Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 06:39 PM JST

PDB ID	:	6K3H
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:

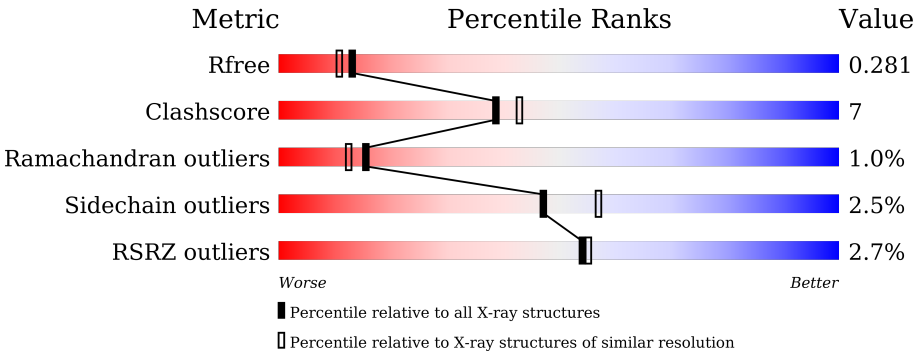
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 <=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	85% 14%
1	B	155	81% 15%
1	C	155	76% 19%
1	D	155	81% 15%
1	E	155	89% 8%
1	F	155	75% 21%

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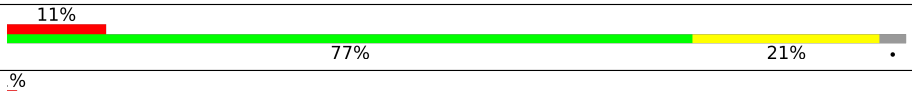
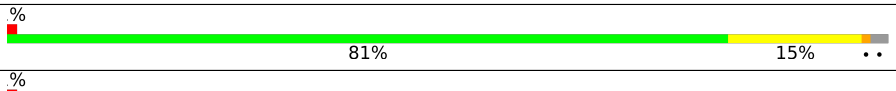
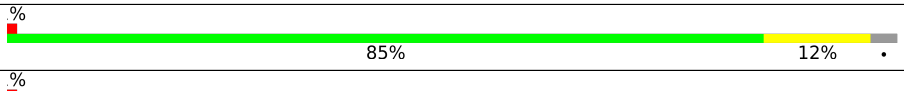
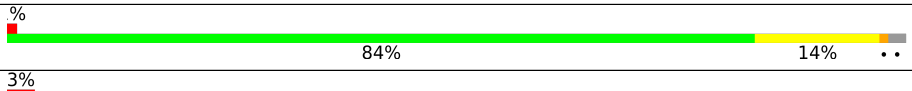
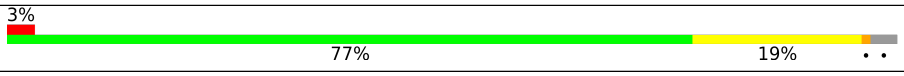
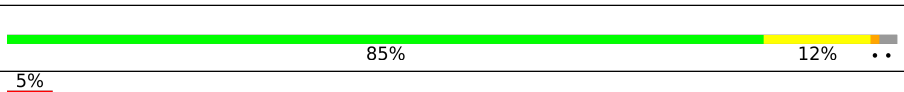
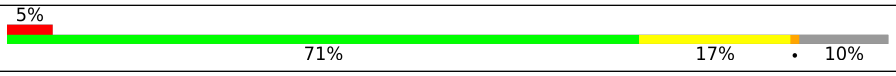
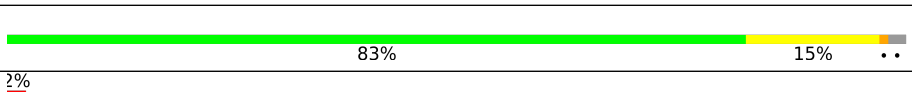
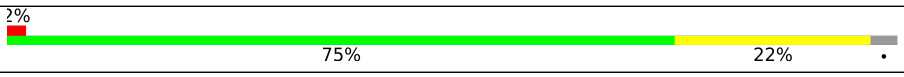
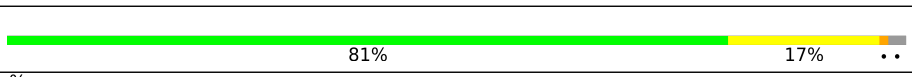
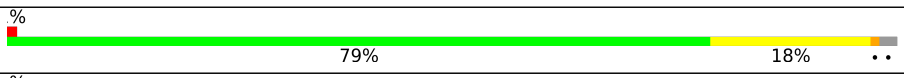
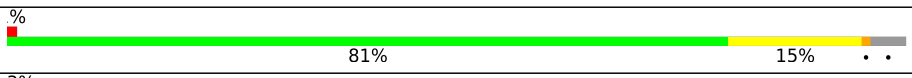
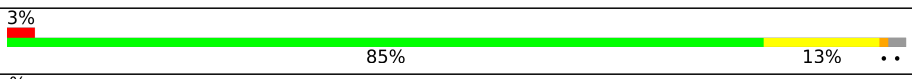
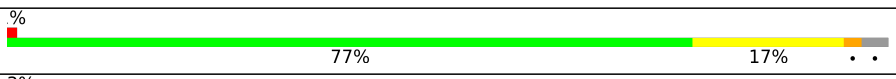
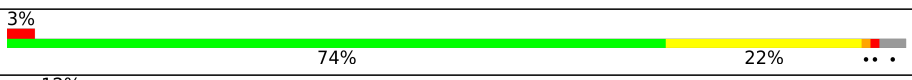
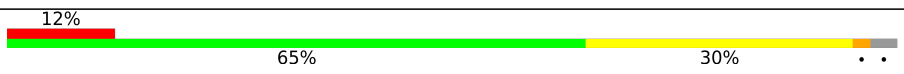
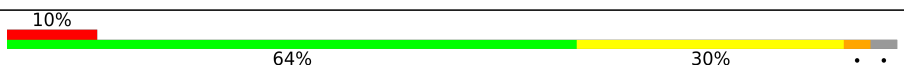
Mol	Chain	Length	Quality of chain
1	G	155	
1	H	155	
1	I	155	
1	J	155	
1	K	155	
1	L	155	
1	M	155	
1	N	155	
1	O	155	
1	P	155	
1	Q	155	
1	R	155	
1	S	155	
1	T	155	
1	U	155	
1	V	155	
1	W	155	
1	X	155	

