:GLU:HB2	2:K:173:PRO:HD3	1.87	0.56
2:L:188:ASP:CG	2:L:189:SER:N	2.60	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: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
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:164:CYS:HB3	2:L:169:GLU:HG2	1.88	0.55
2:N:104:ILE:O	2:N:104:ILE:HG12	2.06	0.55
2:O:336:TYR:CD1	2:O:393:MET:HG2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:GLU:HG3	3:R:15:U:O2'	2.06	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:155:LYS:O	2:M:158:ASP:HB3	2.07	0.54
2:M:84:LEU:HD23	2:M:102:ILE:HD12	1.88	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: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
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:169:GLU:HG2	2:K:170:GLN:N	2.23	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:NE	2:M:317:ARG:H	1.96	0.54
2:O:165:LYS:O	2:O:167:ILE:HG12	2.08	0.54
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
2:M:214:ARG:C	2:M:216:GLY:H	2.11	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
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: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:O	1:D:198:TRP:HE3	1.92	0.52
1:E:215:GLN:HG3	1:E:216:PRO:HD2	1.92	0.52
2:M:132:LYS:HB3	2:M:133:TRP:HD1	1.74	0.52
2:M:42:ILE:HD12	2:M:43:ASN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:342:ALA:O	2:K:343:ASP:C	2.49	0.52
2:O:214:ARG:CA	2:O:217:THR:HG22	2.29	0.52
2:K:117:LEU:N	2:K:118:PRO:HD3	2.23	0.51
1:A:235:GLY:HA2	2:L:364:LEU:HB2	1.93	0.51
2:N:137:TYR:HD1	2:N:163:GLN:HE22	1.58	0.51
1:C:253:LYS:O	1:C:254:LYS:HB2	2.11	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:169:GLU:CD	2:O:170:GLN:H	2.14	0.51
2:O:281:PHE:HB3	2:O:283:LEU:HD21	1.90	0.51
2:O:342:ALA:HB1	2:O:344:LEU:HD23	1.93	0.51
2:L:234:LEU:HD22	2:L:301:GLY:HA2	1.92	0.51
2:L:43:ASN:O	2:L:44:THR:HG23	2.11	0.51
2:M:149:MET:C	2:M:151:GLU:H	2.14	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:M:317:ARG:HH11	3:R:4:U:C5'	2.24	0.51
2:L:317:ARG:CZ	3:R:13:U:H3'	2.41	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:M:224:ASP:CG	3:R:3:U:H4'	2.31	0.51
2:K:37:GLU:HB2	2:K:108:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:113:LEU:HD23	2:K:113:LEU:H	1.75	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
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: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
2:N:233:HIS:HB2	2:N:312:ARG:NH2	2.27	0.49
2:O:336:TYR:CG	2:O:393:MET:HG2	2.48	0.49
2:O:43:ASN:HD22	2:O:111:LYS:HD3	1.77	0.49
1:B:214:LEU:HD13	1:B:262:LYS:HE3	1.95	0.49
2:K:214:ARG:C	2:K:216:GLY:H	2.14	0.49
2:K:43:ASN:HB3	2:K:67:ILE:HG23	1.95	0.49
2:L:43:ASN:CG	2:L:44:THR:N	2.66	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: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:L:306:LEU:HA	2:L:310:SER:HB3	1.95	0.48
2:L:343:ASP:O	2:L:344:LEU:C	2.52	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:K:288:PRO:HG2	2:K:289:TYR:CE2	2.48	0.48
2:K:398:LYS:O	2:K:402:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:ILE:HG22	2:M:349:CYS:SG	2.53	0.48
2:N:275:MET:HB3	2:N:276:PRO:HD3	1.96	0.48
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:NH1	2:L:7:ARG:HG2	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: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:317:ARG:HD3	3:R:22:U:H2'	1.96	0.48
2:K:253:GLU:OE1	2:K:323:GLU:HG2	2.13	0.48
2:K:317:ARG:N	2:K:317:ARG:HE	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:342:ALA:O	2:M:343:ASP:C	2.52	0.48
2:M:395:GLN:HA	2:M:395:GLN:HE21	1.79	0.48
2:N:308:LEU:O	2:N:309:ARG:HB2	2.14	0.48
2:K:108:VAL:O	2:K:108:VAL:HG12	2.14	0.47
2:K:26:GLU:OE1	2:K:285:SER:HB2	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: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: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
1:E:255:LEU:HA	2:O:384:ASP:CG	2.34	0.47
2:K:133:TRP:HE3	2:K:163:GLN:HE21	1.62	0.47
2:K:77:LEU:O	2:K:79:ASP:N	2.46	0.47
2:L:336:TYR:CD1	2:L:393:MET:CE	2.98	0.47
2:L:172:GLU:H	2:L:173:PRO:HD2	1.79	0.47
2:M:162:ASN:C	2:M:164:CYS:N	2.67	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
3:R:8:U:OP2	3:R:8:U:H6	1.98	0.47
2:K:286:LYS:HD2	3:R:20:U:H5''	1.96	0.47
1:A:198:TRP:NE1	1:A:228:ARG:HA	2.30	0.47
2:L:79:ASP:C	2:L:81:ARG:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:270:LYS:HD3	2:K:273:SER:HB2	1.97	0.47
2:L:151:GLU:HA	2:L:154:LYS:HD3	1.97	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:160:LEU:O	2:M:164:CYS:HB3	2.15	0.46
2:M:64:VAL:O	2:M:64:VAL:HG13	2.15	0.46
2:N:346:GLN:NE2	2:N:349:CYS:HB3	2.30	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:162:ASN:OD1	2:K:165:LYS:HD2	2.15	0.46
2:K:9:ILE:HG13	2:L:252:ARG:HH22	1.79	0.46
1:E:234:VAL:O	2:K:364:LEU:HB2	2.14	0.46
