



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:20 PM GMT

PDB ID : 1Q12
Title : Crystal Structure of the ATP-bound E. coli MalK
Authors : Chen, J.; Lu, G.; Lin, J.; Davidson, A.L.; Quiocho, F.A.
Deposited on : 2003-07-18
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

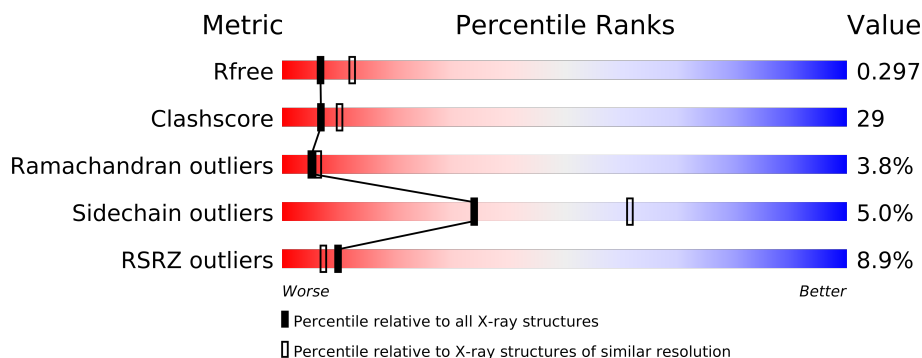
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	381	
1	B	381	
1	C	381	
1	D	381	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11546 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Maltose/maltodextrin transport ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	B	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	C	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	D	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			

There are 40 discrepancies between the modelled and reference sequences:

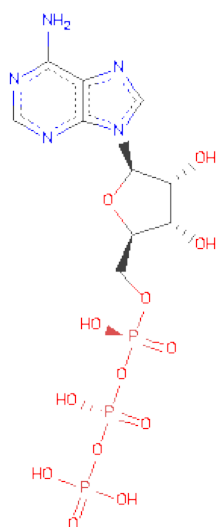
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	UNP P68187
A	379	HIS	-	EXPRESSION TAG	UNP P68187
A	380	HIS	-	EXPRESSION TAG	UNP P68187
A	381	HIS	-	EXPRESSION TAG	UNP P68187
B	372	ALA	-	EXPRESSION TAG	UNP P68187
B	373	SER	-	EXPRESSION TAG	UNP P68187
B	374	ALA	-	EXPRESSION TAG	UNP P68187
B	375	SER	-	EXPRESSION TAG	UNP P68187
B	376	HIS	-	EXPRESSION TAG	UNP P68187
B	377	HIS	-	EXPRESSION TAG	UNP P68187
B	378	HIS	-	EXPRESSION TAG	UNP P68187
B	379	HIS	-	EXPRESSION TAG	UNP P68187
B	380	HIS	-	EXPRESSION TAG	UNP P68187
B	381	HIS	-	EXPRESSION TAG	UNP P68187
C	372	ALA	-	EXPRESSION TAG	UNP P68187

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	EXPRESSION TAG	UNP P68187
C	374	ALA	-	EXPRESSION TAG	UNP P68187
C	375	SER	-	EXPRESSION TAG	UNP P68187
C	376	HIS	-	EXPRESSION TAG	UNP P68187
C	377	HIS	-	EXPRESSION TAG	UNP P68187
C	378	HIS	-	EXPRESSION TAG	UNP P68187
C	379	HIS	-	EXPRESSION TAG	UNP P68187
C	380	HIS	-	EXPRESSION TAG	UNP P68187
C	381	HIS	-	EXPRESSION TAG	UNP P68187
D	372	ALA	-	EXPRESSION TAG	UNP P68187
D	373	SER	-	EXPRESSION TAG	UNP P68187
D	374	ALA	-	EXPRESSION TAG	UNP P68187
D	375	SER	-	EXPRESSION TAG	UNP P68187
D	376	HIS	-	EXPRESSION TAG	UNP P68187
D	377	HIS	-	EXPRESSION TAG	UNP P68187
D	378	HIS	-	EXPRESSION TAG	UNP P68187
D	379	HIS	-	EXPRESSION TAG	UNP P68187
D	380	HIS	-	EXPRESSION TAG	UNP P68187
D	381	HIS	-	EXPRESSION TAG	UNP P68187

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is water.

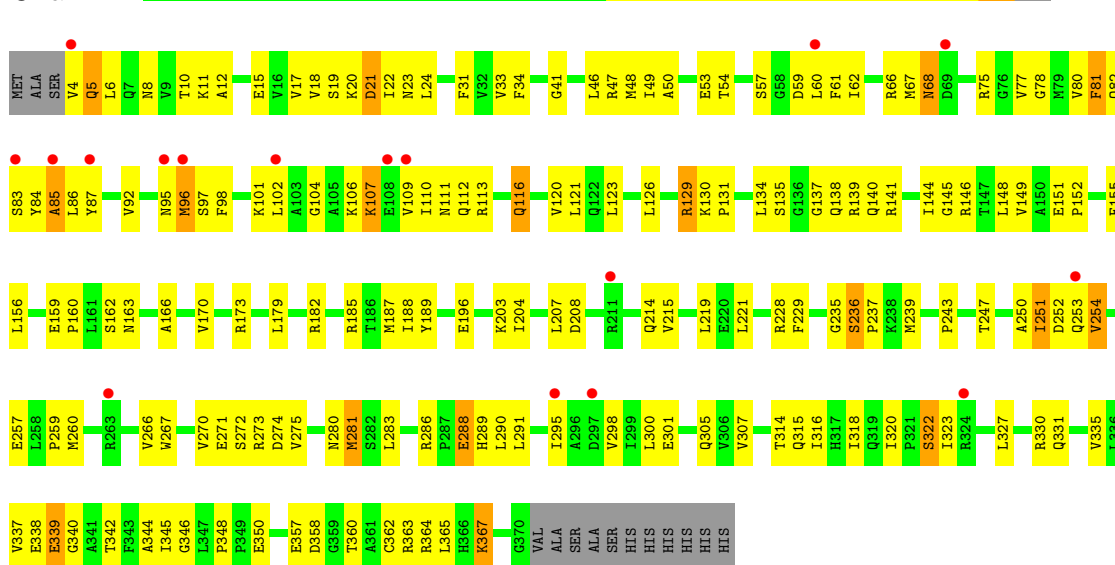
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	9	Total	O	0	0
			9	9		
3	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

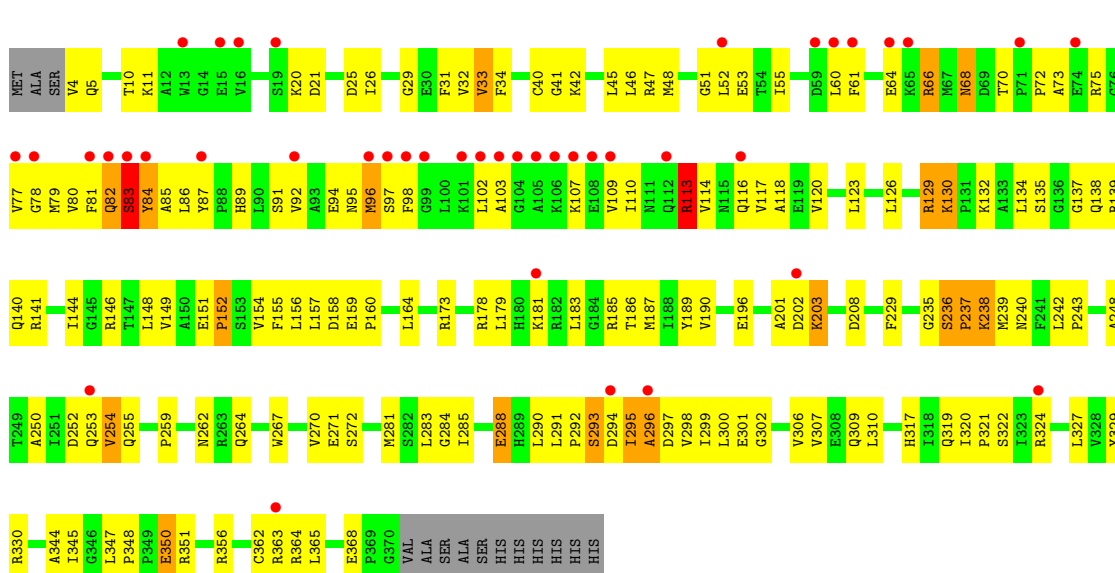
- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

Chain A:



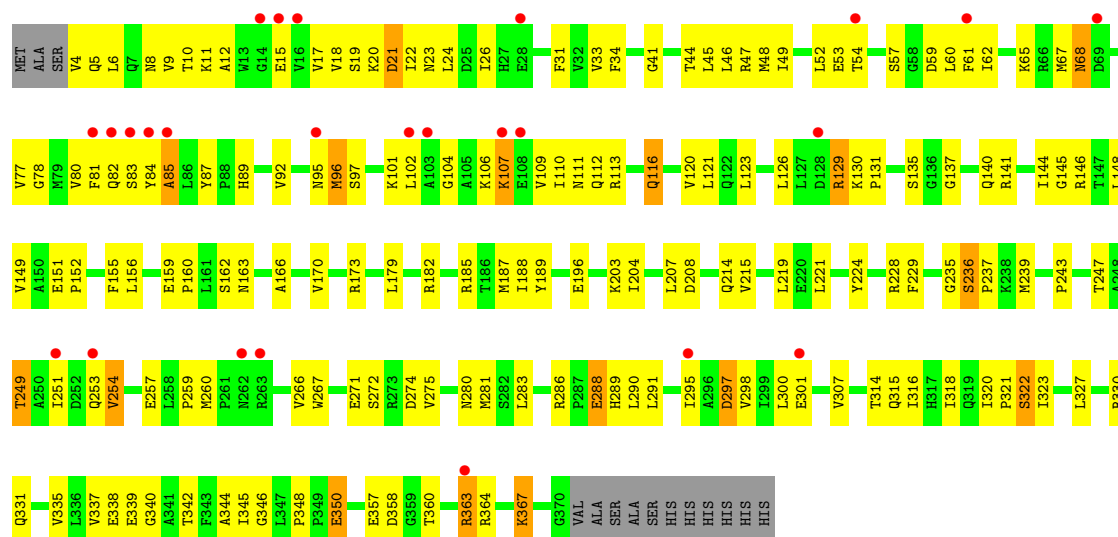
- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

Chain B:



