



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:25 PM UTC

PDB ID : 6K3H / pdb_00006k3h
Title : Crystallographic Analysis of Nucleoside Diphosphate Kinase (NDK) from *Aspergillus Flavus*
Authors : Wang, Y.; Wang, S.; Wang, S.H.
Deposited on : 2019-05-18
Resolution : 2.18 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

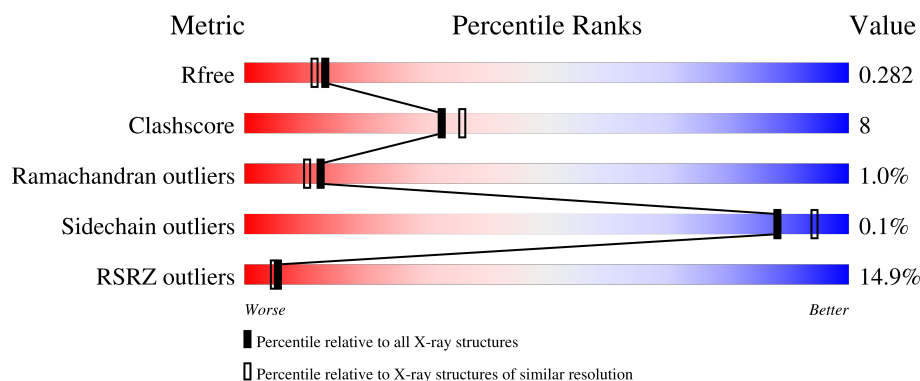
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	155	3% 85% 13% .
1	B	155	9% 79% 19% .
1	C	155	8% 77% 19% ..
1	D	155	11% 80% 18% .
1	E	155	7% 89% 8% .

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Mol	Chain	Length	Quality of chain
1	F	155	
1	G	155	
1	H	155	
1	I	155	
1	J	155	
1	K	155	
1	L	155	
1	M	155	
1	N	155	
1	O	155	
1	P	155	
1	Q	155	
1	R	155	
1	S	155	
1	T	155	
1	U	155	
1	V	155	
1	W	155	
1	X	155	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28318 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1189	763	204	217	5			
1	B	151	Total	C	N	O	S	0	0	0
			1184	759	204	217	4			
1	C	150	Total	C	N	O	S	0	0	0
			1177	755	202	216	4			
1	D	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			
1	E	151	Total	C	N	O	S	0	0	0
			1186	761	204	217	4			
1	F	150	Total	C	N	O	S	0	0	0
			1177	755	202	216	4			
1	G	150	Total	C	N	O	S	0	0	0
			1173	752	202	215	4			
1	H	151	Total	C	N	O	S	0	0	0
			1185	761	204	216	4			
1	I	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			
1	J	150	Total	C	N	O	S	0	0	0
			1177	755	202	216	4			
1	K	152	Total	C	N	O	S	0	0	0
			1190	763	205	217	5			
1	L	151	Total	C	N	O	S	0	0	0
			1177	756	203	213	5			
1	M	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			
1	N	139	Total	C	N	O	S	0	0	0
			1087	693	190	200	4			
1	Q	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			
1	R	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	U	150	Total	C	N	O	S	0	0	0
			1179	757	202	215	5			
1	V	150	Total	C	N	O	S	0	0	0
			1171	750	203	214	4			
1	W	150	Total	C	N	O	S	0	0	0
			1177	755	202	216	4			
1	X	150	Total	C	N	O	S	0	0	0
			1180	758	203	215	4			
1	O	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			
1	P	150	Total	C	N	O	S	0	0	0
			1180	758	203	215	4			
1	S	149	Total	C	N	O	S	0	0	0
			1171	752	201	214	4			
1	T	152	Total	C	N	O	S	0	0	0
			1194	766	205	218	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B8NQF0
A	0	PRO	-	expression tag	UNP B8NQF0
B	-1	GLY	-	expression tag	UNP B8NQF0
B	0	PRO	-	expression tag	UNP B8NQF0
C	-1	GLY	-	expression tag	UNP B8NQF0
C	0	PRO	-	expression tag	UNP B8NQF0
D	-1	GLY	-	expression tag	UNP B8NQF0
D	0	PRO	-	expression tag	UNP B8NQF0
E	-1	GLY	-	expression tag	UNP B8NQF0
E	0	PRO	-	expression tag	UNP B8NQF0
F	-1	GLY	-	expression tag	UNP B8NQF0
F	0	PRO	-	expression tag	UNP B8NQF0
G	-1	GLY	-	expression tag	UNP B8NQF0
G	0	PRO	-	expression tag	UNP B8NQF0
H	-1	GLY	-	expression tag	UNP B8NQF0
H	0	PRO	-	expression tag	UNP B8NQF0
I	-1	GLY	-	expression tag	UNP B8NQF0
I	0	PRO	-	expression tag	UNP B8NQF0
J	-1	GLY	-	expression tag	UNP B8NQF0
J	0	PRO	-	expression tag	UNP B8NQF0
K	-1	GLY	-	expression tag	UNP B8NQF0
K	0	PRO	-	expression tag	UNP B8NQF0
L	-1	GLY	-	expression tag	UNP B8NQF0

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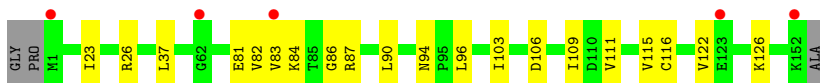
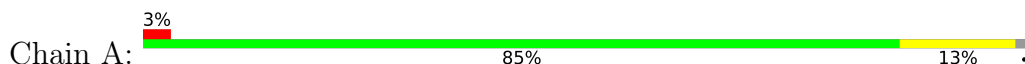
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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	PRO	-	expression tag	UNP B8NQF0
M	-1	GLY	-	expression tag	UNP B8NQF0
M	0	PRO	-	expression tag	UNP B8NQF0
N	-1	GLY	-	expression tag	UNP B8NQF0
N	0	PRO	-	expression tag	UNP B8NQF0
Q	-1	GLY	-	expression tag	UNP B8NQF0
Q	0	PRO	-	expression tag	UNP B8NQF0
R	-1	GLY	-	expression tag	UNP B8NQF0
R	0	PRO	-	expression tag	UNP B8NQF0
U	-1	GLY	-	expression tag	UNP B8NQF0
U	0	PRO	-	expression tag	UNP B8NQF0
V	-1	GLY	-	expression tag	UNP B8NQF0
V	0	PRO	-	expression tag	UNP B8NQF0
W	-1	GLY	-	expression tag	UNP B8NQF0
W	0	PRO	-	expression tag	UNP B8NQF0
X	-1	GLY	-	expression tag	UNP B8NQF0
X	0	PRO	-	expression tag	UNP B8NQF0
O	-1	GLY	-	expression tag	UNP B8NQF0
O	0	PRO	-	expression tag	UNP B8NQF0
P	-1	GLY	-	expression tag	UNP B8NQF0
P	0	PRO	-	expression tag	UNP B8NQF0
S	-1	GLY	-	expression tag	UNP B8NQF0
S	0	PRO	-	expression tag	UNP B8NQF0
T	-1	GLY	-	expression tag	UNP B8NQF0
T	0	PRO	-	expression tag	UNP B8NQF0

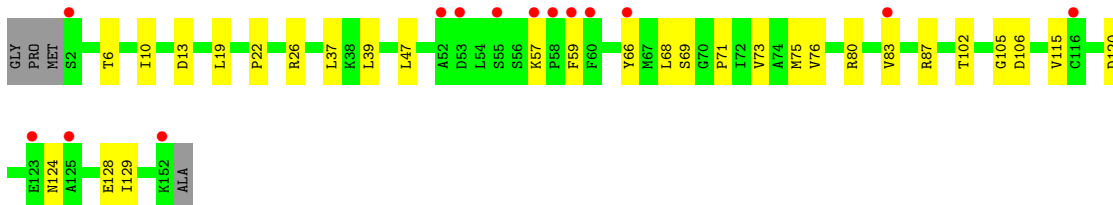
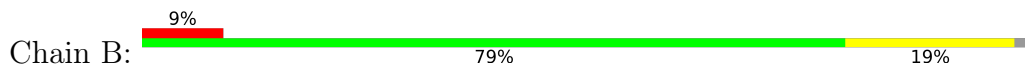
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

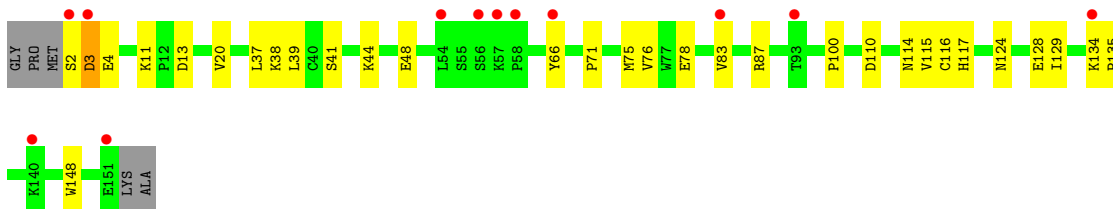
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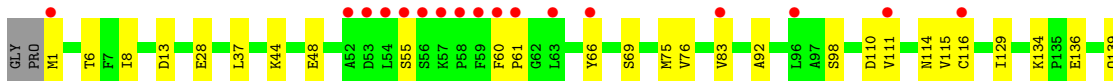
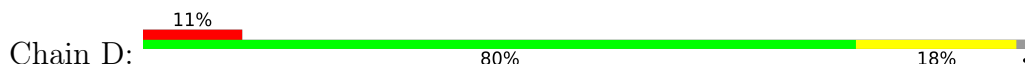
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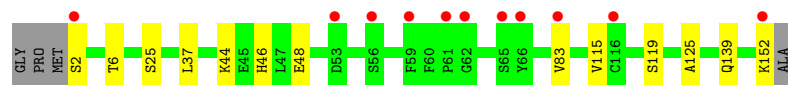
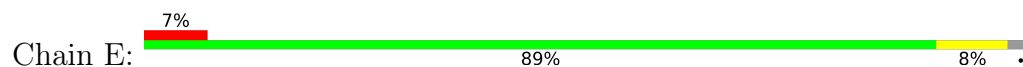


- Molecule 1: Nucleoside diphosphate kinase

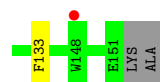
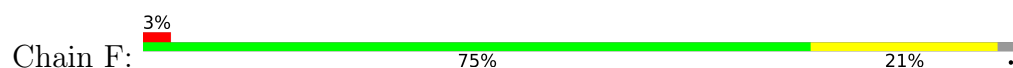