2 Entry composition (i)

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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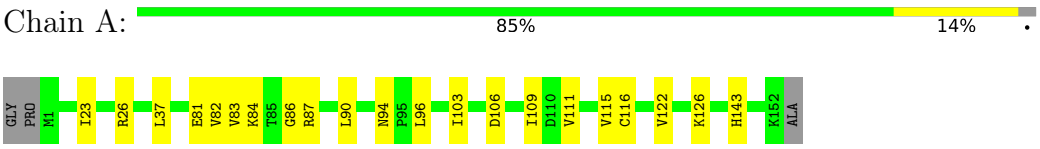
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	PRO	-	expression tag	UNP B8NQF0
M	-1	GLY	-	expression tag	UNP B8NQF0
M	0	PRO	-	expression tag	UNP B8NQF0
N	-1	GLY	-	expression tag	UNP B8NQF0
N	0	PRO	-	expression tag	UNP B8NQF0
Q	-1	GLY	-	expression tag	UNP B8NQF0
Q	0	PRO	-	expression tag	UNP B8NQF0
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.

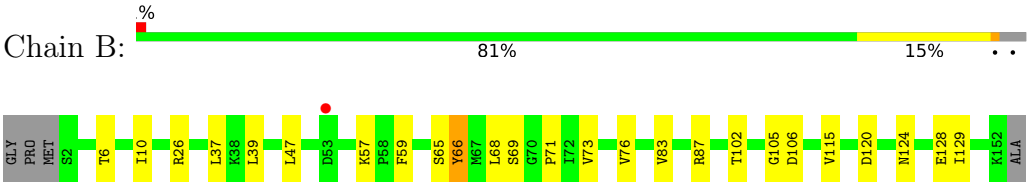
• Molecule 1: Nucleoside diphosphate kinase

Chain A:



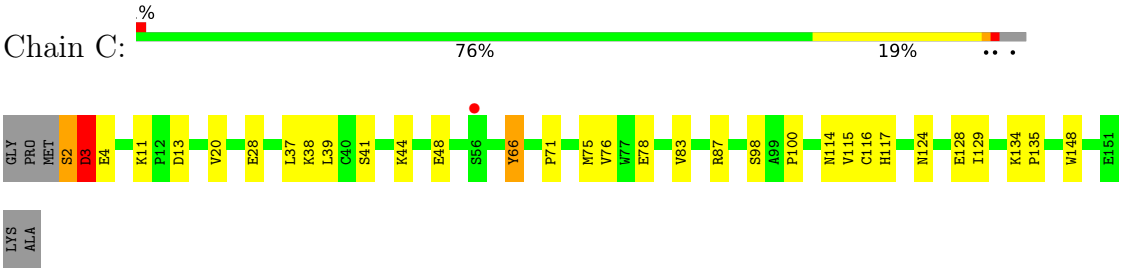
• Molecule 1: Nucleoside diphosphate kinase

Chain B:



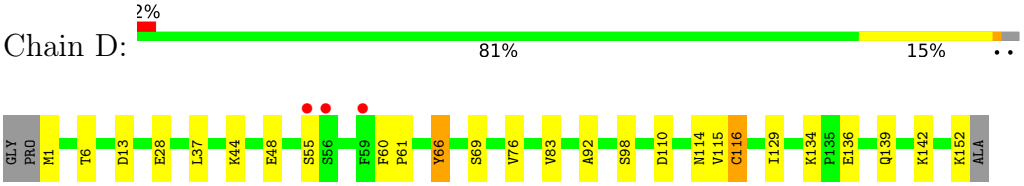
• Molecule 1: Nucleoside diphosphate kinase

Chain C:



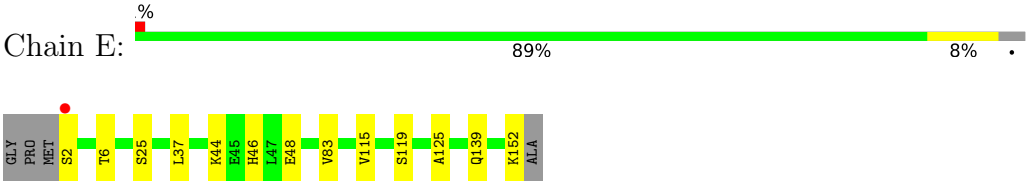
• Molecule 1: Nucleoside diphosphate kinase