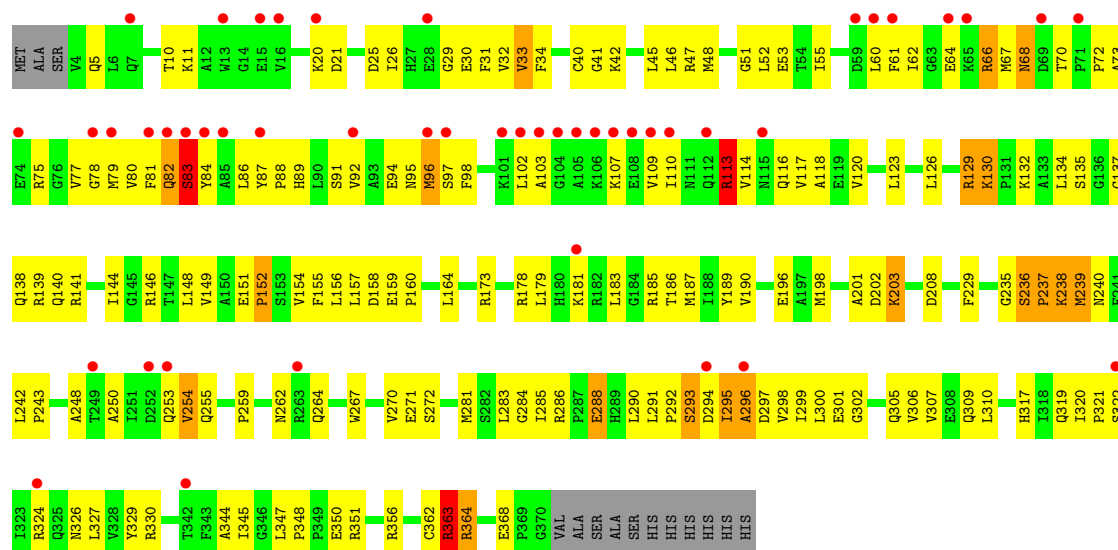
• Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

Chain C: 



• Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.88Å 97.28Å 101.86Å 74.59° 82.47° 76.85°	Depositor
Resolution (Å)	14.80 – 2.60 14.85 – 2.53	Depositor EDS
% Data completeness (in resolution range)	86.4 (14.80-2.60) 85.9 (14.85-2.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.286 0.272 , 0.297	Depositor DCC
R_{free} test set	4645 reflections (8.21%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 124917 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.50	0/2903	0.81	10/3936 (0.3%)
1	B	0.49	0/2903	0.81	6/3936 (0.2%)
1	C	0.47	0/2903	0.75	4/3936 (0.1%)
1	D	0.49	0/2903	0.82	8/3936 (0.2%)
All	All	0.49	0/11612	0.80	28/15744 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	D	363	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	66	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	D	364	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	364	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	A	364	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	363	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	47	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	D	129	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	B	129	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	B	139	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	D	113	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	113	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	D	139	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	C	363	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	273	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	67	MET	CG-SD-CE	6.12	109.99	100.20
1	D	239	MET	CG-SD-CE	6.11	109.98	100.20
1	A	96	MET	CG-SD-CE	6.09	109.95	100.20
1	C	239	MET	CG-SD-CE	6.08	109.93	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	MET	CG-SD-CE	5.98	109.78	100.20
1	A	239	MET	CG-SD-CE	5.83	109.53	100.20
1	C	96	MET	CG-SD-CE	5.83	109.53	100.20
1	B	239	MET	CG-SD-CE	5.80	109.49	100.20
1	B	96	MET	CG-SD-CE	5.77	109.43	100.20
1	D	96	MET	CG-SD-CE	5.76	109.42	100.20
1	D	198	MET	CG-SD-CE	5.73	109.37	100.20
1	A	281	MET	CG-SD-CE	5.67	109.27	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2853	0	2918	172	0
1	B	2853	0	2918	166	1
1	C	2853	0	2918	169	1
1	D	2853	0	2918	165	0
2	A	31	0	12	3	0
2	B	31	0	12	2	0
2	C	31	0	12	3	0
2	D	31	0	12	2	0
3	C	9	0	0	0	0
3	D	1	0	0	0	0
All	All	11546	0	11720	672	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (672) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:GLN:O	1:A:254:VAL:HG23	1.32	1.29
1:D:253:GLN:O	1:D:254:VAL:HG23	1.14	1.25