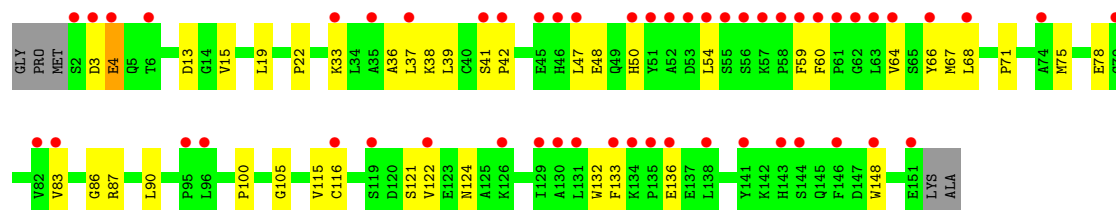
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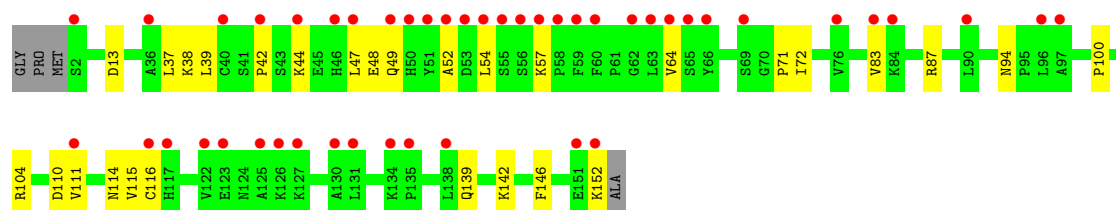
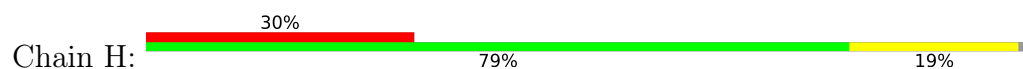
- Molecule 1: Nucleoside diphosphate kinase



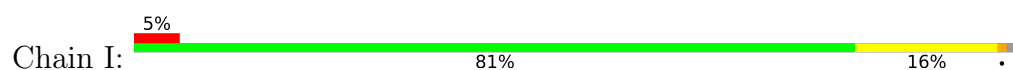
- Molecule 1: Nucleoside diphosphate kinase



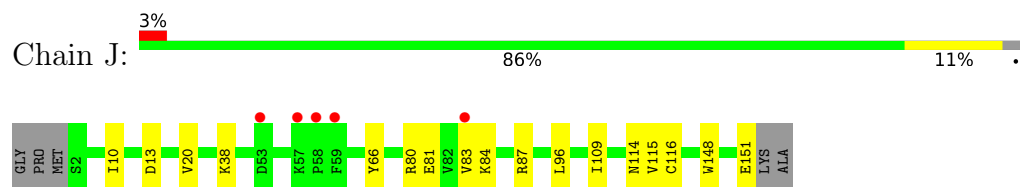
- Molecule 1: Nucleoside diphosphate kinase



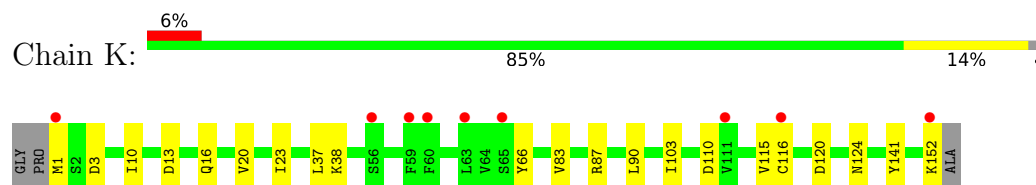
- Molecule 1: Nucleoside diphosphate kinase



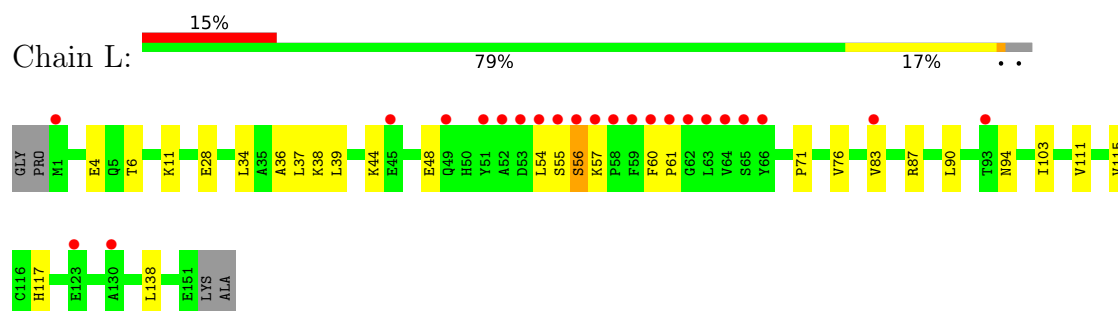
- Molecule 1: Nucleoside diphosphate kinase



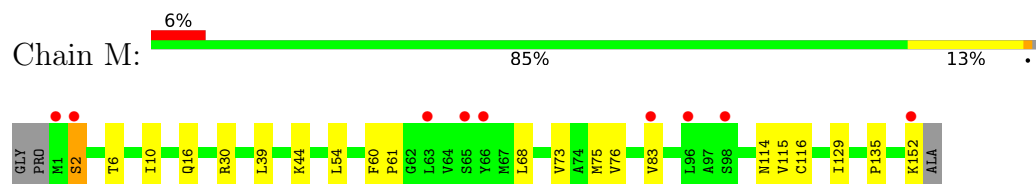
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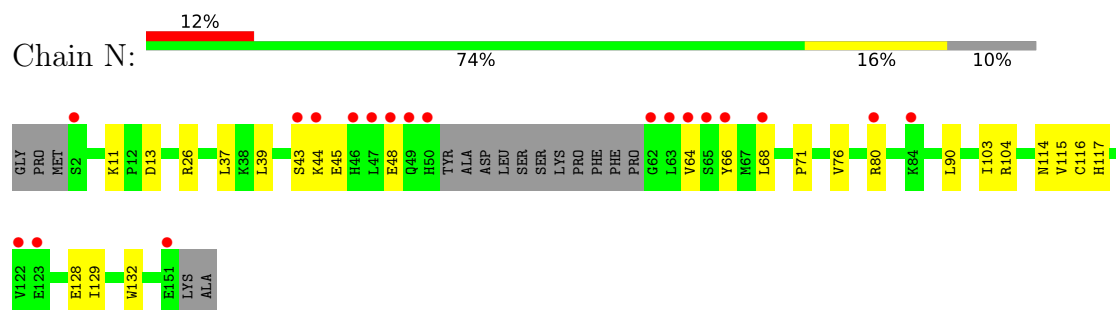
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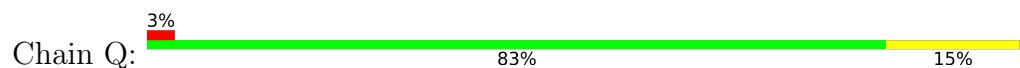
- Molecule 1: Nucleoside diphosphate kinase



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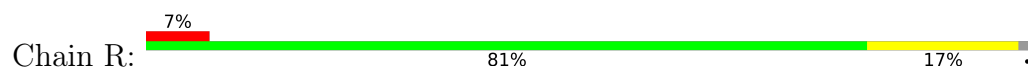


- Molecule 1: Nucleoside diphosphate kinase

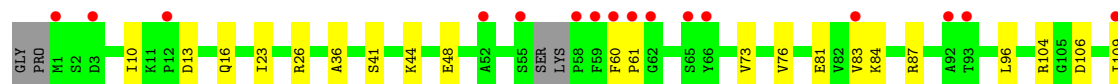
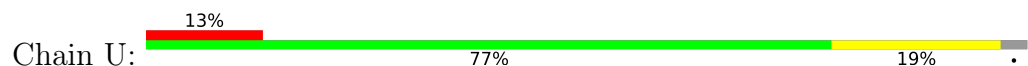




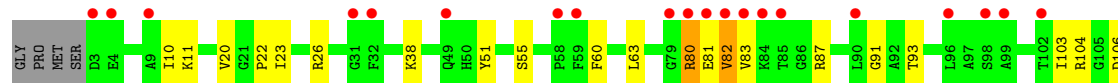
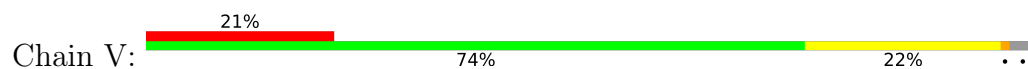
- Molecule 1: Nucleoside diphosphate kinase



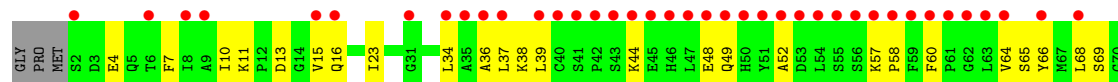
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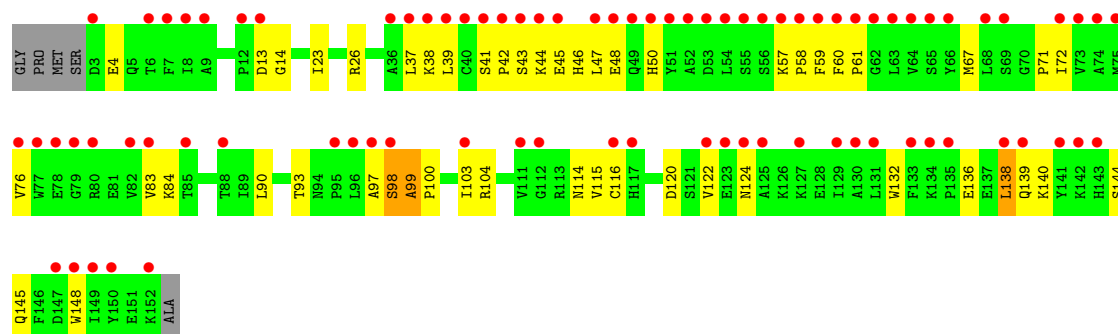


- Molecule 1: Nucleoside diphosphate kinase

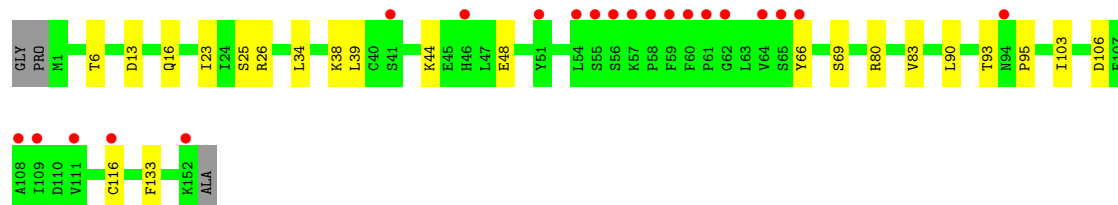
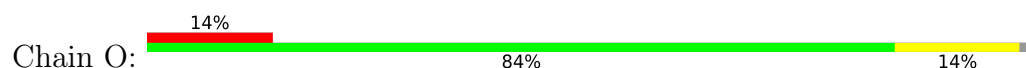


- Molecule 1: Nucleoside diphosphate kinase

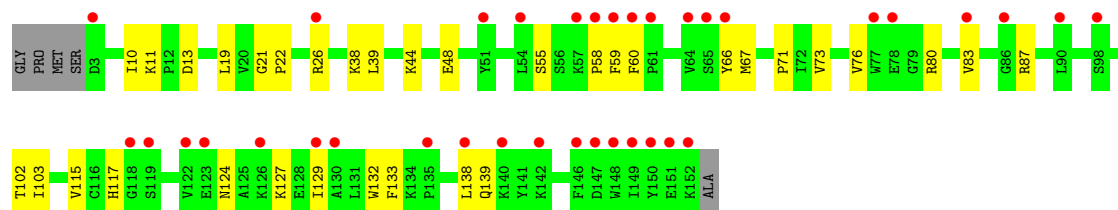
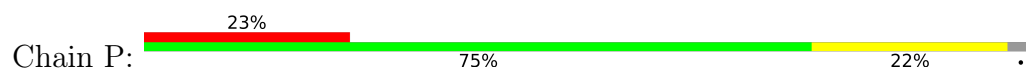