2:O:22:GLU:OE1	2:O:22:GLU:HA	2.16	0.46
2:O:37:GLU:HB2	2:O:108:VAL:HG11	1.97	0.46
2:K:43:ASN:O	2:K:44:THR:C	2.54	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:N:79:ASP:C	2:N:81:ARG:H	2.19	0.46
2:K:14:ILE:HD11	2:L:259:VAL:HG13	1.97	0.46
2:K:380:GLY:HA2	2:L:354:LYS:NZ	2.30	0.46
2:K:43:ASN:HD22	2:K:67:ILE:HG23	1.81	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:N:177:GLU:HG2	2:N:179:ARG:H	1.80	0.46
2:N:57:GLN:HB2	2:N:63:ASN:HD21	1.81	0.46
2:O:34:LYS:HA	2:O:34:LYS:HD2	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:190:ASN:O	2:N:194:ILE:HG12	2.16	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: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:O:312:ARG:O	2:O:313:ALA:C	2.55	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
2:L:113:LEU:O	2:L:114:ASP:HB2	2.16	0.45
2:L:81:ARG:HD3	2:L:208:HIS:NE2	2.32	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:E:254:LYS:O	2:O:384:ASP:HB3	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:299:PHE:HE1	2:K:328:THR:HG22	1.80	0.44
2:L:181:ILE:HG13	2:L:181:ILE:H	1.62	0.44
2:L:7:ARG:HH11	2:L:7:ARG:HG2	1.81	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
2:O:143:ARG:HG2	2:O:216:GLY:HA2	1.99	0.44
2:K:202:PHE:HE2	2:K:208:HIS:ND1	2.16	0.44
2:K:324:TYR:C	2:K:326:SER:H	2.21	0.44
2:M:248:TRP:CZ3	2:M:333:LEU:HD23	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:224:ASP:HB2	2:L:279:ILE:HG13	2.00	0.44
2:N:317:ARG:N	2:N:317:ARG:HE	1.97	0.44
2:K:402:MET:O	2:K:403:SER:C	2.56	0.44
2:K:77:LEU:C	2:K:79:ASP:N	2.70	0.44
2:L:183:ASP:C	2:L:185:TRP:H	2.21	0.44
2:N:379:LEU:HB3	2:O:354:LYS:HD3	2.00	0.44
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:O:397:ALA:O	2:O:398:LYS:C	2.57	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: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: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:K:317:ARG:HH11	3:R:22:U:H3'	1.78	0.43
2:L:312:ARG:HD2	3:R:14:U:C2	2.54	0.43
2:L:336:TYR:CD1	2:L:393:MET:HE2	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:L:214:ARG:C	2:L:216:GLY:H	2.22	0.43
2:M:66:ILE:O	2:M:70:ASN:HB2	2.19	0.43
1:E:198:TRP:C	1:E:200:LEU:H	2.22	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:350:VAL:C	2:K:352:ASP:H	2.22	0.43
2:M:58:GLY:C	2:M:60:LYS:H	2.22	0.43
3:R:4:U:H5'	3:R:5:U:OP2	2.18	0.43
2:L:72:TYR:CE1	2:L:134:LEU:HD12	2.54	0.42
2:N:302:GLN:HE21	2:N:313:ALA:HA	1.84	0.42
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:42:U:H5''	3:R:43:U:H5''	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:8:U:H2'	3:R:9:U:C5'	2.44	0.42
2:K:167:ILE:HG22	2:K:168:ASN:C	2.40	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
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: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:M:246:THR:HG23	2:M:258:MET:HE2	2.02	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:L:238:THR:C	2:L:240:MET:H	2.22	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:73:LEU:HD21	2:M:135:PRO:HA	2.02	0.41
2:M:14:ILE:HD12	2:M:14:ILE:HA	1.97	0.41
2:M:86:LYS:HB3	2:M:87:ASP:H	1.74	0.41
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:L:162:ASN:HB3	2:L:215:TYR:CD1	2.56	0.41
2:M:176:PRO:O	2:M:177:GLU:C	2.58	0.41
2:K:195:VAL:HB	2:K:217:THR:OG1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:HA	1:C:265:LEU:HD22	2.02	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:102:ILE:HG22	2:M:103:GLY:N	2.36	0.41
2:M:36:LYS:HE2	2:M:93:ILE:HD13	2.03	0.41
2:K:354:LYS:HG2	2:O:376:VAL:HG13	2.03	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:L:43:ASN:HA	2:L:112:ALA:HB3	2.02	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: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:349:CYS:SG	2:O:8:ILE:HG22	2.61	0.41
2:L:136:LEU:HG	2:L:163:GLN:CG	2.51	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:O:385:GLN:HE21	2:O:385:GLN:HB2	1.68	0.41
2:L:214:ARG:O	2:L:216:GLY:N	2.54	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
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:395:GLN:NE2	2:L:395:GLN:HA	2.34	0.40
2:L:84:LEU:HD11	2:L:88:TRP:HB2	2.03	0.40
2:M:242:THR:HG23	2:M:243:GLU:OE1	2.21	0.40
2:M:81:ARG:HD2	2:M:81:ARG:N	2.36	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:N:222:PHE:HE2	2:N:275:MET:SD	2.45	0.40
2:M:286:LYS:HZ3	3:R:2:U:H5'	1.86	0.40
2:K:275:MET:O	2:K:278:LEU:HB3	2.20	0.40
2:N:63:ASN:ND2	2:N:63:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:27:TYR:CZ	2:N:263:LEU:HD23	2.57	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:HA	2:O:302:GLN:OE1	2.21	0.40
2:O:57:GLN:NE2	2:O:123:ASP:HB2	2.37	0.40
2:N:143:ARG:NH2	3:R:44:U:H3'	2.30	0.40
2:M:317:ARG:NH1	3:R:4:U:C5'	2.85	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 ⓘ