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:SER:OG	1:B:237:PRO:HD2	1.36	1.25
1:A:236:SER:OG	1:A:237:PRO:HD2	1.36	1.25
1:C:236:SER:OG	1:C:237:PRO:HD2	1.36	1.24
1:D:236:SER:OG	1:D:237:PRO:HD2	1.34	1.24
1:D:253:GLN:O	1:D:254:VAL:CG2	1.89	1.19
1:C:236:SER:HB2	1:C:237:PRO:HD3	1.34	1.08
1:D:236:SER:OG	1:D:237:PRO:CD	2.01	1.08
1:A:236:SER:OG	1:A:237:PRO:CD	2.04	1.06
1:C:236:SER:CB	1:C:237:PRO:CD	2.34	1.05
1:B:236:SER:OG	1:B:237:PRO:CD	2.04	1.05
1:D:83:SER:O	1:D:84:TYR:CD2	2.11	1.04
1:B:83:SER:O	1:B:84:TYR:CD2	2.15	0.99
1:C:253:GLN:O	1:C:254:VAL:HB	1.63	0.99
1:C:68:ASN:H	1:C:68:ASN:HD22	1.12	0.97
1:D:236:SER:CB	1:D:237:PRO:CD	2.42	0.97
1:B:236:SER:CB	1:B:237:PRO:CD	2.44	0.96
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.49	0.94
1:A:288:GLU:HG3	1:A:330:ARG:HD3	1.49	0.94
1:C:236:SER:OG	1:C:237:PRO:CD	2.15	0.94
1:A:253:GLN:O	1:A:254:VAL:CG2	2.17	0.93
1:C:236:SER:HB2	1:C:237:PRO:CD	1.97	0.92
1:C:4:VAL:HG13	1:C:26:ILE:O	1.70	0.91
1:D:236:SER:HB2	1:D:237:PRO:HD3	1.53	0.88
1:D:87:TYR:H	1:D:95:ASN:HD21	1.21	0.88
1:B:236:SER:HB2	1:B:237:PRO:HD3	1.54	0.88
1:C:314:THR:CG2	1:C:316:ILE:HD11	2.05	0.87
1:C:110:ILE:HG12	1:C:111:ASN:H	1.38	0.87
1:A:110:ILE:HG12	1:A:111:ASN:H	1.38	0.87
1:B:87:TYR:H	1:B:95:ASN:HD21	1.21	0.87
1:A:101:LYS:HG3	1:A:102:LEU:H	1.39	0.86
1:C:101:LYS:HG3	1:C:102:LEU:H	1.39	0.86
1:D:236:SER:CB	1:D:237:PRO:HD3	2.06	0.85
1:B:135:SER:H	1:B:138:GLN:HE21	1.22	0.85
1:A:314:THR:CG2	1:A:316:ILE:HD11	2.05	0.85
1:C:314:THR:HG22	1:C:316:ILE:HD11	1.59	0.84
1:D:135:SER:H	1:D:138:GLN:HE21	1.22	0.84
1:A:314:THR:HG22	1:A:316:ILE:HD11	1.59	0.84
1:B:236:SER:CB	1:B:237:PRO:HD3	2.09	0.82
1:A:96:MET:HA	1:A:146:ARG:HA	1.61	0.82
1:D:253:GLN:O	1:D:254:VAL:CB	2.28	0.81
1:D:20:LYS:HG3	1:D:21:ASP:H	1.45	0.81
1:B:253:GLN:O	1:B:254:VAL:HB	1.79	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:253:GLN:C	1:D:254:VAL:HG23	2.01	0.81
1:C:96:MET:HA	1:C:146:ARG:HA	1.61	0.81
1:B:20:LYS:HG3	1:B:21:ASP:H	1.45	0.80
1:C:253:GLN:O	1:C:254:VAL:CB	2.27	0.80
1:A:236:SER:CB	1:A:237:PRO:CD	2.57	0.80
1:B:250:ALA:HB3	1:B:253:GLN:HB2	1.64	0.79
1:C:271:GLU:O	1:C:272:SER:HB3	1.82	0.78
1:D:130:LYS:HD3	1:D:130:LYS:N	1.98	0.78
1:C:68:ASN:N	1:C:68:ASN:HD22	1.79	0.78
1:B:82:GLN:HA	1:B:140:GLN:OE1	1.84	0.78
1:B:130:LYS:N	1:B:130:LYS:HD3	1.98	0.78
1:B:135:SER:H	1:B:138:GLN:NE2	1.82	0.77
1:C:224:TYR:CG	1:C:363:ARG:NH2	2.52	0.77
1:B:68:ASN:N	1:B:68:ASN:HD22	1.80	0.77
1:D:68:ASN:N	1:D:68:ASN:HD22	1.80	0.77
1:C:291:LEU:HG	1:C:348:PRO:HG3	1.65	0.77
1:D:82:GLN:HA	1:D:140:GLN:OE1	1.84	0.77
1:D:86:LEU:HD23	1:D:146:ARG:NH2	2.00	0.77
1:A:68:ASN:H	1:A:68:ASN:HD22	1.30	0.77
1:B:202:ASP:O	1:B:203:LYS:HB2	1.85	0.77
1:B:248:ALA:HB3	1:B:267:TRP:CH2	2.20	0.76
1:A:60:LEU:H	1:A:68:ASN:HD21	1.33	0.76
1:A:271:GLU:O	1:A:272:SER:HB3	1.83	0.76
1:D:135:SER:H	1:D:138:GLN:NE2	1.82	0.76
1:D:86:LEU:HA	1:D:146:ARG:HH22	1.51	0.76
1:A:291:LEU:HG	1:A:348:PRO:HG3	1.68	0.76
1:C:236:SER:CB	1:C:237:PRO:HD2	2.10	0.75
1:A:34:PHE:HD1	1:A:207:LEU:HD11	1.51	0.75
1:B:86:LEU:HD23	1:B:146:ARG:NH2	2.01	0.75
1:C:236:SER:CB	1:C:237:PRO:HD3	2.05	0.75
1:A:4:VAL:HG12	1:A:4:VAL:O	1.88	0.74
1:C:34:PHE:HD1	1:C:207:LEU:HD11	1.51	0.74
1:B:86:LEU:HA	1:B:146:ARG:HH22	1.51	0.73
1:B:78:GLY:HA3	1:B:152:PRO:HG2	1.70	0.73
1:A:250:ALA:HB3	1:A:253:GLN:HB2	1.70	0.73
1:A:78:GLY:HA3	1:A:152:PRO:HG2	1.70	0.73
1:D:78:GLY:HA3	1:D:152:PRO:HG2	1.70	0.72
1:D:173:ARG:NE	1:D:196:GLU:HG3	2.04	0.72
1:A:95:ASN:O	1:A:96:MET:HB2	1.89	0.72
1:B:173:ARG:NE	1:B:196:GLU:HG3	2.04	0.72
1:C:78:GLY:HA3	1:C:152:PRO:HG2	1.70	0.71
1:B:253:GLN:O	1:B:254:VAL:CB	2.38	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:237:PRO:HG2	1:A:330:ARG:HD2	1.73	0.70
1:D:237:PRO:HG2	1:D:330:ARG:HD2	1.74	0.70
1:A:110:ILE:C	1:A:112:GLN:H	1.95	0.70
1:D:283:LEU:C	1:D:283:LEU:HD23	2.13	0.69
1:C:95:ASN:O	1:C:96:MET:HB2	1.92	0.69
1:C:110:ILE:C	1:C:112:GLN:H	1.95	0.69
1:B:283:LEU:C	1:B:283:LEU:HD23	2.13	0.69
1:C:68:ASN:H	1:C:68:ASN:ND2	1.90	0.69
1:C:235:GLY:O	1:C:236:SER:O	2.11	0.68
1:C:300:LEU:HB3	1:C:320:ILE:HD13	1.76	0.68
1:C:60:LEU:H	1:C:68:ASN:HD21	1.41	0.68
1:C:110:ILE:HG12	1:C:111:ASN:N	2.09	0.67
1:A:85:ALA:HB1	1:A:146:ARG:NH1	2.07	0.67
1:A:300:LEU:HB3	1:A:320:ILE:HD13	1.76	0.67
1:C:101:LYS:NZ	1:C:102:LEU:HG	2.10	0.67
1:B:84:TYR:CD1	1:B:84:TYR:O	2.48	0.67
1:D:84:TYR:CD1	1:D:84:TYR:O	2.47	0.67
1:A:101:LYS:NZ	1:A:102:LEU:HG	2.09	0.67
1:A:110:ILE:HG12	1:A:111:ASN:N	2.09	0.67
1:A:33:VAL:CG2	1:A:204:ILE:HG12	2.25	0.67
1:C:208:ASP:HB2	1:C:229:PHE:CE2	2.30	0.67
1:C:155:PHE:HB2	1:C:187:MET:HG2	1.77	0.66
1:B:255:GLN:HB2	1:B:267:TRP:CE3	2.28	0.66
1:A:208:ASP:HB2	1:A:229:PHE:CE2	2.30	0.66
1:A:140:GLN:OE1	1:A:163:ASN:HB2	1.96	0.66
1:A:68:ASN:N	1:A:68:ASN:HD22	1.93	0.66
1:B:270:VAL:HG13	1:B:362:CYS:HB3	1.76	0.66
1:D:87:TYR:H	1:D:95:ASN:ND2	1.93	0.66
1:C:6:LEU:HD22	1:C:22:ILE:HD11	1.78	0.66
1:B:60:LEU:H	1:B:68:ASN:HD21	1.44	0.65
1:A:101:LYS:HZ3	1:A:102:LEU:HG	1.60	0.65
1:B:309:GLN:O	1:B:310:LEU:HD23	1.96	0.65
1:D:60:LEU:H	1:D:68:ASN:HD21	1.44	0.65
1:C:4:VAL:O	1:C:4:VAL:HG12	1.97	0.65
1:A:236:SER:CB	1:A:237:PRO:HD3	2.27	0.65
1:B:148:LEU:HD22	1:B:179:LEU:CD1	2.27	0.65
1:B:237:PRO:HG2	1:B:330:ARG:HD2	1.78	0.65
1:D:254:VAL:HG21	1:D:270:VAL:HG12	1.79	0.64
1:D:130:LYS:HD3	1:D:130:LYS:H	1.62	0.64
1:C:140:GLN:OE1	1:C:163:ASN:HB2	1.96	0.64
1:B:87:TYR:H	1:B:95:ASN:ND2	1.93	0.64
1:B:262:ASN:HD21	1:B:264:GLN:HB2	1.63	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:148:LEU:HD22	1:D:179:LEU:CD1	2.27	0.64
1:B:144:ILE:HD11	1:B:160:PRO:O	1.98	0.64
1:D:270:VAL:HG13	1:D:362:CYS:HB3	1.79	0.64
1:C:243:PRO:O	1:C:259:PRO:HG3	1.97	0.64
1:D:309:GLN:O	1:D:310:LEU:HD23	1.96	0.64
1:D:33:VAL:HG13	1:D:201:ALA:HB2	1.77	0.64
1:B:236:SER:HB2	1:B:237:PRO:CD	2.20	0.64
1:D:288:GLU:HG3	1:D:330:ARG:HD3	1.80	0.64
1:D:144:ILE:HD11	1:D:160:PRO:O	1.98	0.64
1:D:11:LYS:HB2	1:D:48:MET:HE1	1.79	0.64
1:C:33:VAL:CG2	1:C:204:ILE:HG12	2.27	0.64
1:B:248:ALA:CB	1:B:267:TRP:CH2	2.81	0.64
1:A:173:ARG:HE	1:A:196:GLU:HG3	1.63	0.64
1:A:87:TYR:CE1	1:A:98:PHE:CE2	2.86	0.64
1:A:155:PHE:HB2	1:A:187:MET:HG2	1.78	0.64
1:A:236:SER:HG	1:A:237:PRO:HD2	1.57	0.63
1:B:130:LYS:H	1:B:130:LYS:HD3	1.62	0.63
1:A:243:PRO:O	1:A:259:PRO:HG3	1.97	0.63
1:A:123:LEU:HD21	1:A:141:ARG:HB3	1.79	0.63
1:A:214:GLN:HG2	1:A:221:LEU:CD2	2.29	0.63
1:A:331:GLN:OE1	1:A:335:VAL:HG21	1.99	0.63
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.80	0.63
1:C:173:ARG:HE	1:C:196:GLU:HG3	1.63	0.63
1:D:262:ASN:HD21	1:D:264:GLN:HB2	1.63	0.63
1:D:270:VAL:HG22	1:D:362:CYS:O	1.99	0.62
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.80	0.62
1:B:271:GLU:O	1:B:272:SER:HB3	1.99	0.62
1:D:34:PHE:HB2	1:D:190:VAL:HG22	1.80	0.62
1:C:123:LEU:HD21	1:C:141:ARG:HB3	1.79	0.62
1:C:314:THR:HG22	1:C:316:ILE:CD1	2.30	0.62
1:D:155:PHE:O	1:D:156:LEU:HD23	2.00	0.62
1:B:155:PHE:O	1:B:156:LEU:HD23	2.00	0.62
1:D:271:GLU:O	1:D:272:SER:HB3	1.99	0.62
1:C:214:GLN:HG2	1:C:221:LEU:CD2	2.29	0.62
1:C:331:GLN:OE1	1:C:335:VAL:HG21	1.99	0.62
1:B:173:ARG:HE	1:B:196:GLU:HG3	1.65	0.61
1:B:47:ARG:NH2	1:B:52:LEU:HB3	2.15	0.61
1:B:141:ARG:HD2	1:B:164:LEU:HD21	1.82	0.61
1:C:33:VAL:HG22	1:C:204:ILE:HG12	1.82	0.61
1:A:367:LYS:HE3	1:A:367:LYS:HA	1.82	0.61
1:D:173:ARG:HE	1:D:196:GLU:HG3	1.65	0.61
1:C:92:VAL:O	1:C:96:MET:HE2	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:208:ASP:HB2	1:D:229:PHE:CE2	2.36	0.61
1:D:141:ARG:HD2	1:D:164:LEU:HD21	1.82	0.61
1:A:87:TYR:HE1	1:A:98:PHE:CE2	2.19	0.60
1:B:208:ASP:HB2	1:B:229:PHE:CE2	2.36	0.60
1:B:255:GLN:HB2	1:B:267:TRP:CZ3	2.36	0.60
1:C:288:GLU:CG	1:C:330:ARG:HD3	2.28	0.60
1:C:367:LYS:HE3	1:C:367:LYS:HA	1.82	0.60
1:C:253:GLN:HB3	1:C:267:TRP:CE3	2.37	0.60
1:D:47:ARG:NH2	1:D:52:LEU:HB3	2.15	0.60
1:B:262:ASN:ND2	1:B:264:GLN:HB2	2.17	0.60
1:D:301:GLU:HG2	1:D:344:ALA:HB2	1.84	0.60
1:D:281:MET:HE2	1:D:356:ARG:HA	1.84	0.59
1:A:236:SER:HB2	1:A:237:PRO:HD3	1.83	0.59
1:B:248:ALA:CB	1:B:267:TRP:HH2	2.16	0.59
1:B:202:ASP:O	1:B:203:LYS:CB	2.50	0.59
1:A:33:VAL:HG22	1:A:204:ILE:HG12	1.84	0.59
1:D:262:ASN:ND2	1:D:264:GLN:HB2	2.17	0.59
1:B:236:SER:O	1:B:238:LYS:N	2.35	0.59
1:A:126:LEU:O	1:A:129:ARG:HB2	2.03	0.59
1:C:126:LEU:O	1:C:129:ARG:HB2	2.03	0.59
1:A:314:THR:HG22	1:A:316:ILE:CD1	2.30	0.59
1:D:243:PRO:O	1:D:259:PRO:HD3	2.03	0.59
1:D:33:VAL:HA	1:D:189:TYR:O	2.03	0.58
1:B:81:PHE:CE2	1:B:157:LEU:HA	2.38	0.58
1:D:327:LEU:HD23	1:D:345:ILE:HD11	1.85	0.58
1:B:33:VAL:HA	1:B:189:TYR:O	2.03	0.58
1:B:255:GLN:HB2	1:B:267:TRP:CD2	2.38	0.58
1:A:250:ALA:HB3	1:A:253:GLN:CG	2.33	0.58
1:A:250:ALA:HB3	1:A:253:GLN:CB	2.34	0.58
1:A:110:ILE:O	1:A:112:GLN:N	2.37	0.58
1:C:101:LYS:HZ3	1:C:102:LEU:HG	1.68	0.58
1:C:290:LEU:HD13	1:C:345:ILE:HD12	1.85	0.58
1:D:81:PHE:CE2	1:D:157:LEU:HA	2.39	0.58
1:A:203:LYS:HD3	1:A:215:VAL:CG1	2.34	0.58
1:D:250:ALA:HB3	1:D:253:GLN:HB2	1.86	0.58
1:B:281:MET:HE2	1:B:356:ARG:HA	1.86	0.58
1:C:110:ILE:O	1:C:112:GLN:N	2.37	0.58
1:C:228:ARG:HH11	1:C:228:ARG:HG2	1.68	0.58
1:C:68:ASN:ND2	1:C:68:ASN:N	2.50	0.57
1:C:84:TYR:O	1:C:85:ALA:HB2	2.04	0.57
1:B:301:GLU:HG2	1:B:344:ALA:HB2	1.84	0.57
1:A:290:LEU:HD13	1:A:345:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:309:GLN:C	1:D:310:LEU:HD23	2.25	0.57
1:B:243:PRO:O	1:B:259:PRO:HD3	2.03	0.57
1:D:236:SER:O	1:D:238:LYS:N	2.37	0.57
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.68	0.57
1:B:148:LEU:HD22	1:B:179:LEU:HD11	1.86	0.57
1:C:45:LEU:HA	1:C:48:MET:CE	2.34	0.57
1:B:11:LYS:HB2	1:B:48:MET:HE1	1.86	0.57
1:B:327:LEU:HD23	1:B:345:ILE:HD11	1.85	0.57
1:D:68:ASN:N	1:D:68:ASN:ND2	2.52	0.57
1:B:309:GLN:C	1:B:310:LEU:HD23	2.25	0.56
1:A:92:VAL:O	1:A:96:MET:HE2	2.05	0.56
1:D:148:LEU:HD22	1:D:179:LEU:HD11	1.86	0.56
1:C:10:THR:HB	1:C:57:SER:HB2	1.86	0.56