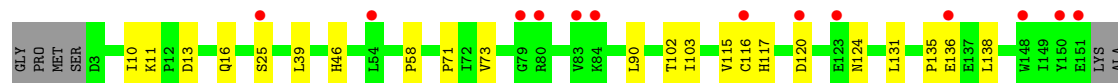
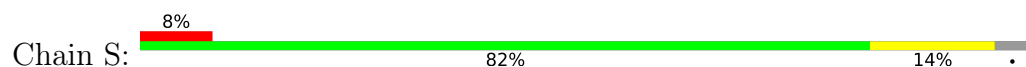
- Molecule 1: Nucleoside diphosphate kinase



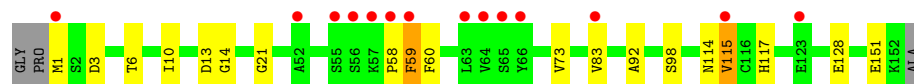
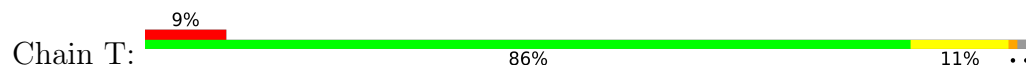
- Molecule 1: Nucleoside diphosphate kinase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.78Å 168.44Å 146.10Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	94.76 – 2.18 94.76 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.3 (94.76-2.18) 99.3 (94.76-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.230 , 0.281 0.233 , 0.282	Depositor DCC
R_{free} test set	11872 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28318	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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	0.36	0/1219	0.57	0/1648
1	B	0.36	0/1213	0.55	0/1638
1	C	0.38	0/1207	0.55	0/1632
1	D	0.34	0/1224	0.58	0/1653
1	E	0.41	0/1216	0.63	0/1643
1	F	0.38	0/1207	0.55	0/1632
1	G	0.36	0/1203	0.64	0/1627
1	H	0.31	0/1215	0.53	0/1642
1	I	0.40	0/1224	0.61	0/1653
1	J	0.35	0/1207	0.51	0/1632
1	K	0.38	0/1220	0.58	0/1648
1	L	0.36	0/1207	0.55	0/1632
1	M	0.38	0/1224	0.55	0/1653
1	N	0.33	0/1111	0.52	0/1499
1	O	0.36	0/1224	0.58	0/1653
1	P	0.33	0/1210	0.54	0/1635
1	Q	0.37	0/1224	0.61	0/1653
1	R	0.34	0/1224	0.54	0/1653
1	S	0.35	0/1201	0.58	0/1624
1	T	0.36	0/1224	0.55	0/1653
1	U	0.37	0/1208	0.58	0/1630
1	V	0.32	0/1199	0.53	0/1619
1	W	0.32	0/1207	0.56	0/1632
1	X	0.37	0/1210	0.61	0/1635
All	All	0.36	0/29028	0.57	0/39219

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
1	X	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	97	ALA	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	1189	0	1180	11	0
1	B	1184	0	1176	18	0
1	C	1177	0	1169	22	0
1	D	1194	0	1194	19	0
1	E	1186	0	1182	11	0
1	F	1177	0	1169	21	0
1	G	1173	0	1157	35	0
1	H	1185	0	1179	21	0
1	I	1194	0	1194	27	0
1	J	1177	0	1169	11	0
1	K	1190	0	1182	16	0
1	L	1177	0	1164	21	0
1	M	1194	0	1194	17	0
1	N	1087	0	1084	15	0
1	O	1194	0	1194	15	0
1	P	1180	0	1177	26	0
1	Q	1194	0	1194	17	0
1	R	1194	0	1194	19	0
1	S	1171	0	1164	14	0
1	T	1194	0	1194	14	0
1	U	1179	0	1176	20	0
1	V	1171	0	1164	32	0
1	W	1177	0	1169	37	0
1	X	1180	0	1177	39	1
All	All	28318	0	28196	446	1

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 8.