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 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	12
1	B	71/87 (82%)	55 (78%)	14 (20%)	2 (3%)	5	32
1	C	71/87 (82%)	60 (84%)	9 (13%)	2 (3%)	5	32
1	D	71/87 (82%)	52 (73%)	17 (24%)	2 (3%)	5	32
1	E	71/87 (82%)	57 (80%)	13 (18%)	1 (1%)	11	46
2	K	419/421 (100%)	338 (81%)	54 (13%)	27 (6%)	1	14
2	L	419/421 (100%)	326 (78%)	72 (17%)	21 (5%)	2	19
2	M	419/421 (100%)	330 (79%)	65 (16%)	24 (6%)	1	16
2	N	419/421 (100%)	333 (80%)	68 (16%)	18 (4%)	2	22
2	O	419/421 (100%)	315 (75%)	82 (20%)	22 (5%)	2	17
All	All	2450/2540 (96%)	1917 (78%)	409 (17%)	124 (5%)	2	19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	57 (89%)	7 (11%)	6	29
1	B	64/77 (83%)	59 (92%)	5 (8%)	12	42
1	C	64/77 (83%)	55 (86%)	9 (14%)	3	19
1	D	64/77 (83%)	60 (94%)	4 (6%)	18	51
1	E	64/77 (83%)	60 (94%)	4 (6%)	18	51
2	K	362/362 (100%)	313 (86%)	49 (14%)	4	21
2	L	362/362 (100%)	325 (90%)	37 (10%)	7	32
2	M	362/362 (100%)	315 (87%)	47 (13%)	4	21
2	N	362/362 (100%)	329 (91%)	33 (9%)	9	36
2	O	362/362 (100%)	320 (88%)	42 (12%)	5	26
All	All	2130/2195 (97%)	1893 (89%)	237 (11%)	6	28