1:C:41:GLY:HA2	2:C:382:ATP:O2A	2.05	0.56
1:A:6:LEU:HD22	1:A:22:ILE:HD11	1.87	0.56
1:A:4:VAL:O	1:A:5:GLN:HB2	2.06	0.56
1:A:253:GLN:O	1:A:272:SER:HB2	2.06	0.56
1:A:288:GLU:CG	1:A:330:ARG:HD3	2.28	0.56
1:A:49:ILE:O	1:A:62:ILE:HD11	2.06	0.56
1:D:60:LEU:HB3	1:D:68:ASN:ND2	2.21	0.56
1:B:60:LEU:HB3	1:B:68:ASN:ND2	2.21	0.56
1:C:44:THR:O	1:C:48:MET:HG3	2.06	0.56
1:C:203:LYS:HD3	1:C:215:VAL:CG1	2.35	0.56
1:B:68:ASN:N	1:B:68:ASN:ND2	2.52	0.55
1:D:290:LEU:HD13	1:D:345:ILE:HD12	1.89	0.55
1:A:10:THR:HB	1:A:57:SER:HB2	1.86	0.55
1:A:41:GLY:HA2	2:A:382:ATP:O2A	2.05	0.55
1:B:270:VAL:HG22	1:B:362:CYS:O	2.05	0.55
1:B:290:LEU:HD13	1:B:345:ILE:HD12	1.88	0.55
1:B:178:ARG:HA	1:B:181:LYS:HG2	1.89	0.55
1:A:250:ALA:HB3	1:A:253:GLN:HG3	1.89	0.54
1:A:87:TYR:HE1	1:A:98:PHE:CD2	2.25	0.54
1:D:183:LEU:HB3	1:D:185:ARG:HG2	1.89	0.54
1:A:85:ALA:O	1:A:146:ARG:NH2	2.40	0.54
1:A:34:PHE:CE2	1:A:188:ILE:HG23	2.43	0.54
1:B:183:LEU:HB3	1:B:185:ARG:HG2	1.89	0.54
1:A:126:LEU:HD22	1:A:129:ARG:HG3	1.89	0.54
1:C:8:ASN:HA	1:C:21:ASP:HB2	1.89	0.54
1:D:178:ARG:HA	1:D:181:LYS:HG2	1.89	0.54
1:A:8:ASN:HA	1:A:21:ASP:HB2	1.90	0.54
1:D:236:SER:HB2	1:D:237:PRO:CD	2.20	0.54
1:D:270:VAL:HG13	1:D:271:GLU:N	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:130:LYS:N	1:B:130:LYS:CD	2.70	0.54
1:A:4:VAL:CG1	1:A:4:VAL:O	2.55	0.54
1:C:126:LEU:HD22	1:C:129:ARG:HG3	1.89	0.54
1:B:126:LEU:HD22	1:B:129:ARG:NH1	2.23	0.54
1:A:83:SER:O	1:A:84:TYR:HB2	2.08	0.53
1:D:81:PHE:CZ	1:D:157:LEU:HD23	2.43	0.53
1:B:81:PHE:CZ	1:B:157:LEU:HD23	2.43	0.53
2:C:382:ATP:H5'1	1:D:135:SER:HB3	1.90	0.53
1:B:130:LYS:H	1:B:130:LYS:CD	2.21	0.53
1:C:275:VAL:HG13	1:C:281:MET:CE	2.39	0.53
1:A:289:HIS:O	1:A:348:PRO:HG2	2.08	0.53
1:C:34:PHE:CE2	1:C:188:ILE:HG23	2.43	0.53
1:B:270:VAL:HG13	1:B:271:GLU:N	2.23	0.53
1:C:45:LEU:HA	1:C:48:MET:HE2	1.90	0.53
1:C:47:ARG:HD2	1:C:52:LEU:HD12	1.91	0.53
1:B:248:ALA:HB1	1:B:267:TRP:HH2	1.73	0.53
1:D:242:LEU:N	1:D:242:LEU:HD12	2.23	0.53
1:C:289:HIS:O	1:C:348:PRO:HG2	2.08	0.53
1:C:327:LEU:HD23	1:C:345:ILE:HD11	1.90	0.53
1:D:5:GLN:HB3	1:D:61:PHE:HB2	1.91	0.53
1:C:110:ILE:C	1:C:112:GLN:N	2.62	0.53
1:C:173:ARG:NE	1:C:196:GLU:HG3	2.23	0.53
1:D:110:ILE:O	1:D:113:ARG:HG2	2.09	0.53
1:A:101:LYS:HG3	1:A:102:LEU:N	2.19	0.53
1:D:130:LYS:CD	1:D:130:LYS:H	2.21	0.53
1:D:126:LEU:HD22	1:D:129:ARG:NH1	2.23	0.53
1:D:351:ARG:NE	1:D:368:GLU:OE2	2.42	0.53
1:D:83:SER:O	1:D:84:TYR:CG	2.60	0.53
2:A:382:ATP:H5'1	1:B:135:SER:HB3	1.90	0.53
1:B:292:PRO:C	1:B:294:ASP:H	2.12	0.52
1:B:242:LEU:N	1:B:242:LEU:HD12	2.23	0.52
1:B:117:VAL:HG13	1:B:118:ALA:N	2.24	0.52
1:A:110:ILE:C	1:A:112:GLN:N	2.62	0.52
1:D:292:PRO:C	1:D:294:ASP:H	2.12	0.52
1:A:34:PHE:HE2	1:A:188:ILE:HG23	1.74	0.52
1:D:97:SER:HB3	1:D:114:VAL:HG21	1.91	0.52
1:D:117:VAL:O	1:D:120:VAL:HG22	2.10	0.52
1:A:286:ARG:HB3	1:A:288:GLU:OE2	2.10	0.52
1:B:295:ILE:O	1:B:296:ALA:HB2	2.09	0.52
1:C:286:ARG:HB3	1:C:288:GLU:OE2	2.10	0.52
1:A:116:GLN:HE22	1:A:182:ARG:HH12	1.58	0.52
1:C:34:PHE:HE2	1:C:188:ILE:HG23	1.73	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:LEU:HD23	1:A:345:ILE:HD11	1.90	0.52
1:D:148:LEU:HD22	1:D:179:LEU:HD13	1.91	0.52
1:B:110:ILE:O	1:B:113:ARG:HG2	2.09	0.52
1:C:249:THR:HA	1:C:254:VAL:HA	1.92	0.52
1:D:321:PRO:O	1:D:322:SER:OG	2.22	0.52
1:D:295:ILE:O	1:D:296:ALA:HB2	2.09	0.52
1:B:97:SER:HB3	1:B:114:VAL:HG21	1.91	0.52
1:C:101:LYS:HG3	1:C:102:LEU:N	2.19	0.52
1:B:117:VAL:O	1:B:120:VAL:HG22	2.10	0.52
1:A:60:LEU:H	1:A:68:ASN:ND2	2.04	0.51
1:C:335:VAL:HG12	1:C:337:VAL:HG23	1.92	0.51
1:D:117:VAL:HG13	1:D:118:ALA:N	2.24	0.51
1:C:96:MET:HA	1:C:146:ARG:CA	2.38	0.51
1:C:80:VAL:HG13	1:C:80:VAL:O	2.10	0.51
1:C:301:GLU:HG3	1:C:344:ALA:HB2	1.91	0.51
1:D:70:THR:HB	1:D:75:ARG:HD3	1.92	0.51
1:A:173:ARG:NE	1:A:196:GLU:HG3	2.23	0.51
1:B:248:ALA:HB3	1:B:255:GLN:HB3	1.93	0.51
1:A:323:ILE:H	1:A:323:ILE:HD12	1.76	0.51
1:D:11:LYS:HB2	1:D:48:MET:CE	2.39	0.51
1:B:11:LYS:HB2	1:B:48:MET:CE	2.39	0.51
1:B:242:LEU:HD11	1:B:327:LEU:HD11	1.93	0.51
1:A:80:VAL:HG13	1:A:80:VAL:O	2.11	0.51
1:C:11:LYS:HD3	1:C:54:THR:O	2.11	0.51
1:B:83:SER:O	1:B:84:TYR:CG	2.62	0.51
1:B:141:ARG:HD2	1:B:164:LEU:CD2	2.41	0.51
1:D:242:LEU:HD11	1:D:327:LEU:HD11	1.93	0.51
1:D:141:ARG:HD2	1:D:164:LEU:CD2	2.41	0.51
1:B:70:THR:HB	1:B:75:ARG:HD3	1.92	0.51
1:C:95:ASN:C	1:C:97:SER:H	2.14	0.51
1:C:280:ASN:O	1:C:357:GLU:HG2	2.11	0.51
1:B:5:GLN:HB3	1:B:61:PHE:HB2	1.91	0.51
1:D:159:GLU:N	1:D:160:PRO:CD	2.74	0.50
1:D:81:PHE:HE2	1:D:156:LEU:O	1.94	0.50
1:B:293:SER:HB3	1:B:345:ILE:HA	1.93	0.50
1:A:280:ASN:O	1:A:357:GLU:HG2	2.11	0.50
1:C:323:ILE:H	1:C:323:ILE:HD12	1.76	0.50
1:B:148:LEU:HD22	1:B:179:LEU:HD13	1.92	0.50
1:A:335:VAL:HG12	1:A:337:VAL:HG23	1.92	0.50
1:B:297:ASP:O	1:B:299:ILE:HG13	2.12	0.50
1:A:358:ASP:OD1	1:A:360:THR:HG23	2.12	0.50
1:A:251:ILE:HD12	1:A:251:ILE:N	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:VAL:HG12	1:A:96:MET:HE2	1.92	0.50
1:C:144:ILE:HD11	1:C:160:PRO:O	2.12	0.50
1:D:293:SER:HB3	1:D:345:ILE:HA	1.93	0.50
1:C:23:ASN:HD22	1:C:23:ASN:N	2.09	0.50
1:A:236:SER:OG	1:A:237:PRO:HD3	2.08	0.50
1:D:84:TYR:CG	1:D:84:TYR:O	2.64	0.50
1:B:84:TYR:CG	1:B:84:TYR:O	2.65	0.50
1:B:81:PHE:HE2	1:B:156:LEU:O	1.94	0.50
1:B:159:GLU:N	1:B:160:PRO:CD	2.74	0.50
1:C:116:GLN:HE22	1:C:182:ARG:HH12	1.58	0.50
1:D:30:GLU:HG2	1:D:202:ASP:OD2	2.12	0.50
1:B:20:LYS:HG3	1:B:21:ASP:N	2.21	0.50
1:B:29:GLY:HA2	1:B:185:ARG:O	2.12	0.50
1:C:4:VAL:O	1:C:4:VAL:CG1	2.60	0.49
1:A:68:ASN:H	1:A:68:ASN:ND2	2.06	0.49
1:D:351:ARG:HH11	1:D:351:ARG:HG3	1.77	0.49
1:D:132:LYS:HG2	1:D:132:LYS:O	2.13	0.49
1:A:11:LYS:HD3	1:A:54:THR:O	2.11	0.49
1:A:96:MET:HA	1:A:146:ARG:CA	2.39	0.49
1:C:5:GLN:C	1:C:6:LEU:HD12	2.32	0.49
1:B:51:GLY:HA3	1:B:72:PRO:HG3	1.94	0.49
1:C:92:VAL:HG12	1:C:96:MET:HE2	1.95	0.49
1:C:260:MET:SD	1:C:300:LEU:HD22	2.52	0.49
1:B:351:ARG:HH11	1:B:351:ARG:HG3	1.77	0.49
1:A:260:MET:SD	1:A:300:LEU:HD22	2.52	0.49
1:D:29:GLY:HA2	1:D:185:ARG:O	2.12	0.49
1:B:252:ASP:HB3	1:B:365:LEU:CD1	2.43	0.49
1:A:23:ASN:N	1:A:23:ASN:HD22	2.09	0.49
1:D:20:LYS:HG3	1:D:21:ASP:N	2.21	0.49
1:D:51:GLY:HA3	1:D:72:PRO:HG3	1.94	0.49
1:D:92:VAL:CG2	1:D:134:LEU:HD11	2.42	0.49
1:B:86:LEU:HA	1:B:146:ARG:NH2	2.25	0.49
1:B:306:VAL:HB	1:B:317:HIS:CG	2.48	0.49
1:C:60:LEU:H	1:C:68:ASN:ND2	2.10	0.49
1:A:214:GLN:HG2	1:A:221:LEU:HD21	1.94	0.49
1:C:275:VAL:HG13	1:C:281:MET:HE1	1.94	0.49
1:A:144:ILE:HD11	1:A:160:PRO:O	2.12	0.48
1:D:96:MET:CE	1:D:117:VAL:HG13	2.43	0.48
1:A:275:VAL:HG13	1:A:281:MET:CE	2.43	0.48
1:B:92:VAL:CG2	1:B:134:LEU:HD11	2.42	0.48
1:A:252:ASP:HB3	1:A:365:LEU:CD1	2.43	0.48
1:B:132:LYS:HG2	1:B:132:LYS:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:135:SER:N	1:D:138:GLN:HE21	2.01	0.48
1:D:297:ASP:O	1:D:299:ILE:HG13	2.12	0.48
1:D:306:VAL:HB	1:D:317:HIS:CG	2.48	0.48
1:D:40:CYS:SG	1:D:42:LYS:HG3	2.53	0.48
1:C:253:GLN:O	1:C:254:VAL:CG2	2.61	0.48
1:D:253:GLN:O	1:D:254:VAL:HB	2.13	0.48
1:B:96:MET:CE	1:B:117:VAL:HG13	2.43	0.48
1:A:301:GLU:HG3	1:A:344:ALA:HB2	1.96	0.48
1:A:5:GLN:C	1:A:6:LEU:HD12	2.34	0.48
1:D:240:ASN:HB2	1:D:285:ILE:O	2.13	0.48
1:C:214:GLN:HG2	1:C:221:LEU:HD21	1.94	0.48
1:C:358:ASP:OD1	1:C:360:THR:HG23	2.13	0.48
1:C:109:VAL:HG13	1:C:110:ILE:N	2.29	0.48
1:C:224:TYR:CD1	1:C:363:ARG:NH2	2.81	0.48
1:B:77:VAL:CG1	1:B:78:GLY:N	2.77	0.48
1:A:84:TYR:HE1	1:A:140:GLN:HG3	1.79	0.48
1:D:77:VAL:CG1	1:D:78:GLY:N	2.77	0.48
1:B:40:CYS:SG	1:B:42:LYS:HG3	2.53	0.48
1:A:140:GLN:HE21	1:A:160:PRO:C	2.18	0.48
1:A:358:ASP:OD1	1:A:358:ASP:C	2.53	0.48
1:C:113:ARG:HA	1:C:116:GLN:HG3	1.96	0.48
1:C:307:VAL:HG13	1:C:316:ILE:CD1	2.44	0.48
1:A:307:VAL:HG13	1:A:316:ILE:CD1	2.44	0.48
1:D:151:GLU:O	1:D:185:ARG:NH1	2.46	0.48
1:C:140:GLN:HE21	1:C:160:PRO:C	2.18	0.48
1:A:145:GLY:O	1:A:149:VAL:HG23	2.14	0.48
1:D:83:SER:C	1:D:84:TYR:CD2	2.86	0.47
1:D:151:GLU:N	1:D:152:PRO:HD3	2.29	0.47
1:C:145:GLY:O	1:C:149:VAL:HG23	2.14	0.47
1:D:253:GLN:OE1	1:D:267:TRP:CE3	2.68	0.47
1:B:135:SER:N	1:B:138:GLN:HE21	2.01	0.47
1:D:77:VAL:HG12	1:D:78:GLY:N	2.29	0.47
1:C:83:SER:O	1:C:84:TYR:HB2	2.14	0.47
1:C:33:VAL:HG12	1:C:189:TYR:HB3	1.96	0.47
1:D:46:LEU:HD11	1:D:156:LEU:HB3	1.97	0.47
1:A:251:ILE:CD1	1:A:251:ILE:H	2.27	0.47
1:A:338:GLU:O	1:A:340:GLY:N	2.47	0.47
1:B:151:GLU:N	1:B:152:PRO:HD3	2.29	0.47
1:B:152:PRO:O	1:B:185:ARG:NH1	2.48	0.47
1:C:283:LEU:HD23	1:C:283:LEU:C	2.34	0.47
1:A:253:GLN:O	1:A:254:VAL:CB	2.62	0.47
1:B:77:VAL:HG12	1:B:78:GLY:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:LEU:C	1:A:283:LEU:HD23	2.34	0.47
1:C:346:GLY:O	1:C:348:PRO:HD3	2.15	0.47
1:B:47:ARG:HG2	1:B:47:ARG:HH11	1.79	0.47
1:C:247:THR:CG2	1:C:257:GLU:HB2	2.45	0.47
1:C:49:ILE:O	1:C:62:ILE:HD11	2.15	0.47
1:B:60:LEU:N	1:B:68:ASN:HD21	2.10	0.47
1:A:113:ARG:HA	1:A:116:GLN:HG3	1.96	0.47
1:C:338:GLU:O	1:C:340:GLY:N	2.47	0.47
2:A:382:ATP:C5'	1:B:135:SER:HB3	2.45	0.47
1:A:68:ASN:ND2	1:A:68:ASN:N	2.62	0.47
1:B:46:LEU:HD11	1:B:156:LEU:HB3	1.97	0.47
1:D:47:ARG:HH11	1:D:47:ARG:HG2	1.79	0.47
1:B:48:MET:HE3	1:B:55:ILE:HA	1.96	0.47
1:B:178:ARG:HG2	1:B:181:LYS:HE2	1.97	0.47
1:A:251:ILE:H	1:A:251:ILE:HD12	1.80	0.47
1:A:109:VAL:HG13	1:A:110:ILE:N	2.29	0.46
1:B:240:ASN:HB2	1:B:285:ILE:O	2.14	0.46
1:C:6:LEU:CD2	1:C:22:ILE:HD11	2.44	0.46
1:C:6:LEU:HB3	1:C:9:VAL:HG21	1.97	0.46
1:D:60:LEU:N	1:D:68:ASN:HD21	2.10	0.46
1:A:50:ALA:O	1:A:75:ARG:HD2	2.15	0.46
1:D:248:ALA:HB3	1:D:255:GLN:HB3	1.97	0.46
1:B:91:SER:H	1:B:94:GLU:HB2	1.81	0.46
1:A:236:SER:O	1:A:237:PRO:C	2.53	0.46
1:D:178:ARG:HG2	1:D:181:LYS:HE2	1.97	0.46
1:C:358:ASP:C	1:C:358:ASP:OD1	2.53	0.46
1:A:247:THR:CG2	1:A:257:GLU:HB2	2.45	0.46
1:A:92:VAL:HG12	1:A:96:MET:CE	2.46	0.46
1:B:283:LEU:C	1:B:283:LEU:CD2	2.83	0.46
1:B:351:ARG:NE	1:B:368:GLU:OE2	2.48	0.46
1:B:154:VAL:HG22	1:B:186:THR:HB	1.97	0.46