All (446) 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)
1:I:80:ARG:HH12	1:I:152:LYS:HE3	0.94	1.10
1:I:80:ARG:NH1	1:I:152:LYS:HE3	1.73	1.03
1:M:2:SER:HB3	1:M:152:LYS:NZ	1.82	0.93
1:V:80:ARG:HH22	1:V:150:TYR:N	1.71	0.89
1:E:2:SER:HA	1:E:152:LYS:HZ2	1.41	0.85
1:I:1:MET:N	1:I:152:LYS:NZ	2.25	0.83
1:P:26:ARG:HG3	1:P:26:ARG:HH11	1.44	0.82
1:X:57:LYS:HD3	1:X:59:PHE:H	1.42	0.81
1:G:41:SER:HB3	1:G:68:LEU:HD21	1.62	0.81
1:I:1:MET:H3	1:I:152:LYS:HZ1	1.25	0.81
1:X:45:GLU:HA	1:X:48:GLU:HB2	1.62	0.80
1:I:1:MET:N	1:I:152:LYS:HZ1	1.78	0.79
1:G:83:VAL:HG22	1:G:87:ARG:HH21	1.47	0.78
1:X:93:THR:HA	1:X:104:ARG:NH1	1.98	0.78
1:M:2:SER:HB3	1:M:152:LYS:HZ2	1.48	0.76
1:W:49:GLN:HA	1:W:52:ALA:HB2	1.67	0.76
1:N:13:ASP:OD1	1:N:66:TYR:OH	2.03	0.76
1:R:134:LYS:NZ	1:R:136:GLU:OE2	2.20	0.74
1:P:58:PRO:O	1:P:60:PHE:N	2.20	0.74
1:I:1:MET:H3	1:I:152:LYS:NZ	1.83	0.73
1:K:20:VAL:HG12	1:L:28:GLU:OE2	1.88	0.73
1:V:80:ARG:HH22	1:V:149:ILE:C	1.97	0.72
1:U:96:LEU:HD21	1:U:109:ILE:HG23	1.70	0.72
1:M:2:SER:HB3	1:M:152:LYS:HZ3	1.52	0.72
1:N:26:ARG:HG3	1:N:26:ARG:HH11	1.55	0.72
1:X:93:THR:HA	1:X:104:ARG:HH11	1.56	0.71
1:H:110:ASP:OD1	1:P:80:ARG:NH2	2.25	0.70
1:H:54:LEU:HB3	1:H:57:LYS:HD2	1.73	0.70
1:J:13:ASP:OD1	1:J:66:TYR:OH	2.11	0.69
1:V:104:ARG:HD3	1:V:114:ASN:HB2	1.75	0.69
1:B:39:LEU:HD11	1:B:71:PRO:HB2	1.76	0.67
1:V:83:VAL:HG12	1:V:87:ARG:HH12	1.60	0.67
1:V:11:LYS:HE3	1:V:117:HIS:HB2	1.75	0.67
1:H:39:LEU:HD11	1:H:71:PRO:HB2	1.75	0.66
1:T:13:ASP:N	1:T:13:ASP:OD1	2.28	0.66
1:O:44:LYS:HE3	1:O:48:GLU:HG3	1.78	0.66
1:S:135:PRO:HA	1:S:138:LEU:HD12	1.76	0.66
1:U:44:LYS:O	1:U:48:GLU:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:39:LEU:HD11	1:X:71:PRO:HB2	1.79	0.65
1:K:23:ILE:HG12	1:K:103:ILE:HD13	1.77	0.65
1:I:83:VAL:HG22	1:I:87:ARG:HH12	1.62	0.64
1:L:94:ASN:HA	1:L:111:VAL:HG22	1.80	0.64
1:W:83:VAL:HG22	1:W:87:ARG:HH12	1.63	0.63
1:D:136:GLU:H	1:D:136:GLU:CD	2.05	0.63
1:H:104:ARG:NH2	1:H:116:CYS:O	2.31	0.63
1:R:1:MET:HG2	1:R:80:ARG:HH11	1.64	0.63
1:G:47:LEU:HD13	1:G:67:MET:HB3	1.80	0.62
1:I:94:ASN:HD21	1:I:96:LEU:HB2	1.63	0.62
1:U:81:GLU:OE1	1:U:84:LYS:NZ	2.32	0.62
1:S:25:SER:HB3	1:T:21:GLY:HA3	1.80	0.62
1:S:90:LEU:HD22	1:S:116:CYS:SG	2.39	0.62
1:X:23:ILE:HG12	1:X:103:ILE:HD12	1.80	0.61
1:I:13:ASP:OD1	1:I:66:TYR:OH	2.19	0.61
1:V:23:ILE:HG12	1:V:103:ILE:HD13	1.82	0.61
1:X:57:LYS:HG2	1:X:58:PRO:HD2	1.83	0.61
1:O:66:TYR:O	1:O:69:SER:HB3	2.00	0.61
1:X:47:LEU:HD13	1:X:67:MET:HB3	1.83	0.60
1:B:66:TYR:O	1:B:69:SER:OG	2.15	0.60
1:T:58:PRO:O	1:T:60:PHE:N	2.34	0.60
1:M:2:SER:CB	1:M:152:LYS:HZ2	2.15	0.60
1:U:41:SER:OG	1:V:139:GLN:OE1	2.19	0.60
1:I:3:ASP:O	1:I:5:GLN:N	2.34	0.60
1:C:3:ASP:HA	1:C:78:GLU:HG2	1.83	0.60
1:W:139:GLN:OE1	1:X:41:SER:OG	2.12	0.60
1:G:42:PRO:O	1:G:68:LEU:HD22	2.02	0.59
1:C:2:SER:O	1:C:4:GLU:N	2.34	0.59
1:L:83:VAL:HG22	1:L:87:ARG:HH12	1.67	0.59
1:H:48:GLU:HG2	1:H:64:VAL:HG11	1.84	0.59
1:M:10:ILE:HG13	1:M:75:MET:HE2	1.82	0.59
1:K:120:ASP:OD1	1:K:124:ASN:ND2	2.36	0.59
1:O:23:ILE:HG12	1:O:103:ILE:HD12	1.86	0.58
1:E:44:LYS:NZ	1:E:48:GLU:OE1	2.37	0.58
1:G:83:VAL:HG22	1:G:87:ARG:NH2	2.18	0.58
1:A:83:VAL:HG12	1:A:87:ARG:NH1	2.18	0.58
1:N:90:LEU:HD22	1:N:116:CYS:SG	2.44	0.57
1:N:90:LEU:HD23	1:N:103:ILE:HD12	1.85	0.57
1:P:58:PRO:C	1:P:60:PHE:H	2.13	0.57
1:C:44:LYS:NZ	1:C:48:GLU:OE2	2.36	0.57
1:X:136:GLU:H	1:X:136:GLU:CD	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:81:GLU:O	1:V:83:VAL:N	2.35	0.57
1:B:10:ILE:HG13	1:B:75:MET:HE2	1.87	0.57
1:J:84:LYS:HD3	1:J:87:ARG:NH2	2.19	0.57
1:K:83:VAL:HG12	1:K:87:ARG:NH2	2.20	0.57
1:U:83:VAL:HG22	1:U:87:ARG:HH12	1.69	0.57
1:B:57:LYS:HD2	1:B:59:PHE:HE1	1.70	0.57
1:U:104:ARG:NH2	1:U:116:CYS:O	2.32	0.56
1:V:80:ARG:NH2	1:V:150:TYR:CB	2.68	0.56
1:X:76:VAL:HG21	1:X:138:LEU:HD21	1.85	0.56
1:V:83:VAL:HG11	1:V:121:SER:O	2.06	0.56
1:W:48:GLU:HG2	1:W:60:PHE:CZ	2.40	0.56
1:D:110:ASP:OD1	1:N:80:ARG:NH2	2.39	0.56
1:I:1:MET:H2	1:I:152:LYS:NZ	2.02	0.56
1:U:13:ASP:OD1	1:U:13:ASP:N	2.38	0.56
1:A:26:ARG:NH2	1:A:106:ASP:OD2	2.39	0.56
1:E:2:SER:HA	1:E:152:LYS:NZ	2.17	0.56
1:I:83:VAL:HG22	1:I:87:ARG:NH1	2.20	0.56
1:J:96:LEU:HD21	1:J:109:ILE:HG23	1.88	0.55
1:R:39:LEU:HD11	1:R:71:PRO:HB2	1.88	0.55
1:X:120:ASP:HB3	1:X:124:ASN:HD22	1.71	0.55
1:U:120:ASP:OD2	1:U:124:ASN:ND2	2.39	0.55
1:L:90:LEU:HD23	1:L:103:ILE:HD12	1.89	0.55
1:V:80:ARG:NH1	1:V:149:ILE:O	2.35	0.55
1:S:120:ASP:HB2	1:S:124:ASN:HD22	1.71	0.55
1:I:1:MET:N	1:I:152:LYS:HZ3	2.02	0.55
1:C:41:SER:OG	1:D:139:GLN:OE1	2.22	0.55
1:H:54:LEU:HD22	1:H:57:LYS:HE3	1.89	0.54
1:W:114:ASN:O	1:W:116:CYS:N	2.38	0.54
1:I:1:MET:HG3	1:I:80:ARG:HD3	1.90	0.54
1:W:60:PHE:O	1:W:64:VAL:HG23	2.07	0.54
1:I:10:ILE:HB	1:I:73:VAL:HB	1.88	0.54
1:Q:126:LYS:HB3	1:U:127:LYS:HD3	1.88	0.54
1:A:122:VAL:HG12	1:A:126:LYS:HE2	1.89	0.54
1:I:121:SER:OG	1:I:123:GLU:HG3	2.07	0.54
1:V:80:ARG:CZ	1:V:149:ILE:HG22	2.39	0.53
1:X:48:GLU:HG2	1:X:60:PHE:CZ	2.43	0.53
1:Q:83:VAL:HG11	1:Q:122:VAL:HG23	1.90	0.53
1:M:6:THR:OG1	1:M:83:VAL:HG23	2.08	0.53
1:R:6:THR:OG1	1:R:83:VAL:HG23	2.07	0.53
1:T:14:GLY:HA2	1:T:115:VAL:HG23	1.90	0.53
1:G:148:TRP:CZ2	1:O:16:GLN:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:VAL:HG22	1:J:87:ARG:NH1	2.24	0.53
1:W:136:GLU:CD	1:W:136:GLU:H	2.16	0.53
1:K:83:VAL:HG12	1:K:87:ARG:HH22	1.73	0.53
1:T:6:THR:OG1	1:T:83:VAL:HG23	2.08	0.53
1:A:83:VAL:HG12	1:A:87:ARG:HH12	1.73	0.53
1:G:90:LEU:HD22	1:G:116:CYS:SG	2.48	0.53
1:H:42:PRO:HG2	1:H:47:LEU:HD11	1.90	0.52
1:X:26:ARG:HG3	1:X:103:ILE:HD11	1.92	0.52
1:U:16:GLN:HG3	1:X:148:TRP:CZ2	2.44	0.52
1:M:114:ASN:O	1:M:116:CYS:N	2.39	0.52
1:O:90:LEU:HD13	1:O:116:CYS:HB3	1.90	0.52
1:L:60:PHE:HB3	1:L:61:PRO:HD3	1.91	0.52
1:L:6:THR:OG1	1:L:83:VAL:HG23	2.09	0.52
1:D:44:LYS:O	1:D:48:GLU:HG3	2.10	0.52
1:S:136:GLU:H	1:S:136:GLU:CD	2.18	0.52
1:E:139:GLN:OE1	1:F:41:SER:OG	2.14	0.51
1:G:50:HIS:CD2	1:G:132:TRP:HE1	2.28	0.51
1:N:104:ARG:HD3	1:N:114:ASN:HB2	1.92	0.51
1:C:20:VAL:HB	1:D:28:GLU:OE2	2.10	0.51
1:P:26:ARG:HH11	1:P:26:ARG:CG	2.20	0.51
1:H:142:LYS:HE2	1:H:146:PHE:CG	2.45	0.51
1:R:104:ARG:NH2	1:R:116:CYS:O	2.35	0.51
1:P:10:ILE:HB	1:P:73:VAL:HB	1.93	0.51
1:V:114:ASN:O	1:V:116:CYS:N	2.44	0.51
1:F:83:VAL:HG12	1:F:87:ARG:HH12	1.75	0.51
1:D:60:PHE:HB3	1:D:61:PRO:HD3	1.93	0.51
1:G:41:SER:OG	1:H:139:GLN:OE1	2.21	0.51
1:C:134:LYS:HE3	1:C:135:PRO:CD	2.41	0.51
1:V:83:VAL:HG12	1:V:87:ARG:NH1	2.26	0.51
1:Q:39:LEU:HD11	1:Q:71:PRO:HB2	1.91	0.50
1:W:39:LEU:HD11	1:W:71:PRO:HB2	1.94	0.50
1:X:83:VAL:HG11	1:X:122:VAL:HG13	1.92	0.50
1:K:37:LEU:O	1:L:38:LYS:HA	2.12	0.50
1:Q:2:SER:HB3	1:Q:152:LYS:HE2	1.92	0.50
1:K:10:ILE:HD13	1:K:20:VAL:HA	1.93	0.50
1:L:83:VAL:HG22	1:L:87:ARG:NH1	2.26	0.50
1:E:46:HIS:HA	1:M:135:PRO:HG2	1.94	0.50
1:K:90:LEU:HD22	1:K:116:CYS:SG	2.52	0.50
1:O:13:ASP:OD1	1:O:66:TYR:OH	2.28	0.50
1:C:38:LYS:HA	1:D:37:LEU:O	2.11	0.50
1:W:139:GLN:HG3	1:X:39:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:123:GLU:HA	1:W:126:LYS:HG3	1.94	0.50
1:C:37:LEU:HD12	1:C:75:MET:HG2	1.94	0.49
1:F:7:PHE:HB2	1:F:129:ILE:HG13	1.94	0.49
1:K:1:MET:H2	1:K:152:LYS:HZ2	1.59	0.49
1:D:136:GLU:OE2	1:D:136:GLU:N	2.43	0.49
1:P:44:LYS:O	1:P:48:GLU:HG3	2.12	0.49
1:L:39:LEU:HD11	1:L:71:PRO:HB2	1.94	0.49
1:U:26:ARG:NH2	1:U:106:ASP:OD2	2.40	0.49
1:F:90:LEU:HD22	1:F:116:CYS:SG	2.52	0.49
1:G:19:LEU:C	1:G:22:PRO:HD2	2.38	0.49
1:I:44:LYS:HG3	1:I:68:LEU:HD11	1.94	0.49
1:Q:104:ARG:NH2	1:Q:116:CYS:O	2.41	0.49
1:C:39:LEU:HD11	1:C:71:PRO:HB2	1.95	0.49
1:V:81:GLU:HG3	1:W:96:LEU:HD13	1.94	0.49
1:G:121:SER:OG	1:G:124:ASN:HB2	2.13	0.49
1:T:14:GLY:CA	1:T:115:VAL:HG23	2.41	0.49
1:F:11:LYS:HE3	1:F:117:HIS:HB2	1.95	0.49
1:F:84:LYS:HD2	1:F:87:ARG:HH21	1.78	0.49
1:X:50:HIS:CG	1:X:132:TRP:HE1	2.31	0.49
1:O:26:ARG:NH2	1:O:106:ASP:OD2	2.45	0.48
1:T:117:HIS:HE1	1:T:128:GLU:OE1	1.96	0.48
1:I:114:ASN:O	1:I:116:CYS:N	2.45	0.48
1:T:58:PRO:C	1:T:60:PHE:H	2.20	0.48
1:K:13:ASP:OD1	1:K:66:TYR:OH	2.27	0.48
1:A:81:GLU:OE2	1:A:84:LYS:NZ	2.46	0.48
1:R:114:ASN:O	1:R:116:CYS:N	2.46	0.48
1:C:83:VAL:HG12	1:C:87:ARG:HH12	1.78	0.48
1:F:26:ARG:NH2	1:F:106:ASP:OD2	2.43	0.48
1:I:44:LYS:HE3	1:I:48:GLU:OE1	2.13	0.48
1:X:83:VAL:HG13	1:X:84:LYS:N	2.28	0.48
1:P:26:ARG:HG3	1:P:26:ARG:NH1	2.23	0.48
1:W:64:VAL:O	1:W:68:LEU:HG	2.14	0.48
1:C:13:ASP:OD1	1:C:66:TYR:OH	2.26	0.48
1:R:10:ILE:HB	1:R:73:VAL:HB	1.96	0.48
1:T:10:ILE:HB	1:T:73:VAL:HB	1.95	0.48
1:H:83:VAL:HG22	1:H:87:ARG:HH12	1.79	0.48
1:X:23:ILE:HD13	1:X:116:CYS:SG	2.54	0.48
1:X:45:GLU:O	1:X:45:GLU:HG2	2.13	0.48
1:P:76:VAL:HG22	1:P:129:ILE:HG12	1.96	0.48
1:U:60:PHE:CD1	1:U:61:PRO:HD3	2.49	0.47
1:O:6:THR:OG1	1:O:83:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ASN:O	1:D:116:CYS:N	2.45	0.47
1:F:76:VAL:HG22	1:F:129:ILE:HG12	1.96	0.47
1:F:110:ASP:OD1	1:O:80:ARG:HD2	2.13	0.47
1:G:136:GLU:O	1:G:136:GLU:HG2	2.13	0.47
1:W:11:LYS:O	1:W:15:VAL:HG23	2.15	0.47
1:X:4:GLU:OE2	1:X:83:VAL:HG12	2.14	0.47
1:R:136:GLU:CD	1:R:136:GLU:H	2.22	0.47
1:P:11:LYS:HE3	1:P:117:HIS:HB2	1.97	0.47
1:P:55:SER:HA	1:P:60:PHE:CD1	2.49	0.47
1:I:87:ARG:HD3	1:I:120:ASP:HA	1.95	0.47
1:R:13:ASP:OD1	1:R:66:TYR:OH	2.30	0.47
1:U:134:LYS:HE2	1:U:137:GLU:OE2	2.15	0.47
1:P:26:ARG:HD2	1:P:103:ILE:HG12	1.97	0.47
1:K:1:MET:C	1:K:3:ASP:H	2.21	0.47
1:Q:124:ASN:O	1:Q:128:GLU:HG3	2.14	0.47
1:P:38:LYS:NZ	1:P:132:TRP:O	2.41	0.47
1:P:39:LEU:HD11	1:P:71:PRO:HB2	1.97	0.47
1:C:114:ASN:O	1:C:116:CYS:N	2.42	0.47
1:D:134:LYS:HB3	1:D:136:GLU:OE1	2.14	0.47
1:V:91:GLY:O	1:V:104:ARG:NH1	2.48	0.47
1:C:2:SER:OG	1:C:3:ASP:N	2.48	0.47