Chain D:



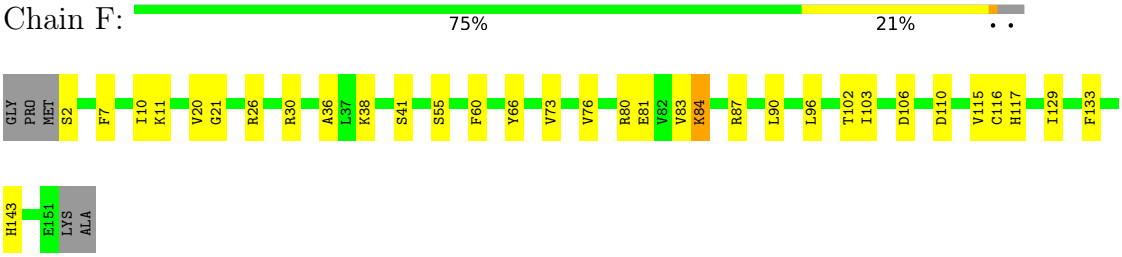
• Molecule 1: Nucleoside diphosphate kinase

Chain E:



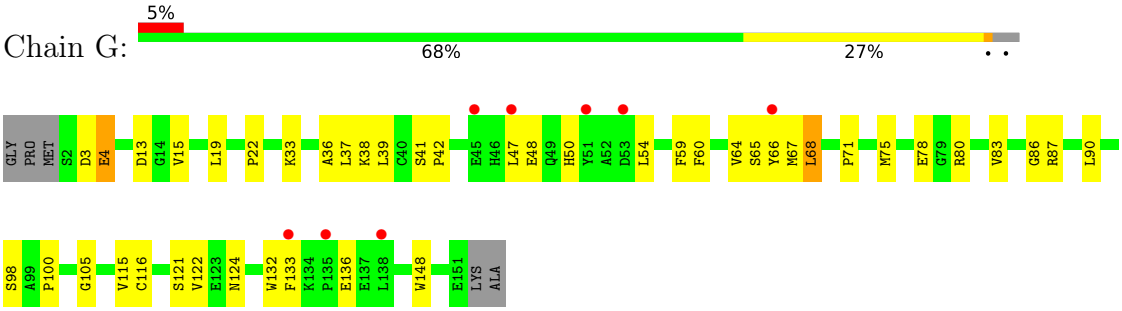
• Molecule 1: Nucleoside diphosphate kinase

Chain F:



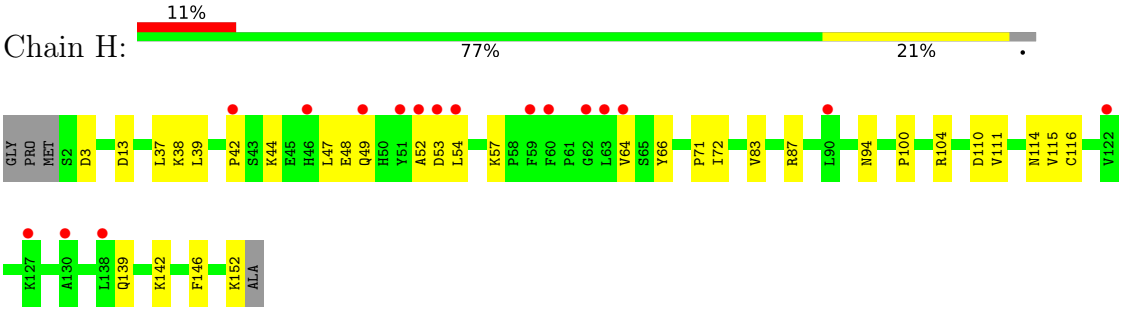
• Molecule 1: Nucleoside diphosphate kinase

Chain G:



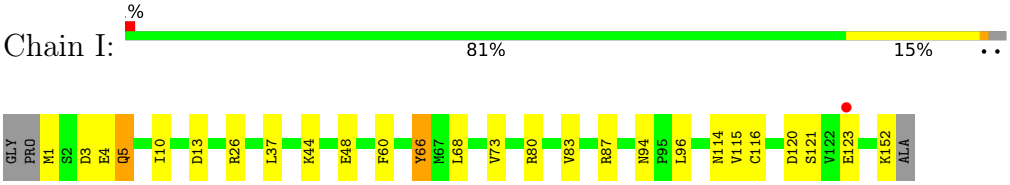
• Molecule 1: Nucleoside diphosphate kinase

Chain H:



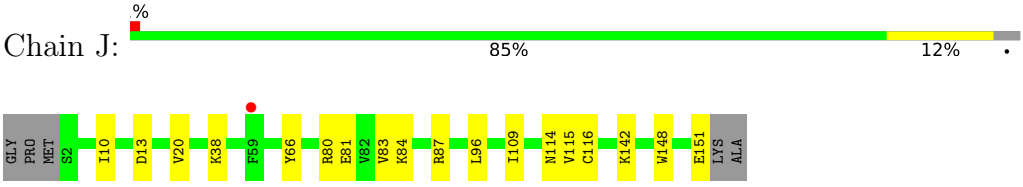
• Molecule 1: Nucleoside diphosphate kinase

Chain I:



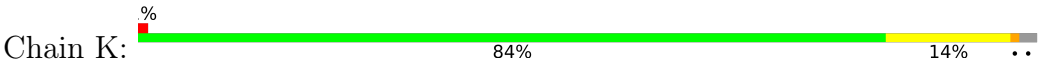
• Molecule 1: Nucleoside diphosphate kinase

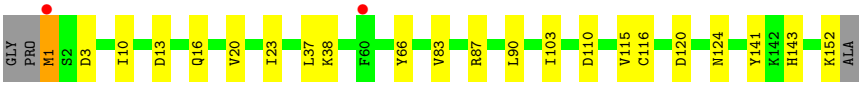
Chain J:



• Molecule 1: Nucleoside diphosphate kinase

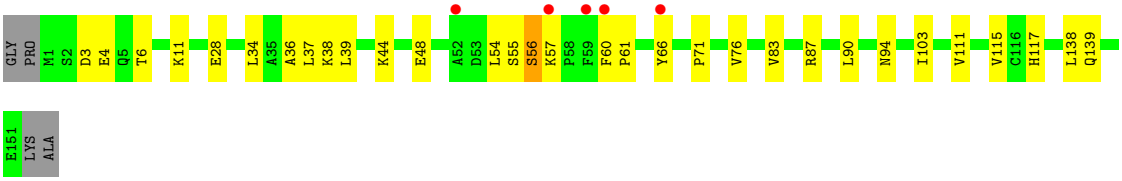
Chain K:





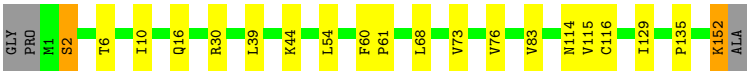
• Molecule 1: Nucleoside diphosphate kinase

Chain L:



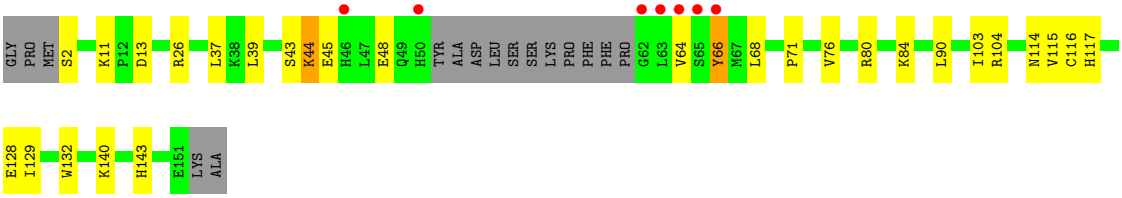
• Molecule 1: Nucleoside diphosphate kinase

Chain M:



• Molecule 1: Nucleoside diphosphate kinase

Chain N:

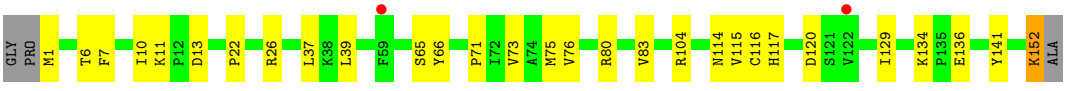


• Molecule 1: Nucleoside diphosphate kinase

Chain Q:

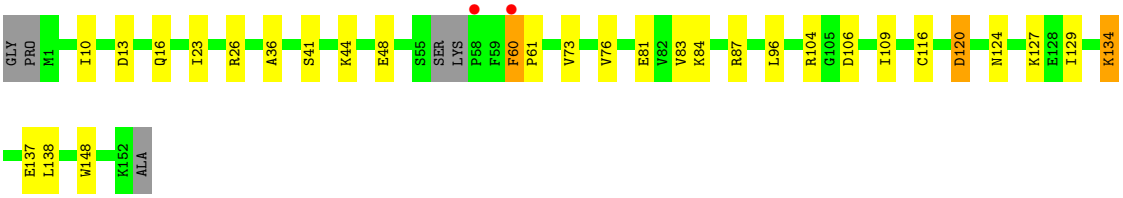
• Molecule 1: Nucleoside diphosphate kinase

Chain R:

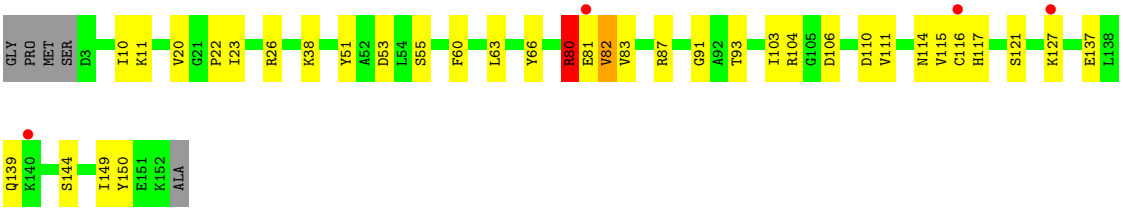


• Molecule 1: Nucleoside diphosphate kinase

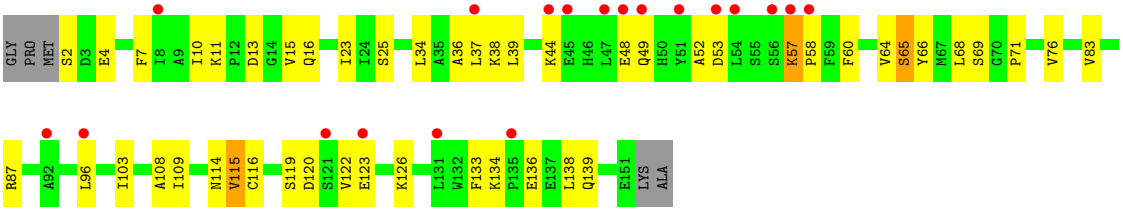
Chain U:



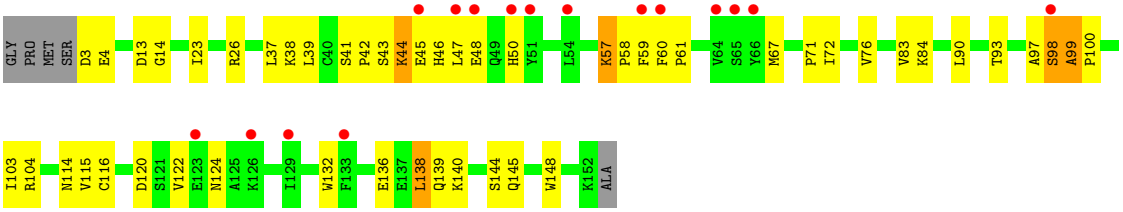
• Molecule 1: Nucleoside diphosphate kinase



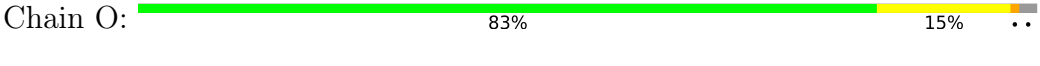
• Molecule 1: Nucleoside diphosphate kinase

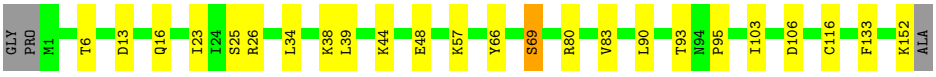


• Molecule 1: Nucleoside diphosphate kinase

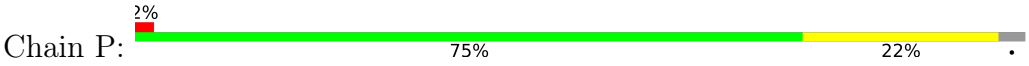


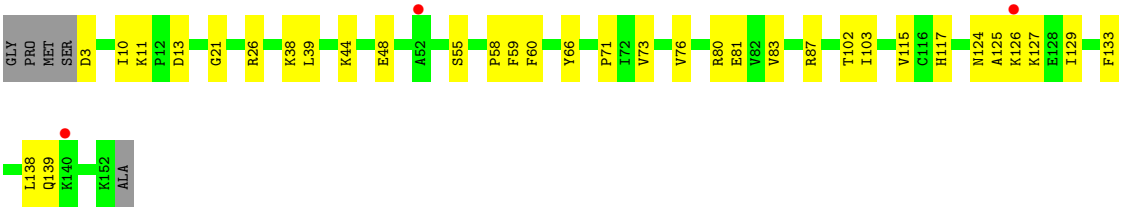
• Molecule 1: Nucleoside diphosphate kinase



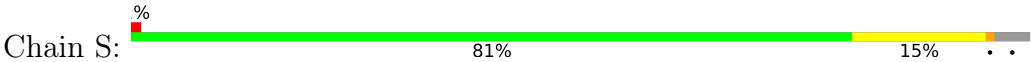


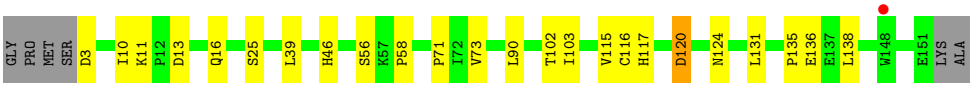
• Molecule 1: Nucleoside diphosphate kinase



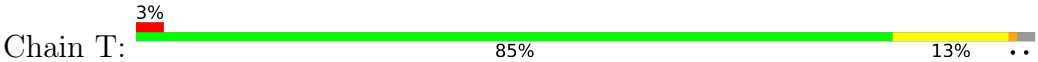


• Molecule 1: Nucleoside diphosphate kinase





• Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics (i)

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) 99.4 (94.76-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.230 , 0.281 0.231 , 0.281	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 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/1219	0.56	0/1648
1	B	0.46	0/1213	0.58	0/1638
1	C	0.46	0/1207	0.54	0/1632
1	D	0.43	0/1224	0.55	0/1653
1	E	0.48	0/1216	0.61	0/1643
1	F	0.46	0/1207	0.56	0/1632
1	G	0.44	0/1203	0.60	1/1627 (0.1%)
1	H	0.38	0/1215	0.54	0/1642
1	I	0.48	0/1224	0.60	0/1653
1	J	0.43	0/1207	0.53	0/1632
1	K	0.45	0/1220	0.61	0/1648
1	L	0.43	0/1207	0.57	0/1632
1	M	0.45	0/1224	0.60	0/1653
1	N	0.40	0/1111	0.58	0/1499
1	O	0.45	0/1224	0.60	0/1653
1	P	0.41	0/1210	0.55	0/1635
1	Q	0.43	0/1224	0.59	0/1653
1	R	0.40	0/1224	0.55	0/1653
1	S	0.42	0/1201	0.59	0/1624
1	T	0.44	0/1224	0.56	0/1653
1	U	0.45	0/1208	0.57	0/1630
1	V	0.41	0/1199	0.56	0/1619
1	W	0.40	0/1207	0.52	0/1632
1	X	0.44	0/1210	0.57	0/1635
All	All	0.44	0/29028	0.57	1/39219 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	68	LEU	CA-CB-CG	-6.38	100.62	115.30