1:C:137:GLY:O	1:C:141:ARG:HD3	2.16	0.46
1:C:77:VAL:HG13	1:C:156:LEU:HG	1.98	0.46
1:A:235:GLY:O	1:A:236:SER:O	2.34	0.46
1:A:33:VAL:HG12	1:A:189:TYR:HB3	1.96	0.46
1:B:102:LEU:O	1:B:103:ALA:HB3	2.16	0.46
1:A:95:ASN:C	1:A:97:SER:H	2.19	0.46
1:B:92:VAL:HG22	1:B:134:LEU:HD11	1.98	0.46
1:B:300:LEU:HB3	1:B:320:ILE:HD13	1.98	0.46
1:D:82:GLN:HA	1:D:140:GLN:CD	2.36	0.46
1:A:152:PRO:O	1:A:185:ARG:NH1	2.47	0.46
1:B:51:GLY:O	1:B:52:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:LEU:CD2	1:A:179:LEU:HD22	2.46	0.46
1:D:48:MET:HE3	1:D:55:ILE:HA	1.98	0.45
1:C:11:LYS:O	1:C:18:VAL:HG12	2.15	0.45
1:D:154:VAL:HG22	1:D:186:THR:HB	1.97	0.45
1:A:11:LYS:O	1:A:18:VAL:HG12	2.15	0.45
1:D:92:VAL:HG22	1:D:134:LEU:HD11	1.98	0.45
1:A:254:VAL:CG2	1:A:272:SER:HA	2.47	0.45
1:A:110:ILE:O	1:A:111:ASN:HB3	2.17	0.45
2:C:382:ATP:C5'	1:D:135:SER:HB3	2.45	0.45
1:C:148:LEU:CD2	1:C:179:LEU:HD22	2.46	0.45
1:C:110:ILE:O	1:C:111:ASN:HB3	2.17	0.45
1:A:315:GLN:C	1:A:316:ILE:HD13	2.37	0.45
1:A:81:PHE:CE1	1:A:83:SER:HB2	2.51	0.45
1:D:51:GLY:O	1:D:52:LEU:HB2	2.16	0.45
1:D:302:GLY:HA3	1:D:319:GLN:O	2.16	0.45
1:D:91:SER:H	1:D:94:GLU:HB2	1.81	0.45
1:D:41:GLY:O	1:D:45:LEU:HB2	2.17	0.45
1:B:283:LEU:HD23	1:B:284:GLY:N	2.31	0.45
1:B:137:GLY:O	1:B:141:ARG:HD3	2.16	0.45
1:B:41:GLY:O	1:B:45:LEU:HB2	2.17	0.45
1:B:302:GLY:HA3	1:B:319:GLN:O	2.16	0.45
1:A:137:GLY:O	1:A:141:ARG:HD3	2.16	0.45
1:C:315:GLN:C	1:C:316:ILE:HD13	2.37	0.45
1:A:102:LEU:C	1:A:104:GLY:H	2.20	0.45
1:A:85:ALA:HB1	1:A:146:ARG:HH12	1.79	0.45
1:A:95:ASN:O	1:A:96:MET:CB	2.59	0.45
1:D:291:LEU:HD11	1:D:348:PRO:HB3	1.99	0.45
1:C:251:ILE:N	1:C:251:ILE:HD12	2.32	0.45
1:D:239:MET:HE3	1:D:286:ARG:CZ	2.47	0.45
1:A:254:VAL:HG23	1:A:272:SER:HB2	1.99	0.45
1:C:107:LYS:HA	1:C:110:ILE:CG2	2.47	0.45
1:A:107:LYS:HA	1:A:110:ILE:CG2	2.46	0.45
1:B:87:TYR:HB3	1:B:89:HIS:CE1	2.52	0.45
1:D:283:LEU:HD23	1:D:284:GLY:N	2.31	0.45
1:D:320:ILE:HG23	1:D:321:PRO:HD2	1.99	0.45
1:C:102:LEU:C	1:C:104:GLY:H	2.20	0.45
1:D:152:PRO:O	1:D:185:ARG:NH1	2.48	0.45
1:D:137:GLY:O	1:D:141:ARG:HD3	2.16	0.45
1:D:300:LEU:HB3	1:D:320:ILE:HD13	1.98	0.45
1:A:77:VAL:HG13	1:A:156:LEU:HG	1.98	0.45
1:B:253:GLN:HB3	1:B:267:TRP:CE3	2.52	0.45
1:D:46:LEU:HD23	1:D:158:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:GLU:O	1:B:185:ARG:NH1	2.46	0.44
1:C:152:PRO:O	1:C:185:ARG:NH1	2.47	0.44
1:C:6:LEU:HB3	1:C:9:VAL:CG2	2.47	0.44
1:C:297:ASP:N	1:C:297:ASP:OD1	2.50	0.44
1:C:84:TYR:HE1	1:C:140:GLN:HG3	1.81	0.44
1:D:102:LEU:O	1:D:103:ALA:HB3	2.16	0.44
1:D:86:LEU:HA	1:D:146:ARG:NH2	2.25	0.44
1:A:151:GLU:O	1:A:185:ARG:NH1	2.51	0.44
1:C:101:LYS:HZ1	1:C:102:LEU:HG	1.80	0.44
1:A:49:ILE:HA	1:A:60:LEU:HD21	1.98	0.44
1:A:87:TYR:CE1	1:A:98:PHE:CD2	3.06	0.44
1:A:18:VAL:HG22	1:A:18:VAL:O	2.17	0.44
1:B:321:PRO:O	1:B:322:SER:OG	2.22	0.44
1:A:236:SER:HG	1:A:237:PRO:CD	2.19	0.44
1:B:82:GLN:HA	1:B:140:GLN:CD	2.36	0.44
1:D:283:LEU:C	1:D:283:LEU:CD2	2.83	0.44
1:A:260:MET:CE	1:A:323:ILE:HD11	2.48	0.44
1:B:157:LEU:HD11	1:B:187:MET:CE	2.48	0.44
1:B:33:VAL:HG13	1:B:201:ALA:HB2	1.98	0.44
1:B:347:LEU:HD13	1:B:347:LEU:O	2.18	0.44
1:B:253:GLN:O	1:B:254:VAL:CG2	2.66	0.44
1:C:151:GLU:O	1:C:185:ARG:NH1	2.51	0.44
1:C:162:SER:O	1:C:163:ASN:HB2	2.18	0.44
1:A:17:VAL:HG11	1:A:20:LYS:HD2	2.00	0.44
1:B:291:LEU:HD11	1:B:348:PRO:HB3	1.99	0.44
1:D:157:LEU:HD11	1:D:187:MET:CE	2.48	0.44
1:A:207:LEU:N	1:A:207:LEU:HD12	2.34	0.43
1:C:260:MET:CE	1:C:323:ILE:HD11	2.48	0.43
1:C:159:GLU:N	1:C:160:PRO:CD	2.81	0.43
1:D:237:PRO:O	1:D:238:LYS:O	2.35	0.43
1:C:49:ILE:HA	1:C:60:LEU:HD21	1.99	0.43
1:A:259:PRO:HD2	1:A:260:MET:HE2	1.99	0.43
1:A:121:LEU:O	1:A:123:LEU:HD22	2.19	0.43
1:C:45:LEU:HA	1:C:48:MET:HE3	2.00	0.43
1:B:320:ILE:HG23	1:B:321:PRO:HD2	1.99	0.43
1:D:347:LEU:O	1:D:347:LEU:HD13	2.18	0.43
1:C:135:SER:HB3	2:D:382:ATP:O5'	2.18	0.43
1:A:159:GLU:N	1:A:160:PRO:CD	2.81	0.43
1:C:121:LEU:O	1:C:123:LEU:HD22	2.18	0.43
1:B:208:ASP:HB2	1:B:229:PHE:CZ	2.53	0.43
1:D:26:ILE:HG23	1:D:32:VAL:HG21	2.00	0.43
1:C:259:PRO:HB2	1:C:322:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:260:MET:HE2	1:A:260:MET:N	2.33	0.43
1:C:350:GLU:H	1:C:350:GLU:HG3	1.48	0.43
1:D:253:GLN:HB3	1:D:267:TRP:HE3	1.84	0.43
1:B:235:GLY:O	1:B:236:SER:O	2.37	0.43
1:D:87:TYR:HB3	1:D:89:HIS:CE1	2.53	0.43
1:D:86:LEU:O	1:D:88:PRO:HD3	2.19	0.43
1:A:346:GLY:O	1:A:348:PRO:HD3	2.18	0.43
1:C:260:MET:HE2	1:C:260:MET:N	2.32	0.43
1:A:162:SER:O	1:A:163:ASN:HB2	2.18	0.43
1:B:270:VAL:CG1	1:B:362:CYS:HB3	2.46	0.43
1:C:18:VAL:HG22	1:C:18:VAL:O	2.17	0.43
1:C:207:LEU:N	1:C:207:LEU:HD12	2.34	0.43
1:C:259:PRO:HD2	1:C:260:MET:HE2	2.01	0.43
1:C:6:LEU:N	1:C:6:LEU:HD12	2.34	0.43
1:C:120:VAL:HG23	1:C:121:LEU:N	2.34	0.43
1:B:46:LEU:HD23	1:B:158:ASP:HB2	1.99	0.43
1:A:10:THR:HA	1:A:19:SER:O	2.19	0.43
1:A:86:LEU:HD12	1:A:139:ARG:HB3	2.00	0.43
1:C:87:TYR:HB3	1:C:89:HIS:CE1	2.54	0.43
1:A:253:GLN:HB3	1:A:267:TRP:CE3	2.54	0.42
1:D:66:ARG:HG3	1:D:68:ASN:ND2	2.34	0.42
1:A:120:VAL:HG23	1:A:121:LEU:N	2.34	0.42
1:A:289:HIS:O	1:A:348:PRO:CG	2.67	0.42
1:A:59:ASP:HB2	1:A:61:PHE:HE1	1.84	0.42
1:A:135:SER:HB3	2:B:382:ATP:O5'	2.18	0.42
1:B:126:LEU:O	1:B:129:ARG:HB2	2.20	0.42
1:D:126:LEU:O	1:D:129:ARG:HB2	2.20	0.42
1:C:17:VAL:HG11	1:C:20:LYS:HD2	2.00	0.42
1:B:350:GLU:CD	1:B:350:GLU:H	2.17	0.42
1:C:107:LYS:HA	1:C:110:ILE:HG22	2.02	0.42
1:A:106:LYS:O	1:A:110:ILE:HG22	2.19	0.42
1:A:107:LYS:HA	1:A:110:ILE:HG22	2.02	0.42
1:B:253:GLN:O	1:B:254:VAL:HG23	2.19	0.42
1:D:47:ARG:NH1	1:D:47:ARG:HG2	2.35	0.42
1:B:117:VAL:HG11	1:B:149:VAL:CG2	2.49	0.42
1:A:101:LYS:HZ3	1:A:102:LEU:CG	2.30	0.42
1:C:260:MET:HE1	1:C:323:ILE:HD11	2.00	0.42
1:A:15:GLU:O	1:A:15:GLU:HG3	2.20	0.42
1:C:24:LEU:HD11	1:C:34:PHE:HE1	1.85	0.42
1:C:321:PRO:O	1:C:322:SER:OG	2.30	0.42
1:D:208:ASP:HB2	1:D:229:PHE:CZ	2.54	0.42
1:D:364:ARG:NH2	1:D:368:GLU:HG3	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:ILE:HG23	1:B:32:VAL:HG21	2.00	0.42
1:B:47:ARG:HG2	1:B:47:ARG:NH1	2.35	0.42
1:C:10:THR:HA	1:C:19:SER:O	2.19	0.42
1:A:113:ARG:HA	1:A:116:GLN:CG	2.50	0.42
1:C:135:SER:HB3	2:D:382:ATP:C5'	2.50	0.42
1:A:135:SER:HB3	2:B:382:ATP:C5'	2.50	0.42
1:D:109:VAL:HG22	1:D:109:VAL:O	2.20	0.42
1:A:24:LEU:HD11	1:A:34:PHE:HE1	1.85	0.42
1:A:259:PRO:HB2	1:A:322:SER:HB3	2.00	0.42
1:D:290:LEU:HB2	1:D:329:TYR:HD1	1.85	0.42
1:B:290:LEU:HB2	1:B:329:TYR:HD1	1.85	0.42
1:C:106:LYS:O	1:C:110:ILE:HG22	2.19	0.42
1:D:157:LEU:HD11	1:D:187:MET:HE2	2.02	0.42
1:B:306:VAL:HG12	1:B:307:VAL:N	2.35	0.42
1:D:117:VAL:HG11	1:D:149:VAL:CG2	2.49	0.42
1:C:113:ARG:HA	1:C:116:GLN:CG	2.50	0.42
1:B:83:SER:C	1:B:84:TYR:CD2	2.89	0.41
1:B:66:ARG:HG3	1:B:68:ASN:ND2	2.34	0.41
1:C:289:HIS:O	1:C:348:PRO:CG	2.68	0.41
1:B:240:ASN:O	1:B:284:GLY:HA2	2.20	0.41
1:B:81:PHE:CE2	1:B:156:LEU:O	2.73	0.41
1:D:202:ASP:OD2	1:D:202:ASP:C	2.58	0.41
1:A:270:VAL:HG13	1:A:362:CYS:HB3	2.03	0.41
1:B:109:VAL:HG22	1:B:109:VAL:O	2.20	0.41
1:C:59:ASP:HB2	1:C:61:PHE:HE1	1.84	0.41
1:D:362:CYS:O	1:D:363:ARG:C	2.58	0.41
1:D:309:GLN:NE2	1:D:309:GLN:HA	2.35	0.41
1:C:12:ALA:HB2	1:C:17:VAL:HA	2.03	0.41
1:C:46:LEU:HD11	1:C:188:ILE:HG22	2.03	0.41
1:C:84:TYR:O	1:C:85:ALA:CB	2.69	0.41
1:D:300:LEU:HD12	1:D:300:LEU:N	2.35	0.41
1:B:306:VAL:HB	1:B:317:HIS:HB2	2.01	0.41
1:A:134:LEU:HD22	1:A:138:GLN:NE2	2.36	0.41
1:D:70:THR:HB	1:D:75:ARG:CD	2.51	0.41
1:C:11:LYS:HG3	1:C:18:VAL:CG1	2.51	0.41
1:D:306:VAL:HB	1:D:317:HIS:HB2	2.01	0.41
1:B:51:GLY:C	1:B:53:GLU:H	2.24	0.41
1:D:240:ASN:O	1:D:284:GLY:HA2	2.20	0.41
1:C:228:ARG:HG2	1:C:228:ARG:NH1	2.35	0.41
1:B:11:LYS:HB2	1:B:48:MET:SD	2.61	0.41
1:B:300:LEU:HD12	1:B:300:LEU:N	2.35	0.41
1:C:166:ALA:O	1:C:170:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:236:SER:O	1:D:237:PRO:C	2.59	0.41
1:C:253:GLN:HB3	1:C:267:TRP:HE3	1.86	0.41
1:C:92:VAL:HG12	1:C:96:MET:CE	2.50	0.41
1:B:309:GLN:NE2	1:B:309:GLN:HA	2.35	0.41
1:A:318:ILE:HD12	1:A:345:ILE:HD13	2.03	0.41
1:A:12:ALA:HB2	1:A:17:VAL:HA	2.03	0.41
1:D:110:ILE:HD12	1:D:110:ILE:C	2.41	0.41
1:B:296:ALA:O	1:B:297:ASP:HB2	2.21	0.41
1:D:321:PRO:O	1:D:322:SER:CB	2.69	0.41
1:D:202:ASP:O	1:D:203:LYS:HB2	2.21	0.41
1:D:306:VAL:HG12	1:D:307:VAL:N	2.35	0.41
1:C:12:ALA:CB	1:C:17:VAL:HA	2.51	0.41
1:A:166:ALA:O	1:A:170:VAL:HG23	2.21	0.41
1:C:15:GLU:O	1:C:15:GLU:HG3	2.20	0.41
1:D:235:GLY:O	1:D:236:SER:O	2.39	0.41
1:D:51:GLY:C	1:D:53:GLU:H	2.24	0.41
1:C:130:LYS:O	1:C:131:PRO:C	2.60	0.41
1:C:65:LYS:O	1:C:67:MET:HG3	2.21	0.41
1:A:101:LYS:NZ	1:A:102:LEU:CG	2.82	0.40
1:D:33:VAL:CG1	1:D:201:ALA:HB2	2.47	0.40
1:B:46:LEU:CD2	1:B:158:ASP:HB2	2.51	0.40
1:C:260:MET:HE2	1:C:260:MET:H	1.86	0.40
1:C:173:ARG:HE	1:C:196:GLU:CG	2.31	0.40
1:C:318:ILE:HD12	1:C:345:ILE:HD13	2.03	0.40
1:B:110:ILE:HD12	1:B:110:ILE:C	2.41	0.40
1:B:4:VAL:O	1:B:26:ILE:O	2.40	0.40
1:A:305:GLN:O	1:A:339:GLU:HG3	2.22	0.40
1:D:62:ILE:O	1:D:67:MET:HE3	2.21	0.40
1:C:11:LYS:HG3	1:C:18:VAL:HG12	2.03	0.40
1:B:70:THR:HB	1:B:75:ARG:CD	2.51	0.40
1:D:305:GLN:HG3	1:D:326:ASN:OD1	2.21	0.40
1:B:255:GLN:HB2	1:B:267:TRP:CE2	2.56	0.40
1:C:95:ASN:O	1:C:96:MET:CB	2.61	0.40
1:A:46:LEU:HD11	1:A:188:ILE:HG22	2.02	0.40
1:A:260:MET:HE2	1:A:260:MET:H	1.86	0.40
1:A:173:ARG:HE	1:A:196:GLU:CG	2.31	0.40
1:A:12:ALA:CB	1:A:17:VAL:HA	2.51	0.40
1:A:20:LYS:O	1:A:21:ASP:C	2.60	0.40
1:D:296:ALA:O	1:D:297:ASP:HB2	2.21	0.40
1:A:130:LYS:O	1:A:131:PRO:C	2.60	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	Distance(Å)	Clash(Å)
1:B:253:GLN:NE2	1:C:85:ALA:CB[1.554]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/381 (96%)	307 (84%)	47 (13%)	11 (3%)	7	10
1	B	365/381 (96%)	305 (84%)	41 (11%)	19 (5%)	3	3
1	C	365/381 (96%)	304 (83%)	52 (14%)	9 (2%)	9	14
1	D	365/381 (96%)	306 (84%)	42 (12%)	17 (5%)	4	4
All	All	1460/1524 (96%)	1222 (84%)	182 (12%)	56 (4%)	5	6