1:Q:143:HIS:CE1	1:Q:145:GLN:HB2	2.50	0.47
1:R:37:LEU:HD12	1:R:75:MET:HG2	1.97	0.47
1:V:26:ARG:NH2	1:V:106:ASP:OD2	2.34	0.46
1:Q:60:PHE:HB3	1:Q:61:PRO:HD3	1.98	0.46
1:V:119:SER:OG	1:V:128:GLU:OE1	2.29	0.46
1:K:141:TYR:CD1	1:L:71:PRO:HG3	2.50	0.46
1:W:7:PHE:HB3	1:W:119:SER:OG	2.15	0.46
1:M:39:LEU:HB2	1:N:37:LEU:HB3	1.98	0.46
1:V:80:ARG:NH1	1:V:149:ILE:HG22	2.31	0.46
1:B:6:THR:OG1	1:B:83:VAL:HG23	2.15	0.46
1:I:94:ASN:ND2	1:I:96:LEU:HB2	2.30	0.46
1:G:41:SER:CB	1:G:68:LEU:HD21	2.41	0.46
1:W:38:LYS:NZ	1:W:132:TRP:O	2.49	0.46
1:C:134:LYS:HA	1:C:134:LYS:CE	2.46	0.46
1:J:83:VAL:HG22	1:J:87:ARG:HH12	1.81	0.46
1:N:11:LYS:HE3	1:N:117:HIS:HB2	1.97	0.46
1:W:44:LYS:HE2	1:W:48:GLU:OE1	2.15	0.46
1:W:134:LYS:HE2	1:W:136:GLU:OE2	2.14	0.46
1:I:48:GLU:HG2	1:I:60:PHE:CZ	2.51	0.46
1:J:148:TRP:CZ2	1:K:16:GLN:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:LEU:O	1:L:56:SER:HB3	2.15	0.46
1:M:44:LYS:HG3	1:M:68:LEU:HD11	1.98	0.46
1:S:10:ILE:HB	1:S:73:VAL:HB	1.97	0.46
1:Q:71:PRO:HG3	1:R:141:TYR:CD1	2.50	0.45
1:R:76:VAL:HG22	1:R:129:ILE:HG12	1.97	0.45
1:R:80:ARG:HH12	1:R:152:LYS:HZ3	1.64	0.45
1:S:39:LEU:HD11	1:S:71:PRO:HB2	1.98	0.45
1:A:94:ASN:HA	1:A:111:VAL:HG22	1.97	0.45
1:G:83:VAL:HG11	1:G:122:VAL:HG12	1.98	0.45
1:T:92:ALA:H	1:T:98:SER:HB3	1.81	0.45
1:M:10:ILE:HB	1:M:73:VAL:HB	1.99	0.45
1:U:120:ASP:OD1	1:U:120:ASP:N	2.47	0.45
1:P:13:ASP:OD1	1:P:66:TYR:OH	2.32	0.45
1:B:76:VAL:HG22	1:B:129:ILE:HG12	1.99	0.45
1:E:152:LYS:HD2	1:E:152:LYS:HA	1.80	0.45
1:J:151:GLU:HG3	1:K:110:ASP:OD2	2.15	0.45
1:Q:90:LEU:HD22	1:Q:116:CYS:HB3	1.99	0.45
1:B:83:VAL:HG22	1:B:87:ARG:HH12	1.81	0.45
1:D:13:ASP:OD1	1:D:66:TYR:OH	2.35	0.45
1:G:3:ASP:OD1	1:G:3:ASP:N	2.49	0.45
1:F:36:ALA:HB1	1:F:133:PHE:CE1	2.52	0.45
1:H:49:GLN:HA	1:H:52:ALA:HB2	1.99	0.45
1:I:13:ASP:OD1	1:I:13:ASP:N	2.50	0.45
1:K:38:LYS:HA	1:L:37:LEU:O	2.16	0.45
1:N:128:GLU:O	1:N:132:TRP:HD1	2.00	0.45
1:V:38:LYS:NZ	1:V:132:TRP:O	2.49	0.45
1:V:55:SER:HA	1:V:60:PHE:CG	2.52	0.45
1:W:83:VAL:HG22	1:W:87:ARG:NH1	2.29	0.45
1:P:38:LYS:HE2	1:P:133:PHE:CE1	2.52	0.45
1:B:87:ARG:HD3	1:B:120:ASP:HA	1.99	0.45
1:M:54:LEU:O	1:M:60:PHE:HB2	2.17	0.45
1:X:60:PHE:HB3	1:X:61:PRO:HD3	1.99	0.45
1:S:46:HIS:HE1	1:S:131:LEU:O	2.00	0.45
1:G:86:GLY:O	1:G:90:LEU:HG	2.17	0.45
1:L:34:LEU:HD21	1:L:37:LEU:HD22	1.99	0.45
1:V:81:GLU:O	1:V:82:VAL:HG12	2.16	0.45
1:B:102:THR:HG22	1:C:100:PRO:HG2	1.99	0.44
1:G:13:ASP:OD1	1:G:13:ASP:N	2.48	0.44
1:H:83:VAL:HG22	1:H:87:ARG:NH1	2.31	0.44
1:U:10:ILE:HB	1:U:73:VAL:HB	1.99	0.44
1:G:47:LEU:HD23	1:G:47:LEU:HA	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:PRO:HG2	1:P:102:THR:HG22	1.98	0.44
1:N:39:LEU:HD11	1:N:71:PRO:HB2	1.99	0.44
1:P:129:ILE:HG21	1:P:138:LEU:HD21	1.99	0.44
1:F:10:ILE:HB	1:F:73:VAL:HB	1.99	0.44
1:W:123:GLU:HG2	1:W:126:LYS:HE3	1.98	0.44
1:D:92:ALA:H	1:D:98:SER:HB3	1.82	0.44
1:G:37:LEU:HD13	1:G:75:MET:HG2	1.99	0.44
1:H:13:ASP:OD1	1:H:13:ASP:N	2.50	0.44
1:U:76:VAL:HG22	1:U:129:ILE:HG12	2.00	0.44
1:W:13:ASP:OD1	1:W:13:ASP:N	2.49	0.44
1:W:66:TYR:O	1:W:69:SER:OG	2.34	0.44
1:V:22:PRO:O	1:V:26:ARG:HG2	2.17	0.44
1:D:55:SER:HA	1:D:60:PHE:CD2	2.52	0.44
1:A:37:LEU:HD21	1:B:37:LEU:HD21	2.00	0.44
1:P:19:LEU:C	1:P:22:PRO:HD2	2.43	0.44
1:J:114:ASN:O	1:J:116:CYS:N	2.50	0.44
1:R:22:PRO:O	1:R:26:ARG:HG2	2.17	0.44
1:W:65:SER:HA	1:W:68:LEU:HG	1.99	0.44
1:X:139:GLN:O	1:X:140:LYS:HE2	2.17	0.44
1:W:37:LEU:O	1:X:38:LYS:HA	2.18	0.44
1:E:37:LEU:O	1:F:38:LYS:HA	2.18	0.43
1:I:3:ASP:OD1	1:I:3:ASP:N	2.51	0.43
1:I:8:ILE:HB	1:I:75:MET:HE3	1.99	0.43
1:Q:120:ASP:HB2	1:Q:124:ASN:HD22	1.83	0.43
1:V:80:ARG:HH22	1:V:150:TYR:CA	2.29	0.43
1:V:110:ASP:OD2	1:T:151:GLU:HG2	2.18	0.43
1:F:55:SER:HA	1:F:60:PHE:CG	2.53	0.43
1:H:152:LYS:HA	1:H:152:LYS:HD3	1.54	0.43
1:W:76:VAL:HG21	1:W:138:LEU:HD21	1.99	0.43
1:X:42:PRO:HG2	1:X:47:LEU:HD21	2.00	0.43
1:S:11:LYS:HE3	1:S:117:HIS:HB2	1.99	0.43
1:V:144:SER:OG	1:X:145:GLN:NE2	2.43	0.43
1:O:26:ARG:HG3	1:O:103:ILE:HD11	2.00	0.43
1:P:83:VAL:CG1	1:P:87:ARG:HH12	2.32	0.43
1:F:80:ARG:HG2	1:F:81:GLU:HG2	2.00	0.43
1:G:36:ALA:HB1	1:G:133:PHE:CE1	2.54	0.43
1:G:38:LYS:HA	1:H:37:LEU:O	2.18	0.43
1:S:13:ASP:OD1	1:S:13:ASP:N	2.51	0.43
1:R:13:ASP:OD1	1:R:13:ASP:N	2.46	0.43
1:A:82:VAL:O	1:A:86:GLY:N	2.40	0.43
1:E:25:SER:OG	1:F:21:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:GLU:HG2	1:G:60:PHE:CZ	2.53	0.43
1:Q:114:ASN:O	1:Q:116:CYS:N	2.47	0.43
1:W:23:ILE:HG12	1:W:103:ILE:HD12	2.00	0.43
1:W:38:LYS:HA	1:X:37:LEU:O	2.19	0.43
1:B:10:ILE:HB	1:B:73:VAL:HB	2.01	0.43
1:C:124:ASN:O	1:C:128:GLU:HG3	2.17	0.43
1:N:26:ARG:HG3	1:N:26:ARG:NH1	2.29	0.43
1:N:43:SER:OG	1:N:45:GLU:OE1	2.37	0.43
1:O:34:LEU:HG	1:P:39:LEU:HD22	1.99	0.43
1:P:67:MET:HE3	1:P:67:MET:HB3	1.93	0.43
1:F:10:ILE:HD13	1:F:20:VAL:HA	2.00	0.43
1:L:36:ALA:HB3	1:L:76:VAL:HG23	2.01	0.43
1:C:11:LYS:HE3	1:C:117:HIS:HB2	2.01	0.43
1:D:76:VAL:HG22	1:D:129:ILE:HG12	2.00	0.43
1:F:90:LEU:HD23	1:F:103:ILE:HD12	2.00	0.43
1:B:124:ASN:O	1:B:128:GLU:HG3	2.18	0.43
1:C:76:VAL:HG22	1:C:129:ILE:HG12	2.00	0.43
1:C:134:LYS:HE3	1:C:135:PRO:HD3	2.00	0.43
1:I:3:ASP:O	1:I:4:GLU:C	2.61	0.43
1:J:10:ILE:HD13	1:J:20:VAL:HA	2.00	0.43
1:J:80:ARG:HG2	1:J:81:GLU:HG3	2.01	0.43
1:W:36:ALA:HB1	1:W:133:PHE:CE1	2.54	0.43
1:E:6:THR:HA	1:E:125:ALA:HB1	2.01	0.42
1:H:39:LEU:HD12	1:H:72:ILE:O	2.18	0.42
1:W:10:ILE:HG12	1:W:23:ILE:HD13	2.00	0.42
1:W:16:GLN:OE1	1:X:144:SER:HB3	2.18	0.42
1:W:108:ALA:HB2	1:W:115:VAL:HG23	2.01	0.42
1:F:102:THR:HG22	1:G:100:PRO:HG2	2.01	0.42
1:G:15:VAL:HG11	1:G:71:PRO:O	2.19	0.42
1:Q:38:LYS:HE2	1:Q:133:PHE:CE1	2.54	0.42
1:X:44:LYS:O	1:X:48:GLU:HB2	2.19	0.42
1:S:90:LEU:HD23	1:S:103:ILE:HD12	2.00	0.42
1:A:90:LEU:HD23	1:A:103:ILE:HD12	2.00	0.42
1:I:37:LEU:O	1:J:38:LYS:HA	2.19	0.42
1:L:55:SER:HA	1:L:60:PHE:CD1	2.54	0.42
1:N:64:VAL:O	1:N:68:LEU:HG	2.20	0.42
1:V:80:ARG:HD3	1:W:109:ILE:HG21	2.00	0.42
1:U:36:ALA:HB2	1:U:138:LEU:HD23	2.02	0.42
1:X:13:ASP:OD1	1:X:14:GLY:N	2.53	0.42
1:F:19:LEU:C	1:F:22:PRO:HD2	2.44	0.42
1:U:148:TRP:CZ2	1:S:16:GLN:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:36:ALA:HB2	1:W:138:LEU:HD23	2.01	0.42
1:A:23:ILE:HD13	1:A:116:CYS:SG	2.59	0.42
1:A:96:LEU:HD21	1:A:109:ILE:HG23	2.00	0.42
1:H:44:LYS:O	1:H:48:GLU:HG3	2.20	0.42
1:Q:136:GLU:CD	1:Q:136:GLU:H	2.27	0.42
1:D:13:ASP:OD1	1:D:13:ASP:N	2.51	0.42
1:L:4:GLU:OE2	1:L:83:VAL:HG12	2.19	0.42
1:R:7:PHE:HB2	1:R:129:ILE:HG13	2.02	0.42
1:B:105:GLY:O	1:M:30:ARG:NH1	2.53	0.42
1:X:46:HIS:HD1	1:X:46:HIS:C	2.27	0.42
1:X:98:SER:HB3	1:X:99:ALA:H	1.56	0.42
1:G:13:ASP:OD1	1:G:66:TYR:OH	2.35	0.42
1:K:141:TYR:CE1	1:L:71:PRO:HG3	2.54	0.42
1:X:90:LEU:HA	1:X:103:ILE:HB	2.00	0.42
1:V:38:LYS:HD3	1:V:137:GLU:OE1	2.20	0.41
1:G:4:GLU:O	1:G:78:GLU:HG3	2.20	0.41
1:G:37:LEU:O	1:H:38:LYS:HA	2.19	0.41
1:Q:80:ARG:HG3	1:Q:80:ARG:HH11	1.86	0.41
1:O:25:SER:OG	1:P:21:GLY:HA3	2.19	0.41
1:B:19:LEU:C	1:B:22:PRO:HD2	2.45	0.41
1:U:23:ILE:HD13	1:U:116:CYS:SG	2.60	0.41
1:W:34:LEU:HD21	1:W:37:LEU:HD22	2.03	0.41
1:T:59:PHE:CD1	1:T:59:PHE:C	2.99	0.41
1:B:26:ARG:NH2	1:B:106:ASP:OD2	2.52	0.41
1:H:94:ASN:HA	1:H:111:VAL:HG22	2.02	0.41
1:L:55:SER:O	1:L:57:LYS:N	2.53	0.41
1:W:57:LYS:HG3	1:W:58:PRO:HD2	2.01	0.41
1:W:83:VAL:HG11	1:W:122:VAL:HG22	2.02	0.41
1:D:1:MET:SD	1:D:152:LYS:NZ	2.94	0.41
1:D:8:ILE:HB	1:D:75:MET:HE3	2.02	0.41
1:Q:71:PRO:HG3	1:R:141:TYR:CE1	2.55	0.41
1:U:16:GLN:HG3	1:X:148:TRP:CE2	2.55	0.41
1:V:51:TYR:CE2	1:V:63:LEU:HD11	2.55	0.41
1:W:49:GLN:HG3	1:W:52:ALA:HB2	2.02	0.41
1:T:114:ASN:O	1:T:115:VAL:HG12	2.21	0.41
1:G:68:LEU:HA	1:G:68:LEU:HD12	1.57	0.41
1:O:38:LYS:HE2	1:O:133:PHE:CE1	2.55	0.41
1:S:46:HIS:CE1	1:S:131:LEU:HG	2.55	0.41
1:B:13:ASP:OD1	1:B:66:TYR:OH	2.27	0.41
1:B:47:LEU:HD12	1:B:68:LEU:HD12	2.03	0.41
1:V:80:ARG:H	1:V:80:ARG:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:67:MET:HG3	1:X:72:ILE:HD11	2.01	0.41
1:C:148:TRP:CZ2	1:M:16:GLN:HG3	2.56	0.41
1:D:6:THR:OG1	1:D:83:VAL:HG23	2.21	0.41
1:E:6:THR:OG1	1:E:83:VAL:HG23	2.20	0.41
1:F:30:ARG:NH1	1:G:105:GLY:O	2.53	0.41
1:G:33:LYS:HB3	1:G:33:LYS:HE2	1.85	0.41
1:G:39:LEU:HD11	1:G:71:PRO:HB2	2.02	0.41
1:L:11:LYS:HE3	1:L:117:HIS:HB2	2.02	0.41
1:L:36:ALA:HB2	1:L:138:LEU:HD23	2.02	0.41
1:N:44:LYS:O	1:N:48:GLU:HG2	2.21	0.41
1:R:11:LYS:HE3	1:R:117:HIS:HB2	2.03	0.41
1:V:93:THR:O	1:V:111:VAL:HG23	2.20	0.41
1:O:93:THR:O	1:O:95:PRO:HD3	2.20	0.41
1:D:66:TYR:O	1:D:69:SER:OG	2.33	0.41
1:G:83:VAL:HG11	1:G:122:VAL:CG1	2.51	0.41
1:G:83:VAL:HG21	1:G:121:SER:C	2.46	0.41
1:L:44:LYS:O	1:L:48:GLU:HG3	2.21	0.41
1:M:2:SER:CB	1:M:152:LYS:NZ	2.68	0.41
1:X:100:PRO:HG2	1:S:102:THR:HG22	2.03	0.41
1:T:1:MET:O	1:T:3:ASP:N	2.44	0.41
1:M:76:VAL:HG22	1:M:129:ILE:HG12	2.03	0.40
1:R:80:ARG:HH12	1:R:152:LYS:NZ	2.18	0.40
1:B:80:ARG:HH21	1:C:110:ASP:CG	2.28	0.40
1:F:96:LEU:HD23	1:F:96:LEU:HA	1.86	0.40
1:G:60:PHE:O	1:G:64:VAL:HG23	2.22	0.40
1:X:114:ASN:O	1:X:116:CYS:N	2.53	0.40
1:E:119:SER:OG	1:E:125:ALA:HA	2.21	0.40
1:M:60:PHE:HB3	1:M:61:PRO:HD3	2.02	0.40
1:Q:30:ARG:O	1:Q:30:ARG:HG3	2.22	0.40
1:G:54:LEU:HD23	1:G:59:PHE:HE1	1.87	0.40
1:W:4:GLU:OE2	1:W:83:VAL:HG12	2.22	0.40
1:X:139:GLN:C	1:X:140:LYS:HE2	2.46	0.40
1:O:39:LEU:HG	1:P:139:GLN:HG3	2.03	0.40
1:C:134:LYS:HE3	1:C:134:LYS:HA	2.04	0.40
1:H:114:ASN:O	1:H:116:CYS:N	2.49	0.40
1:N:76:VAL:HG22	1:N:129:ILE:HG12	2.04	0.40
1:V:10:ILE:HD13	1:V:20:VAL:HA	2.02	0.40
1:P:55:SER:HA	1:P:60:PHE:CG	2.57	0.40
1:P:124:ASN:HA	1:P:127:LYS:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:43:SER:OG	1:X:136:GLU:OE1[2_456]	2.06	0.14