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	14	0
1	C	1177	0	1169	21	0
1	D	1194	0	1194	17	0
1	E	1186	0	1182	11	0
1	F	1177	0	1169	20	0
1	G	1173	0	1157	33	0
1	H	1185	0	1179	21	0
1	I	1194	0	1194	25	0
1	J	1177	0	1169	11	0
1	K	1190	0	1182	15	0
1	L	1177	0	1164	21	0
1	M	1194	0	1194	16	0
1	N	1087	0	1084	15	0
1	O	1194	0	1194	15	0
1	P	1180	0	1177	24	0
1	Q	1194	0	1194	16	0
1	R	1194	0	1194	18	0
1	S	1171	0	1164	14	0
1	T	1194	0	1194	13	0
1	U	1179	0	1176	20	0
1	V	1171	0	1164	30	0
1	W	1177	0	1169	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	1180	0	1177	37	1
All	All	28318	0	28196	423	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 7.

All (423) 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:I:1:MET:N	1:I:152:LYS:NZ	2.25	0.83
1:E:2:SER:HA	1:E:152:LYS:HZ2	1.42	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: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:V:80:ARG:HH22	1:V:149:ILE:C	1.97	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:2:SER:HA	1:E:152:LYS:NZ	2.17	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:K:120:ASP:OD1	1:K:124:ASN:ND2	2.36	0.59
1:D:136:GLU:H	1:D:136:GLU:CD	2.05	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG12	1:A:87:ARG:NH1	2.18	0.58
1:N:90:LEU:HD23	1:N:103:ILE:HD12	1.85	0.57
1:N:90:LEU:HD22	1:N:116:CYS:SG	2.44	0.57
1:C:44:LYS:NZ	1:C:48:GLU:OE2	2.36	0.57
1:V:81:GLU:O	1:V:83:VAL:N	2.35	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: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:C:13:ASP:OD1	1:C:66:TYR:OH	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:83:VAL:HG22	1:J:87:ARG:NH1	2.24	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:X:136:GLU:H	1:X:136:GLU:CD	2.13	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: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:C:38:LYS:HA	1:D:37:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:139:GLN:HG3	1:X:39:LEU:HG	1.94	0.50
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: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: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:G:136:GLU:O	1:G:136:GLU:HG2	2.13	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: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:136:GLU:CD	1:W:136:GLU:H	2.16	0.48
1:W:64:VAL:O	1:W:68:LEU:HG	2.14	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
1:D:114:ASN:O	1:D:116:CYS:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:U:134:LYS:HE2	1:U:137:GLU:OE2	2.15	0.47
1:O:13:ASP:OD1	1:O:66:TYR:OH	2.28	0.47
1:P:26:ARG:HD2	1:P:103:ILE:HG12	1.97	0.47
1:S:136:GLU:H	1:S:136:GLU:CD	2.18	0.47
1:Q:124:ASN:O	1:Q:128:GLU:HG3	2.14	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:P:58:PRO:C	1:P:60:PHE:H	2.13	0.46
1:Q:60:PHE:HB3	1:Q:61:PRO:HD3	1.98	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:19:LEU:C	1:G:22:PRO:HD2	2.38	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
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:R:13:ASP:OD1	1:R:13:ASP:N	2.46	0.44
1:W:123:GLU:HG2	1:W:126:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:T:58:PRO:C	1:T:60:PHE:H	2.20	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:R:136:GLU:CD	1:R:136:GLU:H	2.22	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:K:1:MET:C	1:K:3:ASP:H	2.21	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:U:148:TRP:CZ2	1:S:16:GLN:HG3	2.55	0.42
1:W:36:ALA:HB2	1:W:138:LEU:HD23	2.01	0.42
1:P:125:ALA:HB3	1:P:126:LYS:HZ2	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLY:O	1:M:30:ARG:NH1	2.53	0.42
1:X:98:SER:HB3	1:X:99:ALA:H	1.56	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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:VAL:HG11	1:G:122:VAL:CG1	2.51	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: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: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%)	22	20
1	B	149/155 (96%)	143 (96%)	5 (3%)	1 (1%)	22	20
1	C	148/155 (96%)	141 (95%)	5 (3%)	2 (1%)	11	8
1	D	150/155 (97%)	145 (97%)	4 (3%)	1 (1%)	22	20
1	E	149/155 (96%)	146 (98%)	2 (1%)	1 (1%)	22	20
1	F	148/155 (96%)	142 (96%)	5 (3%)	1 (1%)	22	20
1	G	148/155 (96%)	141 (95%)	5 (3%)	2 (1%)	11	8
1	H	149/155 (96%)	142 (95%)	6 (4%)	1 (1%)	22	20
1	I	150/155 (97%)	143 (95%)	4 (3%)	3 (2%)	7	4
1	J	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	20
1	K	150/155 (97%)	146 (97%)	3 (2%)	1 (1%)	22	20
1	L	149/155 (96%)	139 (93%)	8 (5%)	2 (1%)	12	8
1	M	150/155 (97%)	146 (97%)	3 (2%)	1 (1%)	22	20
1	N	135/155 (87%)	132 (98%)	2 (2%)	1 (1%)	22	20
1	O	150/155 (97%)	147 (98%)	3 (2%)	0	100	100
1	P	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	11	8
1	Q	150/155 (97%)	147 (98%)	2 (1%)	1 (1%)	22	20
1	R	150/155 (97%)	144 (96%)	5 (3%)	1 (1%)	22	20
1	S	147/155 (95%)	140 (95%)	5 (3%)	2 (1%)	11	8
1	T	150/155 (97%)	144 (96%)	4 (3%)	2 (1%)	12	8
1	U	146/155 (94%)	141 (97%)	5 (3%)	0	100	100
1	V	148/155 (96%)	141 (95%)	4 (3%)	3 (2%)	7	4
1	W	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	22	20
1	X	148/155 (96%)	134 (90%)	10 (7%)	4 (3%)	5	2
All	All	3558/3720 (96%)	3408 (96%)	115 (3%)	35 (1%)	15	12