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	SER
1	A	254	VAL
1	A	322	SER
1	B	73	ALA
1	B	83	SER
1	B	203	LYS
1	B	236	SER
1	B	238	LYS
1	B	324	ARG
1	C	85	ALA
1	C	236	SER
1	C	254	VAL
1	C	322	SER
1	D	73	ALA
1	D	83	SER
1	D	236	SER
1	D	238	LYS
1	D	254	VAL
1	D	324	ARG
1	A	21	ASP

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	251	ILE
1	A	339	GLU
1	B	66	ARG
1	B	107	LYS
1	B	254	VAL
1	B	295	ILE
1	C	21	ASP
1	C	107	LYS
1	C	339	GLU
1	D	66	ARG
1	D	107	LYS
1	D	203	LYS
1	D	295	ILE
1	A	5	GLN
1	A	85	ALA
1	B	64	GLU
1	B	82	GLN
1	B	296	ALA
1	D	64	GLU
1	D	82	GLN
1	D	296	ALA
1	B	80	VAL
1	D	80	VAL
1	D	363	ARG
1	B	84	TYR
1	B	152	PRO
1	B	363	ARG
1	C	298	VAL
1	D	152	PRO
1	A	298	VAL
1	B	85	ALA
1	B	237	PRO
1	D	237	PRO
1	A	295	ILE
1	C	295	ILE