All (237) 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	255	LEU
1	A	265	LEU
1	B	196	ASP
1	B	211	LYS
1	B	231	PHE
1	B	244	GLU
1	B	250	LEU
1	C	194	VAL
1	C	200	LEU
1	C	215	GLN
1	C	223	GLU

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Mol	Chain	Res	Type
1	C	228	ARG
1	C	251	ARG
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	198	TRP
1	E	214	LEU
1	E	224	LEU
2	K	6	LYS
2	K	9	ILE
2	K	13	VAL
2	K	14	ILE
2	K	18	LEU
2	K	40	LEU
2	K	50	ASP
2	K	66	ILE
2	K	79	ASP
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	119	ASP
2	K	126	ARG
2	K	134	LEU
2	K	151	GLU
2	K	152	TYR
2	K	168	ASN
2	K	172	GLU
2	K	181	ILE
2	K	192	THR
2	K	199	ASP
2	K	220	SER
2	K	228	LEU

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Mol	Chain	Res	Type
2	K	237	ILE
2	K	241	SER
2	K	243	GLU
2	K	258	MET
2	K	278	LEU
2	K	294	ASN
2	K	307	LEU
2	K	317	ARG
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	403	SER
2	K	404	LEU
2	K	410	LYS
2	K	411	THR
2	L	7	ARG
2	L	15	VAL
2	L	42	ILE
2	L	45	THR
2	L	59	LEU
2	L	67	ILE
2	L	78	LYS
2	L	83	LYS
2	L	94	ASN
2	L	104	ILE
2	L	108	VAL
2	L	113	LEU
2	L	114	ASP
2	L	134	LEU
2	L	144	VAL
2	L	148	GLN
2	L	152	TYR
2	L	160	LEU
2	L	181	ILE
2	L	183	ASP
2	L	188	ASP
2	L	199	ASP

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Mol	Chain	Res	Type
2	L	242	THR
2	L	268	ILE
2	L	293	LYS
2	L	307	LEU
2	L	308	LEU
2	L	311	THR
2	L	317	ARG
2	L	321	ASP
2	L	323	GLU
2	L	325	THR
2	L	327	LEU
2	L	355	TYR
2	L	390	THR
2	L	399	ARG
2	L	414	LYS
2	M	8	ILE
2	M	15	VAL
2	M	23	ASP
2	M	50	ASP
2	M	60	LYS
2	M	66	ILE
2	M	70	ASN
2	M	81	ARG
2	M	84	LEU
2	M	86	LYS
2	M	90	SER
2	M	94	ASN
2	M	97	LYS
2	M	104	ILE
2	M	113	LEU
2	M	134	LEU
2	M	147	THR
2	M	158	ASP
2	M	181	ILE
2	M	182	PHE
2	M	230	THR
2	M	241	SER
2	M	243	GLU
2	M	268	ILE
2	M	269	ASP
2	M	291	SER
2	M	293	LYS

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Mol	Chain	Res	Type
2	M	307	LEU
2	M	308	LEU
2	M	309	ARG
2	M	314	ARG
2	M	317	ARG
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	355	TYR
2	M	365	THR
2	M	383	GLU
2	M	386	ASN
2	M	395	GLN
2	M	402	MET
2	M	409	GLU
2	M	410	LYS
2	N	11	ASN
2	N	22	GLU
2	N	23	ASP
2	N	51	LEU
2	N	54	TYR
2	N	56	TYR
2	N	57	GLN
2	N	59	LEU
2	N	63	ASN
2	N	69	VAL
2	N	84	LEU
2	N	87	ASP
2	N	119	ASP
2	N	133	TRP
2	N	134	LEU
2	N	138	LEU
2	N	183	ASP
2	N	193	LYS
2	N	206	LYS
2	N	241	SER
2	N	250	LEU
2	N	278	LEU

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Mol	Chain	Res	Type
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	327	LEU
2	N	329	THR
2	N	332	LEU
2	N	334	TYR
2	N	340	SER
2	O	4	THR
2	O	13	VAL
2	O	30	ASP
2	O	34	LYS
2	O	40	LEU
2	O	85	ASP
2	O	106	ASP
2	O	107	LEU
2	O	117	LEU
2	O	126	ARG
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	177	GLU
2	O	183	ASP
2	O	247	THR
2	O	253	GLU
2	O	270	LYS
2	O	283	LEU
2	O	291	SER
2	O	292	VAL
2	O	307	LEU
2	O	311	THR
2	O	317	ARG
2	O	321	ASP
2	O	329	THR
2	O	332	LEU