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	150/155 (97%)	145 (97%)	4 (3%)	1 (1%)	18	17
1	B	149/155 (96%)	143 (96%)	5 (3%)	1 (1%)	18	17
1	C	148/155 (96%)	141 (95%)	5 (3%)	2 (1%)	9	6
1	D	150/155 (97%)	145 (97%)	4 (3%)	1 (1%)	18	17
1	E	149/155 (96%)	146 (98%)	2 (1%)	1 (1%)	18	17
1	F	148/155 (96%)	142 (96%)	5 (3%)	1 (1%)	18	17
1	G	148/155 (96%)	141 (95%)	5 (3%)	2 (1%)	9	6
1	H	149/155 (96%)	142 (95%)	6 (4%)	1 (1%)	18	17
1	I	150/155 (97%)	143 (95%)	4 (3%)	3 (2%)	6	3
1	J	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	17
1	K	150/155 (97%)	146 (97%)	3 (2%)	1 (1%)	18	17
1	L	149/155 (96%)	139 (93%)	8 (5%)	2 (1%)	9	7
1	M	150/155 (97%)	146 (97%)	3 (2%)	1 (1%)	18	17
1	N	135/155 (87%)	132 (98%)	2 (2%)	1 (1%)	18	17
1	O	150/155 (97%)	147 (98%)	3 (2%)	0	100	100
1	P	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	9	6
1	Q	150/155 (97%)	147 (98%)	2 (1%)	1 (1%)	18	17
1	R	150/155 (97%)	144 (96%)	5 (3%)	1 (1%)	18	17
1	S	147/155 (95%)	140 (95%)	5 (3%)	2 (1%)	9	6
1	T	150/155 (97%)	144 (96%)	4 (3%)	2 (1%)	9	7
1	U	146/155 (94%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	148/155 (96%)	141 (95%)	4 (3%)	3 (2%)	6	3
1	W	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	18	17
1	X	148/155 (96%)	134 (90%)	10 (7%)	4 (3%)	4	2
All	All	3558/3720 (96%)	3408 (96%)	115 (3%)	35 (1%)	12	10