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	312/323 (97%)	298 (96%)	14 (4%)	38	67
1	B	312/323 (97%)	296 (95%)	16 (5%)	33	60
1	C	312/323 (97%)	296 (95%)	16 (5%)	33	60
1	D	312/323 (97%)	296 (95%)	16 (5%)	33	60
All	All	1248/1292 (97%)	1186 (95%)	62 (5%)	34	61

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	53	GLU
1	A	68	ASN
1	A	81	PHE
1	A	82	GLN
1	A	116	GLN
1	A	129	ARG
1	A	219	LEU
1	A	266	VAL
1	A	274	ASP
1	A	288	GLU
1	A	342	THR
1	A	350	GLU
1	A	367	LYS
1	B	10	THR
1	B	25	ASP
1	B	31	PHE
1	B	33	VAL
1	B	68	ASN
1	B	79	MET
1	B	83	SER
1	B	98	PHE
1	B	113	ARG
1	B	116	GLN
1	B	123	LEU
1	B	130	LYS
1	B	288	GLU
1	B	293	SER
1	B	298	VAL
1	B	350	GLU
1	C	31	PHE
1	C	53	GLU
1	C	68	ASN

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Mol	Chain	Res	Type
1	C	81	PHE
1	C	82	GLN
1	C	116	GLN
1	C	129	ARG
1	C	219	LEU
1	C	249	THR
1	C	266	VAL
1	C	274	ASP
1	C	288	GLU
1	C	297	ASP
1	C	342	THR
1	C	350	GLU
1	C	367	LYS
1	D	10	THR
1	D	25	ASP
1	D	31	PHE
1	D	33	VAL
1	D	68	ASN
1	D	79	MET
1	D	83	SER
1	D	98	PHE
1	D	113	ARG
1	D	116	GLN
1	D	123	LEU
1	D	130	LYS
1	D	288	GLU
1	D	293	SER
1	D	298	VAL
1	D	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	68	ASN
1	A	82	GLN
1	A	253	GLN
1	A	255	GLN
1	A	276	GLN
1	A	309	GLN
1	B	7	GLN
1	B	68	ASN

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Mol	Chain	Res	Type
1	B	82	GLN
1	B	95	ASN
1	B	138	GLN
1	B	163	ASN
1	B	180	HIS
1	B	264	GLN
1	B	309	GLN
1	B	325	GLN
1	B	331	GLN
1	C	23	ASN
1	C	68	ASN
1	C	82	GLN
1	C	255	GLN
1	C	309	GLN
1	D	7	GLN
1	D	68	ASN
1	D	82	GLN
1	D	95	ASN
1	D	138	GLN
1	D	163	ASN
1	D	180	HIS
1	D	264	GLN
1	D	309	GLN
1	D	325	GLN
1	D	331	GLN
1	D	366	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ATP	A	382	-	33,33,33	2.11	10 (30%)	52,52,52	2.69	17 (32%)
2	ATP	B	382	-	33,33,33	2.16	10 (30%)	52,52,52	2.70	15 (28%)
2	ATP	C	382	-	33,33,33	2.11	11 (33%)	52,52,52	2.69	17 (32%)
2	ATP	D	382	-	33,33,33	2.16	10 (30%)	52,52,52	2.70	15 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	382	-	-	0/22/38/38	0/1/3/3
2	ATP	B	382	-	-	0/22/38/38	0/1/3/3
2	ATP	C	382	-	-	0/22/38/38	0/1/3/3
2	ATP	D	382	-	-	0/22/38/38	0/1/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	382	ATP	C4-N3	5.48	1.44	1.35
2	C	382	ATP	C4-N3	5.48	1.44	1.35
2	B	382	ATP	C4-N3	5.37	1.43	1.35
2	D	382	ATP	C4-N3	5.35	1.43	1.35
2	D	382	ATP	PB-O3A	5.20	1.69	1.59
2	B	382	ATP	PB-O3A	5.19	1.69	1.59
2	A	382	ATP	PB-O3A	5.13	1.69	1.59
2	C	382	ATP	PB-O3A	5.12	1.69	1.59
2	D	382	ATP	O5'-C5'	-4.42	1.26	1.44
2	B	382	ATP	O5'-C5'	-4.42	1.26	1.44
2	C	382	ATP	O5'-C5'	-4.24	1.27	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	382	ATP	O5'-C5'	-4.23	1.27	1.44
2	D	382	ATP	O4'-C1'	3.49	1.46	1.41
2	B	382	ATP	O4'-C1'	3.49	1.46	1.41
2	C	382	ATP	O4'-C1'	3.35	1.46	1.41
2	A	382	ATP	O4'-C1'	3.34	1.46	1.41
2	B	382	ATP	C8-N9	3.04	1.41	1.36
2	D	382	ATP	C8-N9	3.04	1.41	1.36
2	C	382	ATP	C8-N9	2.94	1.41	1.36
2	A	382	ATP	C8-N9	2.89	1.40	1.36
2	B	382	ATP	PA-O5'	-2.87	1.46	1.59
2	D	382	ATP	PA-O5'	-2.86	1.46	1.59
2	C	382	ATP	PA-O5'	-2.62	1.47	1.59
2	A	382	ATP	PA-O5'	-2.62	1.47	1.59
2	B	382	ATP	PB-O1B	-2.35	1.42	1.51
2	D	382	ATP	PB-O1B	-2.34	1.42	1.51
2	D	382	ATP	C8-N7	-2.26	1.30	1.34
2	D	382	ATP	C2'-C1'	2.23	1.56	1.53
2	B	382	ATP	C8-N7	-2.23	1.30	1.34
2	B	382	ATP	C2'-C1'	2.23	1.56	1.53
2	D	382	ATP	PB-O2B	-2.17	1.45	1.55
2	B	382	ATP	PB-O2B	-2.16	1.45	1.55
2	A	382	ATP	PB-O1B	-2.11	1.43	1.51
2	C	382	ATP	PB-O1B	-2.10	1.43	1.51
2	C	382	ATP	C2'-C1'	2.09	1.56	1.53
2	C	382	ATP	C3'-C4'	-2.08	1.47	1.53
2	A	382	ATP	C2'-C1'	2.07	1.56	1.53
2	A	382	ATP	C3'-C4'	-2.06	1.47	1.53
2	C	382	ATP	C8-N7	-2.02	1.30	1.34
2	C	382	ATP	PB-O2B	-2.01	1.46	1.55
2	A	382	ATP	PB-O2B	-2.01	1.46	1.55