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Mol	Chain	Res	Type
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	388	LYS
2	O	408	ARG
2	O	412	ILE
2	O	418	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	258	GLN
1	D	208	GLN
1	D	215	GLN
2	K	148	GLN
2	K	187	ASN
2	K	266	GLN
2	K	347	GLN
2	K	367	ASN
2	L	94	ASN
2	L	203	HIS
2	L	251	ASN
2	L	266	GLN
2	L	347	GLN
2	L	395	GLN
2	M	68	HIS
2	M	163	GLN
2	M	203	HIS
2	M	266	GLN
2	M	347	GLN
2	M	353	ASN
2	M	367	ASN
2	M	395	GLN
2	N	63	ASN
2	N	148	GLN
2	N	163	GLN
2	N	266	GLN

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Mol	Chain	Res	Type
2	N	294	ASN
2	N	302	GLN
2	N	315	ASN
2	N	346	GLN
2	N	347	GLN
2	N	385	GLN
2	N	386	ASN
2	O	11	ASN
2	O	43	ASN
2	O	266	GLN
2	O	315	ASN
2	O	318	GLN
2	O	347	GLN
2	O	385	GLN
2	O	395	GLN

5.3.3 RNA [i](#)

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

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Mol	Chain	Res	Type
3	R	22	U
3	R	23	U
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 carbohydrates 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%)	0.62	8 (10%) 5 6	58, 60, 61, 62	0
1	B	73/87 (83%)	1.92	27 (36%) 0 0	57, 62, 64, 65	0
1	C	73/87 (83%)	0.65	6 (8%) 11 12	58, 60, 63, 65	0
1	D	73/87 (83%)	1.88	27 (36%) 0 0	59, 62, 64, 64	0
1	E	73/87 (83%)	1.06	14 (19%) 1 1	55, 61, 64, 65	0
2	K	421/421 (100%)	-0.21	11 (2%) 56 49	53, 63, 69, 73	0
2	L	421/421 (100%)	-0.16	6 (1%) 75 69	57, 65, 69, 72	0
2	M	421/421 (100%)	-0.20	13 (3%) 49 43	55, 64, 67, 69	0
2	N	421/421 (100%)	-0.00	20 (4%) 30 27	57, 63, 67, 71	0
2	O	421/421 (100%)	-0.17	13 (3%) 49 43	57, 64, 67, 72	0
3	R	45/45 (100%)	2.76	36 (80%) 0 0	99, 108, 127, 139	0
All	All	2515/2585 (97%)	0.10	181 (7%) 15 15	53, 63, 69, 139	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ALA	10.3
1	B	252	TYR	9.8
1	D	215	GLN	8.6
1	E	193	ALA	7.6
1	D	216	PRO	7.5
1	B	222	ASP	6.7
1	B	233	SER	6.6
2	N	357	PRO	6.3
2	K	179	ARG	6.2
1	D	212	ALA	6.0
1	D	195	SER	5.8
2	L	357	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	194	VAL	5.5
1	E	253	LYS	5.5
2	M	178	GLY	5.4
1	B	200	LEU	5.3
1	C	193	ALA	5.3
2	K	178	GLY	5.0
1	D	260	ARG	4.9
3	R	18	U	4.8
1	E	252	TYR	4.8
1	C	213	SER	4.8
1	A	252	TYR	4.8
1	B	253	LYS	4.7
1	C	212	ALA	4.6
1	B	229	GLY	4.6
1	B	213	SER	4.6
3	R	42	U	4.5
3	R	1	U	4.4
1	B	228	ARG	4.3
1	B	199	SER	4.3
2	M	180	ASP	4.2
2	N	130	ASP	4.1
1	D	261	VAL	4.1
1	C	194	VAL	4.1
1	B	230	GLU	4.0
2	K	2	SER	4.0
3	R	28	U	4.0