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	B	115	VAL
1	C	3	ASP
1	C	115	VAL
1	D	115	VAL
1	G	115	VAL
1	I	4	GLU
1	I	115	VAL
1	L	56	SER
1	R	115	VAL
1	V	115	VAL
1	S	58	PRO
1	E	115	VAL
1	F	115	VAL
1	I	5	GLN
1	L	115	VAL
1	Q	115	VAL
1	P	59	PHE
1	P	115	VAL
1	S	115	VAL
1	T	59	PHE
1	V	80	ARG
1	X	98	SER
1	X	115	VAL
1	X	138	LEU
1	J	115	VAL
1	K	115	VAL
1	V	82	VAL
1	X	99	ALA
1	T	115	VAL
1	G	4	GLU
1	H	115	VAL
1	M	115	VAL

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Mol	Chain	Res	Type
1	W	115	VAL
1	N	115	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	126/129 (98%)	126 (100%)	0	100	100
1	B	126/129 (98%)	126 (100%)	0	100	100
1	C	126/129 (98%)	126 (100%)	0	100	100
1	D	128/129 (99%)	127 (99%)	1 (1%)	73	83
1	E	127/129 (98%)	127 (100%)	0	100	100
1	F	126/129 (98%)	125 (99%)	1 (1%)	73	83
1	G	124/129 (96%)	124 (100%)	0	100	100
1	H	126/129 (98%)	126 (100%)	0	100	100
1	I	128/129 (99%)	128 (100%)	0	100	100
1	J	126/129 (98%)	126 (100%)	0	100	100
1	K	126/129 (98%)	126 (100%)	0	100	100
1	L	123/129 (95%)	123 (100%)	0	100	100
1	M	128/129 (99%)	127 (99%)	1 (1%)	73	83
1	N	116/129 (90%)	116 (100%)	0	100	100
1	O	128/129 (99%)	128 (100%)	0	100	100
1	P	126/129 (98%)	126 (100%)	0	100	100
1	Q	128/129 (99%)	128 (100%)	0	100	100
1	R	128/129 (99%)	128 (100%)	0	100	100
1	S	125/129 (97%)	125 (100%)	0	100	100
1	T	128/129 (99%)	128 (100%)	0	100	100
1	U	126/129 (98%)	126 (100%)	0	100	100
1	V	124/129 (96%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	126/129 (98%)	125 (99%)	1 (1%)	73	83
1	X	126/129 (98%)	126 (100%)	0	100	100
All	All	3021/3096 (98%)	3017 (100%)	4 (0%)	88	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	111	VAL
1	F	119	SER
1	M	2	SER
1	W	75	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	94	ASN
1	I	46	HIS
1	J	117	HIS
1	K	5	GLN
1	M	5	GLN
1	M	49	GLN
1	M	145	GLN
1	N	124	ASN
1	Q	49	GLN
1	W	145	GLN
1	X	117	HIS
1	X	124	ASN
1	X	145	GLN
1	O	5	GLN
1	O	94	ASN
1	P	46	HIS
1	S	5	GLN
1	S	46	HIS
1	S	124	ASN
1	T	46	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	152/155 (98%)	0.58	5 (3%)	49	48	33, 42, 57, 62	0
1	B	151/155 (97%)	0.61	14 (9%)	14	13	33, 43, 66, 81	0
1	C	150/155 (96%)	0.75	12 (8%)	18	17	33, 44, 65, 78	0
1	D	152/155 (98%)	0.90	17 (11%)	10	9	33, 47, 78, 93	0
1	E	151/155 (97%)	0.57	11 (7%)	21	20	30, 40, 55, 66	0
1	F	150/155 (96%)	0.41	4 (2%)	56	55	28, 40, 54, 64	0
1	G	150/155 (96%)	1.60	53 (35%)	1	1	36, 52, 72, 83	0
1	H	151/155 (97%)	1.63	46 (30%)	1	1	38, 55, 93, 99	0
1	I	152/155 (98%)	0.55	7 (4%)	37	36	33, 43, 52, 61	0
1	J	150/155 (96%)	0.66	5 (3%)	49	48	33, 45, 63, 87	0
1	K	152/155 (98%)	0.67	9 (5%)	28	27	30, 43, 54, 61	0
1	L	151/155 (97%)	1.10	23 (15%)	5	4	33, 47, 83, 105	0
1	M	152/155 (98%)	0.60	9 (5%)	28	27	32, 41, 52, 58	0
1	N	139/155 (89%)	1.07	19 (13%)	6	6	32, 49, 94, 115	0
1	O	152/155 (98%)	1.03	21 (13%)	6	6	32, 46, 67, 78	0
1	P	150/155 (96%)	1.26	36 (24%)	2	1	33, 54, 70, 81	0
1	Q	152/155 (98%)	0.49	4 (2%)	57	56	33, 41, 54, 60	0
1	R	152/155 (98%)	0.66	11 (7%)	21	21	32, 45, 61, 69	0
1	S	149/155 (96%)	0.70	13 (8%)	16	15	32, 45, 60, 74	0
1	T	152/155 (98%)	0.82	14 (9%)	14	13	34, 46, 62, 77	0
1	U	150/155 (96%)	1.10	20 (13%)	7	6	33, 45, 63, 154	0
1	V	150/155 (96%)	1.30	33 (22%)	2	2	38, 55, 71, 78	0
1	W	150/155 (96%)	2.13	70 (46%)	0	0	45, 60, 106, 123	0
1	X	150/155 (96%)	2.33	82 (54%)	0	0	44, 59, 91, 107	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3610/3720 (97%)	0.98	538 (14%) 5 5	28, 46, 71, 154	0