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	382	ATP	O5'-C5'-C4'	11.54	151.30	108.94
2	A	382	ATP	O5'-C5'-C4'	11.53	151.27	108.94
2	D	382	ATP	O5'-C5'-C4'	11.43	150.89	108.94
2	B	382	ATP	O5'-C5'-C4'	11.42	150.87	108.94
2	D	382	ATP	O5'-PA-O1A	-7.29	80.80	109.37
2	B	382	ATP	O5'-PA-O1A	-7.29	80.83	109.37
2	A	382	ATP	O5'-PA-O1A	-6.57	83.64	109.37
2	C	382	ATP	O5'-PA-O1A	-6.56	83.68	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	382	ATP	C5'-C4'-C3'	-5.14	94.63	115.21
2	B	382	ATP	C5'-C4'-C3'	-5.14	94.63	115.21
2	A	382	ATP	C5'-C4'-C3'	-4.91	95.53	115.21
2	C	382	ATP	C5'-C4'-C3'	-4.90	95.57	115.21
2	B	382	ATP	PA-O5'-C5'	4.77	156.31	122.03
2	D	382	ATP	PA-O5'-C5'	4.76	156.29	122.03
2	C	382	ATP	O4'-C4'-C3'	4.60	114.49	105.17
2	A	382	ATP	O4'-C4'-C3'	4.58	114.46	105.17
2	C	382	ATP	PA-O5'-C5'	4.56	154.85	122.03
2	A	382	ATP	PA-O5'-C5'	4.56	154.83	122.03
2	D	382	ATP	O4'-C4'-C3'	4.21	113.71	105.17
2	B	382	ATP	O4'-C4'-C3'	4.20	113.68	105.17
2	D	382	ATP	O3A-PB-O3B	-4.08	93.37	101.66
2	B	382	ATP	O3A-PB-O3B	-4.07	93.39	101.66
2	A	382	ATP	O3A-PB-O3B	-3.88	93.77	101.66
2	C	382	ATP	O3A-PB-O3B	-3.87	93.80	101.66
2	D	382	ATP	C3'-C2'-C1'	3.82	106.89	100.91
2	B	382	ATP	C3'-C2'-C1'	3.81	106.87	100.91
2	D	382	ATP	O3A-PB-O1B	-3.57	85.69	111.28
2	B	382	ATP	O3A-PB-O1B	-3.56	85.72	111.28
2	C	382	ATP	C3'-C2'-C1'	3.48	106.35	100.91
2	A	382	ATP	C3'-C2'-C1'	3.47	106.33	100.91
2	A	382	ATP	O3A-PB-O1B	-3.44	86.56	111.28
2	C	382	ATP	O3A-PB-O1B	-3.44	86.56	111.28
2	A	382	ATP	O2A-PA-O3A	3.16	120.16	105.14
2	C	382	ATP	O2A-PA-O3A	3.16	120.12	105.14
2	A	382	ATP	C4-C5-N7	3.14	112.21	109.52
2	C	382	ATP	C4-C5-N7	3.14	112.21	109.52
2	D	382	ATP	O2B-PB-O3B	3.13	119.99	105.14
2	B	382	ATP	O2B-PB-O3B	3.13	119.97	105.14
2	D	382	ATP	O2A-PA-O3A	2.98	119.28	105.14
2	B	382	ATP	O2A-PA-O3A	2.98	119.27	105.14
2	A	382	ATP	O2B-PB-O3B	2.96	119.20	105.14
2	C	382	ATP	O2B-PB-O3B	2.96	119.19	105.14
2	A	382	ATP	N3-C2-N1	-2.88	126.30	128.71
2	B	382	ATP	N3-C2-N1	-2.87	126.31	128.71
2	C	382	ATP	N3-C2-N1	-2.82	126.35	128.71
2	D	382	ATP	N3-C2-N1	-2.80	126.37	128.71
2	D	382	ATP	C4-C5-N7	2.75	111.88	109.52
2	B	382	ATP	C4-C5-N7	2.74	111.87	109.52
2	C	382	ATP	O3A-PA-O5'	-2.57	91.90	103.41
2	A	382	ATP	O3A-PA-O5'	-2.57	91.93	103.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	ATP	C8-N9-C1'	2.50	131.31	126.38
2	D	382	ATP	C8-N9-C1'	2.50	131.31	126.38
2	C	382	ATP	C8-N9-C1'	2.46	131.23	126.38
2	A	382	ATP	C8-N9-C1'	2.45	131.21	126.38
2	A	382	ATP	O2G-PG-O1G	2.23	117.72	110.44
2	C	382	ATP	O2G-PG-O1G	2.22	117.69	110.44
2	B	382	ATP	O3A-PA-O5'	-2.17	93.70	103.41
2	D	382	ATP	O3A-PA-O5'	-2.17	93.71	103.41
2	C	382	ATP	O2A-PA-O5'	-2.14	97.71	108.51
2	A	382	ATP	O2A-PA-O5'	-2.14	97.73	108.51
2	B	382	ATP	C8-N9-C4	-2.14	105.27	106.90
2	D	382	ATP	C8-N9-C4	-2.09	105.30	106.90
2	C	382	ATP	C4'-O4'-C1'	-2.03	107.54	109.75
2	A	382	ATP	C4'-O4'-C1'	-2.02	107.56	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/381 (96%)	0.16	17 (4%) 31 27	29, 62, 99, 121	0
1	B	367/381 (96%)	0.56	42 (11%) 6 4	36, 71, 130, 149	0
1	C	367/381 (96%)	0.23	25 (6%) 17 14	29, 62, 99, 121	0
1	D	367/381 (96%)	0.62	47 (12%) 4 3	36, 71, 130, 149	0
All	All	1468/1524 (96%)	0.39	131 (8%) 10 7	29, 67, 117, 149	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	ALA	16.4
1	B	104	GLY	11.2
1	B	105	ALA	11.2
1	B	103	ALA	11.2
1	B	84	TYR	9.3
1	B	102	LEU	9.2
1	D	82	GLN	8.2
1	D	102	LEU	8.1
1	D	84	TYR	7.6
1	D	105	ALA	7.3
1	B	82	GLN	6.7
1	B	101	LYS	6.6
1	D	83	SER	5.6
1	B	106	LYS	4.8
1	D	324	ARG	4.8
1	D	104	GLY	4.7
1	B	59	ASP	4.6
1	D	109	VAL	4.4
1	B	61	PHE	4.4
1	D	85	ALA	4.2
1	B	202	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	108	GLU	4.0
1	B	60	LEU	4.0
1	A	108	GLU	4.0
1	B	15	GLU	3.8
1	C	295	ILE	3.8
1	A	4	VAL	3.8
1	B	78	GLY	3.8
1	B	296	ALA	3.8
1	D	78	GLY	3.8
1	D	74	GLU	3.8
1	D	69	ASP	3.7
1	D	20	LYS	3.7
1	D	59	ASP	3.7
1	B	87	TYR	3.7
1	C	263	ARG	3.6
1	C	69	ASP	3.5
1	D	112	GLN	3.5
1	B	52	LEU	3.5
1	A	253	GLN	3.4
1	C	102	LEU	3.4
1	D	101	LYS	3.4
1	B	83	SER	3.4
1	D	108	GLU	3.4
1	A	295	ILE	3.4
1	C	82	GLN	3.2
1	D	7	GLN	3.2
1	D	28	GLU	3.1
1	B	99	GLY	3.1
1	B	112	GLN	3.1
1	D	65	LYS	3.0
1	B	108	GLU	3.0
1	C	262	ASN	3.0
1	D	107	LYS	3.0
1	B	363	ARG	3.0
1	D	296	ALA	3.0
1	C	83	SER	3.0
1	D	97	SER	2.9
1	C	253	GLN	2.9
1	C	81	PHE	2.9
1	B	64	GLU	2.9
1	D	71	PRO	2.8
1	B	324	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	128	ASP	2.8
1	A	102	LEU	2.8
1	D	13	TRP	2.7
1	B	98	PHE	2.7
1	A	85	ALA	2.7
1	D	60	LEU	2.7
1	D	16	VAL	2.7
1	D	64	GLU	2.7
1	D	61	PHE	2.7
1	B	71	PRO	2.7
1	C	15	GLU	2.7
1	D	106	LYS	2.6
1	B	77	VAL	2.6
1	B	96	MET	2.6
1	C	84	TYR	2.5
1	C	103	ALA	2.5
1	B	65	LYS	2.5
1	A	263	ARG	2.5
1	D	79	MET	2.5
1	D	181	LYS	2.5
1	D	294	ASP	2.5
1	D	253	GLN	2.5
1	A	60	LEU	2.4
1	D	15	GLU	2.4
1	D	81	PHE	2.4
1	D	263	ARG	2.4
1	B	19	SER	2.4
1	A	211	ARG	2.4
1	A	83	SER	2.4
1	B	97	SER	2.4
1	B	107	LYS	2.4
1	B	16	VAL	2.3
1	D	115	ASN	2.3
1	B	116	GLN	2.3
1	B	109	VAL	2.3
1	A	69	ASP	2.3
1	D	110	ILE	2.3
1	B	181	LYS	2.3
1	B	92	VAL	2.2
1	C	251	ILE	2.2
1	C	54	THR	2.2
1	C	61	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	363	ARG	2.2
1	C	107	LYS	2.1
1	D	87	TYR	2.1
1	D	249	THR	2.1
1	A	87	TYR	2.1
1	D	92	VAL	2.1
1	D	96	MET	2.1
1	D	322	SER	2.1
1	A	324	ARG	2.1
1	C	95	ASN	2.1
1	A	297	ASP	2.1
1	B	74	GLU	2.1
1	B	13	TRP	2.1
1	B	294	ASP	2.1
1	D	252	ASP	2.1
1	B	81	PHE	2.1
1	C	28	GLU	2.1
1	C	14	GLY	2.1
1	B	253	GLN	2.0
1	C	16	VAL	2.0
1	A	109	VAL	2.0
1	A	96	MET	2.0
1	D	342	THR	2.0
1	C	85	ALA	2.0
1	A	95	ASN	2.0
1	C	301	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ATP	C	382	31/31	0.18	0.02	38,78,91,92	0
2	ATP	B	382	31/31	0.15	-0.29	63,87,98,98	0
2	ATP	D	382	31/31	0.16	-0.33	63,87,98,98	0
2	ATP	A	382	31/31	0.14	-0.36	38,78,91,92	0

6.5 Other polymers ⓘ

There are no such residues in this entry.