3	R	27	U	3.9
2	M	179	ARG	3.9
3	R	41	U	3.8
3	R	19	U	3.8
1	B	206	THR	3.8
3	R	6	U	3.7
1	B	251	ARG	3.7
2	N	49	SER	3.7
1	D	214	LEU	3.6
2	M	358	ASP	3.6
3	R	45	U	3.6
3	R	40	U	3.5
3	R	5	U	3.5
1	B	193	ALA	3.5
2	K	43	ASN	3.4
2	K	180	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
3	R	17	U	3.4
1	B	234	VAL	3.4
1	E	229	GLY	3.4
1	A	215	GLN	3.4
1	D	217	LEU	3.4
1	D	252	TYR	3.4
2	L	128	SER	3.3
2	O	180	ASP	3.3
2	M	123	ASP	3.3
3	R	33	U	3.3
2	O	96	GLY	3.3
1	B	231	PHE	3.3
3	R	10	U	3.3
3	R	24	U	3.2
3	R	14	U	3.2
3	R	37	U	3.2
1	C	195	SER	3.2
1	D	211	LYS	3.2
2	M	114	ASP	3.1
2	N	89	SER	3.1
3	R	15	U	3.1
2	O	83	LYS	3.1
2	L	131	ASP	3.1
1	B	215	GLN	3.0
1	B	198	TRP	3.0
2	M	357	PRO	3.0
2	N	114	ASP	3.0
1	D	213	SER	2.9
2	M	121	VAL	2.9
2	N	58	GLY	2.9
2	K	177	GLU	2.9
1	D	264	SER	2.9
2	N	128	SER	2.9
1	A	213	SER	2.9
1	B	195	SER	2.9
1	D	199	SER	2.9
1	E	260	ARG	2.8
2	O	166	MET	2.8
3	R	29	U	2.8
2	N	178	GLY	2.8
1	D	230	GLU	2.7
1	E	194	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	221	LEU	2.7
3	R	3	U	2.7
2	K	357	PRO	2.7
1	D	201	SER	2.7
3	R	13	U	2.7
2	N	362	GLY	2.7
3	R	22	U	2.7
1	D	253	LYS	2.7
2	N	154	LYS	2.7
2	O	53	GLY	2.7
3	R	39	U	2.7
2	M	2	SER	2.7
3	R	23	U	2.6
2	O	43	ASN	2.6
1	A	264	SER	2.6
1	E	228	ARG	2.6
1	B	204	SER	2.6
1	D	239	ARG	2.6
2	N	127	THR	2.6
3	R	44	U	2.6
1	D	229	GLY	2.6
3	R	32	U	2.6
1	B	214	LEU	2.5
1	D	218	THR	2.5
1	C	215	GLN	2.5
2	M	176	PRO	2.5
1	D	225	PHE	2.5
2	N	187	ASN	2.5
1	E	210	LYS	2.5
2	M	119	ASP	2.5
1	D	231	PHE	2.4
1	E	195	SER	2.4
1	D	203	THR	2.4
2	O	130	ASP	2.4
3	R	20	U	2.4
1	B	212	ALA	2.4
3	R	9	U	2.4
2	O	68	HIS	2.3
3	R	4	U	2.3
2	K	176	PRO	2.3
1	A	212	ALA	2.3
1	B	223	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	R	7	U	2.3
1	D	193	ALA	2.3
1	B	224	LEU	2.3
2	N	92	GLY	2.2
2	L	122	SER	2.2
1	D	206	THR	2.2
3	R	31	U	2.2
3	R	36	U	2.2
1	B	226	SER	2.2
2	N	125	SER	2.2
1	B	194	VAL	2.2
1	D	196	ASP	2.2
2	N	109	SER	2.2
3	R	43	U	2.2
2	O	122	SER	2.2
1	B	225	PHE	2.2
1	E	258	GLN	2.2
1	E	222	ASP	2.2
2	K	119	ASP	2.2
3	R	11	U	2.2
2	M	122	SER	2.1
2	L	178	GLY	2.1
2	K	131	ASP	2.1
1	E	202	LYS	2.1
2	K	44	THR	2.1
1	A	260	ARG	2.1
2	O	362	GLY	2.1
2	N	102	ILE	2.1
1	A	194	VAL	2.1
2	O	47	SER	2.1
2	N	180	ASP	2.1
2	N	358	ASP	2.0
2	N	47	SER	2.0
2	O	121	VAL	2.0
2	O	363	GLY	2.0
3	R	2	U	2.0
3	R	16	U	2.0
1	E	259	ALA	2.0
1	D	204	SER	2.0
1	E	214	LEU	2.0
2	L	125	SER	2.0
2	M	45	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	183	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.