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

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Mol	Chain	Res	Type
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
1	W	115	VAL
1	N	115	VAL

5.3.2 Protein sidechains (i)

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%)	125 (99%)	1 (1%)	81 89
1	B	126/129 (98%)	124 (98%)	2 (2%)	62 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	126/129 (98%)	121 (96%)	5 (4%)	31	37
1	D	128/129 (99%)	125 (98%)	3 (2%)	50	60
1	E	127/129 (98%)	127 (100%)	0	100	100
1	F	126/129 (98%)	122 (97%)	4 (3%)	39	47
1	G	124/129 (96%)	120 (97%)	4 (3%)	39	47
1	H	126/129 (98%)	123 (98%)	3 (2%)	49	59
1	I	128/129 (99%)	126 (98%)	2 (2%)	62	74
1	J	126/129 (98%)	125 (99%)	1 (1%)	81	89
1	K	126/129 (98%)	123 (98%)	3 (2%)	49	59
1	L	123/129 (95%)	120 (98%)	3 (2%)	49	59
1	M	128/129 (99%)	126 (98%)	2 (2%)	62	74
1	N	116/129 (90%)	110 (95%)	6 (5%)	23	26
1	O	128/129 (99%)	125 (98%)	3 (2%)	50	60
1	P	126/129 (98%)	124 (98%)	2 (2%)	62	74
1	Q	128/129 (99%)	123 (96%)	5 (4%)	32	38
1	R	128/129 (99%)	124 (97%)	4 (3%)	40	48
1	S	125/129 (97%)	122 (98%)	3 (2%)	49	59
1	T	128/129 (99%)	126 (98%)	2 (2%)	62	74
1	U	126/129 (98%)	123 (98%)	3 (2%)	49	59
1	V	124/129 (96%)	120 (97%)	4 (3%)	39	47
1	W	126/129 (98%)	120 (95%)	6 (5%)	25	29
1	X	126/129 (98%)	122 (97%)	4 (3%)	39	47
All	All	3021/3096 (98%)	2946 (98%)	75 (2%)	47	57

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	B	65	SER
1	B	66	TYR
1	C	2	SER
1	C	3	ASP
1	C	28	GLU
1	C	66	TYR

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Mol	Chain	Res	Type
1	C	98	SER
1	D	66	TYR
1	D	116	CYS
1	D	142	LYS
1	F	2	SER
1	F	66	TYR
1	F	84	LYS
1	F	143	HIS
1	G	65	SER
1	G	66	TYR
1	G	80	ARG
1	G	98	SER
1	H	3	ASP
1	H	53	ASP
1	H	66	TYR
1	I	26	ARG
1	I	66	TYR
1	J	142	LYS
1	K	1	MET
1	K	143	HIS
1	K	152	LYS
1	L	3	ASP
1	L	66	TYR
1	L	139	GLN
1	M	2	SER
1	M	152	LYS
1	N	2	SER
1	N	44	LYS
1	N	66	TYR
1	N	84	LYS
1	N	140	LYS
1	N	143	HIS
1	Q	28	GLU
1	Q	30	ARG
1	Q	65	SER
1	Q	69	SER
1	Q	140	LYS
1	R	65	SER
1	R	66	TYR
1	R	120	ASP
1	R	152	LYS
1	U	60	PHE