All (538) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	58	PRO	11.3
1	X	59	PHE	8.5
1	H	54	LEU	8.2
1	N	63	LEU	7.3
1	U	59	PHE	7.1
1	D	59	PHE	6.7
1	J	59	PHE	6.6
1	N	64	VAL	6.5
1	L	54	LEU	6.3
1	R	59	PHE	6.0
1	L	53	ASP	6.0
1	L	55	SER	5.9
1	N	62	GLY	5.8
1	X	60	PHE	5.6
1	D	57	LYS	5.6
1	V	58	PRO	5.4
1	U	60	PHE	5.3
1	W	2	SER	5.2
1	L	66	TYR	5.2
1	U	55	SER	5.1
1	X	133	PHE	5.1
1	X	58	PRO	5.0
1	D	58	PRO	4.9
1	L	60	PHE	4.8
1	U	61	PRO	4.8
1	L	62	GLY	4.8
1	L	56	SER	4.7
1	W	8	ILE	4.7
1	N	46	HIS	4.7
1	N	50	HIS	4.7
1	G	68	LEU	4.7
1	X	56	SER	4.6
1	X	63	LEU	4.6
1	W	61	PRO	4.6
1	D	54	LEU	4.5
1	G	56	SER	4.5
1	E	2	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	59	PHE	4.5
1	T	58	PRO	4.5
1	X	54	LEU	4.5
1	H	42	PRO	4.4
1	W	47	LEU	4.4
1	T	59	PHE	4.4
1	X	64	VAL	4.4
1	X	134	LYS	4.4
1	N	66	TYR	4.4
1	C	2	SER	4.3
1	W	59	PHE	4.3
1	X	74	ALA	4.3
1	X	98	SER	4.3
1	W	52	ALA	4.3
1	P	58	PRO	4.3
1	W	54	LEU	4.2
1	X	83	VAL	4.2
1	K	1	MET	4.1
1	X	51	TYR	4.1
1	W	131	LEU	4.1
1	X	47	LEU	4.1
1	X	65	SER	4.1
1	G	133	PHE	4.1
1	W	83	VAL	4.1
1	W	62	GLY	4.0
1	X	127	LYS	4.0
1	G	135	PRO	4.0
1	X	131	LEU	4.0
1	L	61	PRO	4.0
1	N	68	LEU	3.9
1	X	111	VAL	3.9
1	H	56	SER	3.9
1	H	47	LEU	3.9
1	X	61	PRO	3.9
1	G	79	GLY	3.9
1	H	65	SER	3.9
1	G	47	LEU	3.9
1	X	68	LEU	3.9
1	X	55	SER	3.8
1	N	47	LEU	3.8
1	H	58	PRO	3.8
1	W	135	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	152	LYS	3.8
1	O	116	CYS	3.8
1	X	88	THR	3.8
1	H	60	PHE	3.8
1	X	42	PRO	3.8
1	G	122	VAL	3.8
1	X	73	VAL	3.8
1	T	1	MET	3.8
1	W	40	CYS	3.7
1	P	151	GLU	3.7
1	W	9	ALA	3.7
1	O	61	PRO	3.7
1	S	151	GLU	3.7
1	W	37	LEU	3.7
1	B	58	PRO	3.7
1	W	53	ASP	3.7
1	H	62	GLY	3.6
1	X	72	ILE	3.6
1	H	125	ALA	3.6
1	D	61	PRO	3.6
1	H	63	LEU	3.6
1	V	116	CYS	3.6
1	O	66	TYR	3.6
1	S	148	TRP	3.6
1	X	52	ALA	3.6
1	G	58	PRO	3.6
1	W	51	TYR	3.6
1	V	127	LYS	3.5
1	W	68	LEU	3.5
1	H	152	LYS	3.5
1	V	152	LYS	3.5
1	P	59	PHE	3.5
1	L	63	LEU	3.5
1	N	43	SER	3.5
1	H	116	CYS	3.5
1	P	150	TYR	3.5
1	L	58	PRO	3.4
1	H	59	PHE	3.4
1	V	122	VAL	3.4
1	O	58	PRO	3.4
1	K	65	SER	3.4
1	V	148	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	148	TRP	3.4
1	H	138	LEU	3.4
1	X	6	THR	3.4
1	T	56	SER	3.4
1	L	123	GLU	3.4
1	H	122	VAL	3.4
1	V	83	VAL	3.4
1	W	58	PRO	3.4
1	W	44	LYS	3.4
1	G	52	ALA	3.4
1	V	80	ARG	3.3
1	J	57	LYS	3.3
1	H	55	SER	3.3
1	L	83	VAL	3.3
1	L	52	ALA	3.3
1	O	55	SER	3.3
1	W	50	HIS	3.3
1	X	122	VAL	3.3
1	X	9	ALA	3.3
1	D	60	PHE	3.3
1	H	57	LYS	3.3
1	N	49	GLN	3.3
1	H	46	HIS	3.2
1	J	58	PRO	3.2
1	G	51	TYR	3.2
1	W	74	ALA	3.2
1	N	2	SER	3.2
1	V	81	GLU	3.2
1	C	56	SER	3.2
1	W	56	SER	3.2
1	W	121	SER	3.2
1	X	135	PRO	3.2
1	L	57	LYS	3.2
1	O	152	LYS	3.2
1	G	138	LEU	3.2
1	X	8	ILE	3.2
1	I	3	ASP	3.2
1	X	117	HIS	3.2
1	O	62	GLY	3.2
1	P	140	LYS	3.2
1	F	116	CYS	3.2
1	U	66	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	152	LYS	3.1
1	G	37	LEU	3.1
1	W	63	LEU	3.1
1	X	66	TYR	3.1
1	B	152	LYS	3.1
1	P	57	LYS	3.1
1	P	142	LYS	3.1
1	L	64	VAL	3.1
1	P	83	VAL	3.1
1	D	56	SER	3.1
1	H	51	TYR	3.1
1	G	143	HIS	3.1
1	X	36	ALA	3.1
1	G	134	LYS	3.1
1	X	3	ASP	3.0
1	W	73	VAL	3.0
1	T	65	SER	3.0
1	X	112	GLY	3.0
1	G	60	PHE	3.0
1	O	59	PHE	3.0
1	C	3	ASP	3.0
1	P	126	LYS	3.0
1	W	138	LEU	3.0
1	X	138	LEU	3.0
1	H	135	PRO	3.0
1	W	132	TRP	3.0
1	T	66	TYR	3.0
1	R	152	LYS	3.0
1	M	65	SER	3.0
1	G	83	VAL	3.0
1	H	131	LEU	3.0
1	W	76	VAL	3.0
1	X	39	LEU	3.0
1	V	149	ILE	3.0
1	X	62	GLY	3.0
1	B	66	TYR	3.0
1	W	49	GLN	2.9
1	H	130	ALA	2.9
1	M	2	SER	2.9
1	T	52	ALA	2.9
1	W	46	HIS	2.9
1	B	123	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	2	SER	2.9
1	W	35	ALA	2.9
1	G	126	LYS	2.9
1	X	116	CYS	2.9
1	H	111	VAL	2.9
1	C	93	THR	2.9
1	X	95	PRO	2.9
1	H	134	LYS	2.9
1	C	83	VAL	2.9
1	H	53	ASP	2.9
1	W	16	GLN	2.9
1	G	45	GLU	2.9
1	V	126	LYS	2.9
1	W	43	SER	2.9
1	H	52	ALA	2.9
1	D	63	LEU	2.8
1	X	147	ASP	2.8
1	P	147	ASP	2.8
1	L	93	THR	2.8
1	C	151	GLU	2.8
1	F	2	SER	2.8
1	B	60	PHE	2.8
1	X	7	PHE	2.8
1	G	131	LEU	2.8
1	X	123	GLU	2.8
1	R	83	VAL	2.8
1	D	55	SER	2.8
1	H	49	GLN	2.8
1	E	59	PHE	2.8
1	F	3	ASP	2.8
1	J	53	ASP	2.8
1	X	79	GLY	2.8
1	A	123	GLU	2.8
1	G	130	ALA	2.8
1	O	108	ALA	2.8
1	W	41	SER	2.8
1	G	50	HIS	2.8
1	N	48	GLU	2.8
1	S	79	GLY	2.8
1	W	72	ILE	2.8
1	X	77	TRP	2.8
1	R	120	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	W	105	GLY	2.7
1	X	125	ALA	2.7
1	D	96	LEU	2.7
1	W	93	THR	2.7
1	X	12	PRO	2.7
1	S	80	ARG	2.7
1	D	83	VAL	2.7
1	H	83	VAL	2.7
1	W	129	ILE	2.7
1	B	2	SER	2.7
1	G	41	SER	2.7
1	X	75	MET	2.7
1	I	4	GLU	2.7
1	E	152	LYS	2.7
1	V	84	LYS	2.7
1	X	57	LYS	2.7
1	K	60	PHE	2.7
1	X	37	LEU	2.7
1	W	66	TYR	2.7
1	X	141	TYR	2.7
1	P	66	TYR	2.7
1	E	83	VAL	2.7
1	R	1	MET	2.7
1	U	1	MET	2.7
1	X	50	HIS	2.7
1	R	116	CYS	2.7
1	X	129	ILE	2.7
1	X	149	ILE	2.7
1	W	42	PRO	2.7
1	I	1	MET	2.7
1	G	2	SER	2.7
1	H	69	SER	2.7
1	U	65	SER	2.7
1	G	129	ILE	2.7
1	Q	152	LYS	2.7
1	P	146	PHE	2.6
1	P	61	PRO	2.6
1	D	66	TYR	2.6
1	X	53	ASP	2.6
1	P	51	TYR	2.6
1	B	83	VAL	2.6
1	W	111	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	X	130	ALA	2.6
1	W	60	PHE	2.6
1	L	65	SER	2.6
1	U	152	LYS	2.6
1	V	140	LYS	2.6
1	W	55	SER	2.6
1	T	57	LYS	2.6
1	U	83	VAL	2.6
1	G	62	GLY	2.6
1	U	52	ALA	2.6
1	V	9	ALA	2.6
1	B	53	ASP	2.6
1	C	54	LEU	2.6
1	G	42	PRO	2.6
1	H	126	LYS	2.6
1	N	65	SER	2.6
1	V	98	SER	2.6
1	W	133	PHE	2.6
1	O	56	SER	2.6
1	T	83	VAL	2.6
1	H	117	HIS	2.6
1	H	36	ALA	2.6
1	S	120	ASP	2.6
1	I	123	GLU	2.5
1	X	78	GLU	2.5
1	P	64	VAL	2.5
1	M	66	TYR	2.5
1	L	1	MET	2.5
1	S	116	CYS	2.5
1	G	95	PRO	2.5
1	R	52	ALA	2.5
1	W	88	THR	2.5
1	P	130	ALA	2.5
1	O	65	SER	2.5
1	V	96	LEU	2.5
1	H	64	VAL	2.5
1	I	66	TYR	2.5
1	N	44	LYS	2.5
1	D	53	ASP	2.5
1	W	6	THR	2.5
1	E	65	SER	2.5
1	V	4	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	43	SER	2.5
1	W	96	LEU	2.5
1	B	59	PHE	2.5
1	V	32	PHE	2.5
1	M	152	LYS	2.5
1	S	84	LYS	2.5
1	A	83	VAL	2.5
1	G	64	VAL	2.5
1	G	82	VAL	2.5
1	G	3	ASP	2.5
1	W	48	GLU	2.5
1	X	49	GLN	2.5
1	P	78	GLU	2.5
1	S	123	GLU	2.5
1	A	152	LYS	2.5
1	X	152	LYS	2.5
1	P	77	TRP	2.5
1	D	111	VAL	2.4
1	X	76	VAL	2.4
1	G	136	GLU	2.4
1	X	13	ASP	2.4
1	G	66	TYR	2.4
1	G	116	CYS	2.4
1	G	61	PRO	2.4
1	B	57	LYS	2.4
1	G	146	PHE	2.4
1	W	31	GLY	2.4
1	W	79	GLY	2.4
1	P	119	SER	2.4
1	H	127	LYS	2.4
1	K	152	LYS	2.4
1	X	45	GLU	2.4
1	P	123	GLU	2.4
1	W	82	VAL	2.4
1	M	1	MET	2.4
1	C	134	LYS	2.4
1	H	44	LYS	2.4
1	X	142	LYS	2.4
1	G	35	ALA	2.4
1	H	90	LEU	2.4
1	H	96	LEU	2.4
1	L	45	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	W	45	GLU	2.4
1	G	53	ASP	2.4
1	U	110	ASP	2.4
1	V	147	ASP	2.4
1	W	120	ASP	2.4
1	O	111	VAL	2.4
1	C	140	LYS	2.4
1	P	98	SER	2.4
1	L	51	TYR	2.3
1	H	123	GLU	2.3
1	G	54	LEU	2.3
1	W	34	LEU	2.3
1	P	3	ASP	2.3
1	D	1	MET	2.3
1	K	56	SER	2.3
1	V	82	VAL	2.3
1	W	64	VAL	2.3
1	W	98	SER	2.3
1	X	82	VAL	2.3
1	G	6	THR	2.3
1	X	85	THR	2.3
1	E	116	CYS	2.3
1	R	123	GLU	2.3
1	L	49	GLN	2.3
1	X	148	TRP	2.3
1	G	96	LEU	2.3
1	K	63	LEU	2.3
1	V	79	GLY	2.3
1	X	44	LYS	2.3
1	E	56	SER	2.3
1	G	144	SER	2.3
1	O	46	HIS	2.3
1	N	122	VAL	2.3
1	W	15	VAL	2.3
1	O	64	VAL	2.3
1	S	83	VAL	2.3
1	X	97	ALA	2.3
1	E	66	TYR	2.3
1	R	66	TYR	2.3
1	W	39	LEU	2.3
1	P	26	ARG	2.3
1	X	41	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	48	GLU	2.3
1	V	49	GLN	2.3
1	T	115	VAL	2.3
1	B	52	ALA	2.3
1	B	125	ALA	2.3
1	D	52	ALA	2.3
1	G	33	LYS	2.3
1	W	140	LYS	2.3
1	P	54	LEU	2.3
1	G	151	GLU	2.2
1	P	60	PHE	2.2
1	I	83	VAL	2.2
1	U	12	PRO	2.2
1	H	84	LYS	2.2
1	O	57	LYS	2.2
1	A	1	MET	2.2
1	B	116	CYS	2.2
1	Q	1	MET	2.2
1	Q	130	ALA	2.2
1	U	116	CYS	2.2
1	W	92	ALA	2.2
1	P	86	GLY	2.2
1	T	63	LEU	2.2
1	G	141	TYR	2.2
1	N	123	GLU	2.2
1	W	123	GLU	2.2
1	W	137	GLU	2.2
1	O	51	TYR	2.2
1	G	148	TRP	2.2
1	G	55	SER	2.2
1	G	59	PHE	2.2
1	G	57	LYS	2.2
1	H	76	VAL	2.2
1	K	111	VAL	2.2
1	P	135	PRO	2.2
1	D	116	CYS	2.2
1	H	151	GLU	2.2
1	S	136	GLU	2.2
1	P	138	LEU	2.2
1	G	46	HIS	2.2
1	S	150	TYR	2.2
1	W	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	124	ASN	2.2
1	E	53	ASP	2.2
1	U	3	ASP	2.2
1	M	83	VAL	2.2
1	W	122	VAL	2.2
1	P	118	GLY	2.2
1	T	123	GLU	2.2
1	V	99	ALA	2.2
1	K	116	CYS	2.2
1	B	55	SER	2.2
1	W	75	MET	2.2
1	V	3	ASP	2.2
1	V	85	THR	2.2
1	V	123	GLU	2.1
1	X	103	ILE	2.1
1	R	122	VAL	2.1
1	U	111	VAL	2.1
1	U	62	GLY	2.1
1	M	63	LEU	2.1
1	X	96	LEU	2.1
1	S	54	LEU	2.1
1	G	119	SER	2.1
1	M	98	SER	2.1
1	N	84	LYS	2.1
1	H	66	TYR	2.1
1	O	94	ASN	2.1
1	U	93	THR	2.1
1	K	59	PHE	2.1
1	V	59	PHE	2.1
1	P	149	ILE	2.1
1	A	62	GLY	2.1
1	J	83	VAL	2.1
1	L	130	ALA	2.1
1	G	63	LEU	2.1
1	X	40	CYS	2.1
1	X	124	ASN	2.1
1	X	150	TYR	2.1
1	V	102	THR	2.1
1	E	62	GLY	2.1
1	X	80	ARG	2.1
1	P	129	ILE	2.1
1	O	60	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	122	VAL	2.1
1	W	108	ALA	2.1
1	V	90	LEU	2.1
1	V	121	SER	2.1
1	V	138	LEU	2.1
1	O	41	SER	2.1
1	N	151	GLU	2.1
1	R	124	ASN	2.1
1	X	139	GLN	2.1
1	C	66	TYR	2.1
1	W	141	TYR	2.1
1	X	143	HIS	2.1
1	C	57	LYS	2.1
1	G	4	GLU	2.0
1	V	119	SER	2.1
1	P	65	SER	2.1
1	S	25	SER	2.1
1	H	40	CYS	2.0
1	N	80	ARG	2.0
1	H	50	HIS	2.0
1	C	58	PRO	2.0
1	E	61	PRO	2.0
1	X	38	LYS	2.0
1	V	31	GLY	2.0
1	U	109	ILE	2.0
1	O	109	ILE	2.0
1	Q	136	GLU	2.0
1	T	64	VAL	2.0
1	X	69	SER	2.0
1	T	55	SER	2.0
1	F	148	TRP	2.0
1	G	74	ALA	2.0
1	H	97	ALA	2.0
1	U	92	ALA	2.0
1	W	36	ALA	2.0
1	W	77	TRP	2.0
1	M	96	LEU	2.0
1	O	54	LEU	2.0
1	P	90	LEU	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 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.