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Mol	Chain	Res	Type
1	U	120	ASP
1	U	134	LYS
1	V	53	ASP
1	V	66	TYR
1	V	80	ARG
1	V	127	LYS
1	W	2	SER
1	W	25	SER
1	W	53	ASP
1	W	57	LYS
1	W	65	SER
1	W	120	ASP
1	X	3	ASP
1	X	44	LYS
1	X	46	HIS
1	X	57	LYS
1	O	57	LYS
1	O	69	SER
1	O	152	LYS
1	P	3	ASP
1	P	81	GLU
1	S	3	ASP
1	S	56	SER
1	S	120	ASP
1	T	66	TYR
1	T	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	94	ASN
1	N	124	ASN
1	X	124	ASN
1	P	5	GLN
1	S	46	HIS
1	S	124	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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 monosaccharides 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, 95^{th} 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%)	0.25	0 100 100	33, 42, 57, 62	0
1	B	151/155 (97%)	0.27	1 (0%) 87 88	33, 43, 66, 81	0
1	C	150/155 (96%)	0.24	1 (0%) 87 88	33, 44, 65, 78	0
1	D	152/155 (98%)	0.32	3 (1%) 65 66	33, 47, 78, 93	0
1	E	151/155 (97%)	0.31	1 (0%) 87 88	30, 40, 55, 66	0
1	F	150/155 (96%)	0.33	0 100 100	28, 40, 54, 64	0
1	G	150/155 (96%)	0.60	8 (5%) 26 27	36, 52, 72, 83	0
1	H	151/155 (97%)	0.72	17 (11%) 5 5	38, 55, 93, 99	0
1	I	152/155 (98%)	0.18	1 (0%) 87 88	33, 43, 52, 61	0
1	J	150/155 (96%)	0.24	1 (0%) 87 88	33, 45, 63, 87	0
1	K	152/155 (98%)	0.18	2 (1%) 77 77	30, 43, 54, 61	0
1	L	151/155 (97%)	0.38	5 (3%) 46 47	33, 47, 83, 105	0
1	M	152/155 (98%)	0.23	0 100 100	32, 41, 52, 58	0
1	N	139/155 (89%)	0.50	7 (5%) 28 30	32, 49, 94, 115	0
1	O	152/155 (98%)	0.31	0 100 100	32, 46, 67, 78	0
1	P	150/155 (96%)	0.49	3 (2%) 65 66	33, 54, 70, 81	0
1	Q	152/155 (98%)	0.25	0 100 100	33, 41, 54, 60	0
1	R	152/155 (98%)	0.27	2 (1%) 77 77	32, 45, 61, 69	0
1	S	149/155 (96%)	0.28	1 (0%) 87 88	32, 45, 60, 74	0
1	T	152/155 (98%)	0.32	4 (2%) 56 56	34, 46, 62, 77	0
1	U	150/155 (96%)	0.38	2 (1%) 77 77	33, 45, 63, 154	0
1	V	150/155 (96%)	0.45	4 (2%) 54 55	38, 55, 71, 78	0
1	W	150/155 (96%)	1.00	19 (12%) 3 3	45, 60, 106, 123	0
1	X	150/155 (96%)	0.98	16 (10%) 6 6	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%)	0.39	98 (2%) 54 55	28, 46, 71, 154	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	56	SER	8.3
1	W	54	LEU	7.7
1	J	59	PHE	5.7
1	U	58	PRO	5.0
1	X	59	PHE	4.9
1	W	58	PRO	4.5
1	L	60	PHE	4.3
1	W	45	GLU	4.3
1	H	51	TYR	4.2
1	X	66	TYR	4.2
1	U	60	PHE	4.2
1	W	49	GLN	3.9
1	X	54	LEU	3.8
1	G	133	PHE	3.8
1	H	54	LEU	3.7
1	P	126	LYS	3.7
1	L	52	ALA	3.7
1	P	140	LYS	3.6
1	W	8	ILE	3.6
1	W	47	LEU	3.6
1	V	127	LYS	3.5
1	W	135	PRO	3.5
1	N	62	GLY	3.4
1	G	138	LEU	3.4
1	H	59	PHE	3.3
1	X	45	GLU	3.2
1	N	65	SER	3.2
1	R	59	PHE	3.1
1	W	51	TYR	3.1
1	X	60	PHE	3.1
1	X	47	LEU	3.1
1	W	123	GLU	3.0
1	H	60	PHE	3.0
1	G	47	LEU	3.0
1	D	56	SER	3.0
1	W	96	LEU	3.0
1	G	51	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	133	PHE	2.9
1	G	45	GLU	2.9
1	V	140	LYS	2.9
1	H	53	ASP	2.8
1	H	62	GLY	2.8
1	L	59	PHE	2.8
1	T	96	LEU	2.8
1	W	131	LEU	2.8
1	L	66	TYR	2.7
1	T	56	SER	2.7
1	D	55	SER	2.7
1	H	63	LEU	2.7
1	H	49	GLN	2.7
1	X	64	VAL	2.7
1	H	90	LEU	2.7
1	N	66	TYR	2.6
1	X	123	GLU	2.6
1	W	48	GLU	2.6
1	X	129	ILE	2.6
1	H	52	ALA	2.6
1	C	56	SER	2.6
1	X	98	SER	2.6
1	X	51	TYR	2.5
1	W	44	LYS	2.5
1	X	50	HIS	2.4
1	S	148	TRP	2.4
1	K	1	MET	2.4
1	N	50	HIS	2.4
1	E	2	SER	2.4
1	H	64	VAL	2.4
1	H	42	PRO	2.4
1	I	123	GLU	2.4
1	N	46	HIS	2.4
1	G	135	PRO	2.3
1	X	65	SER	2.3
1	W	92	ALA	2.3
1	R	122	VAL	2.2
1	D	59	PHE	2.2
1	L	57	LYS	2.2
1	X	126	LYS	2.2
1	W	37	LEU	2.2
1	W	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	66	TYR	2.2
1	N	63	LEU	2.2
1	T	54	LEU	2.2
1	W	53	ASP	2.2
1	W	121	SER	2.2
1	H	138	LEU	2.1
1	T	63	LEU	2.1
1	H	130	ALA	2.1
1	K	60	PHE	2.1
1	V	116	CYS	2.1
1	H	127	LYS	2.0
1	N	64	VAL	2.0
1	G	53	ASP	2.0
1	P	52	ALA	2.0
1	X	48	GLU	2.0
1	B	53	ASP	2.0
1	H	46	HIS	2.0
1	V	81	GLU	2.0
1	H	122	VAL	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 monosaccharides 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.