



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2016 – 03:00 PM EDT

PDB ID : 4WYB  
Title : Structure of the Bud6 flank domain in complex with actin  
Authors : Eck, M.J.; Park, E.; Zheng, W.  
Deposited on : 2014-11-17  
Resolution : 3.49 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

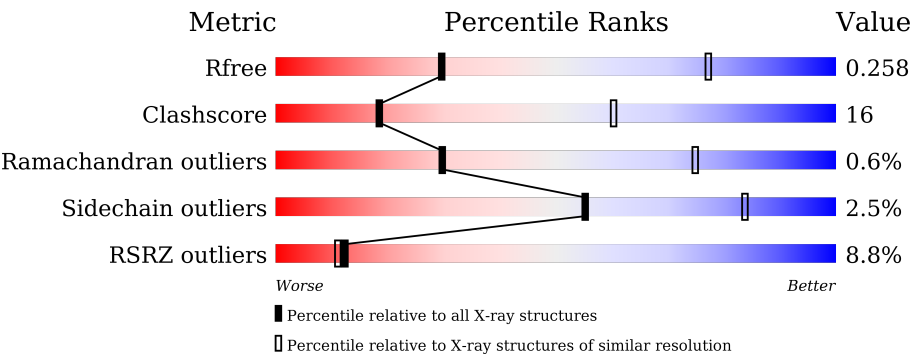
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>75%19%• 5%</div></div>
1	C	377	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>75%20%• 5%</div></div>
1	E	377	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>70%22%• 5%</div></div>
1	G	377	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>69%23%• 6%</div></div>
1	I	377	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>72%22%5%</div></div>
1	K	377	<div><div>10%</div><div><div></div><div></div><div></div><div></div></div><div>64%27%• • 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	M	377	
1	O	377	
1	Q	377	
1	S	377	
1	U	377	
1	X	377	
2	B	92	
2	D	92	
2	F	92	
2	H	92	
2	J	92	
2	L	92	
2	N	92	
2	P	92	
2	R	92	
2	T	92	
2	V	92	
2	Y	92	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37515 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2792	1770	468	536	18			
1	C	358	Total	C	N	O	S	0	0	0
			2803	1776	472	537	18			
1	E	358	Total	C	N	O	S	0	0	0
			2797	1773	469	537	18			
1	G	356	Total	C	N	O	S	0	0	0
			2765	1755	461	531	18			
1	I	358	Total	C	N	O	S	0	0	0
			2803	1776	472	537	18			
1	K	357	Total	C	N	O	S	0	0	0
			2782	1764	464	536	18			
1	M	358	Total	C	N	O	S	0	0	0
			2803	1776	472	537	18			
1	O	355	Total	C	N	O	S	0	0	0
			2768	1756	462	532	18			
1	Q	357	Total	C	N	O	S	0	0	0
			2787	1767	466	536	18			
1	S	358	Total	C	N	O	S	0	0	0
			2793	1771	469	535	18			
1	U	358	Total	C	N	O	S	0	0	0
			2787	1767	465	537	18			
1	X	358	Total	C	N	O	S	0	0	0
			2796	1772	471	535	18			

- Molecule 2 is a protein called Bud site selection protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	40	Total	C	N	O	S	0	0	0
			331	204	60	64	3			
2	D	38	Total	C	N	O	S	0	0	0
			314	192	57	62	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	37	Total	C	N	O	S	0	0	0
			303	186	53	61	3			
2	H	37	Total	C	N	O	S	0	0	0
			295	182	52	58	3			
2	J	39	Total	C	N	O	S	0	0	0
			309	189	54	63	3			
2	L	37	Total	C	N	O	S	0	0	0
			296	181	52	61	2			
2	N	37	Total	C	N	O	S	0	0	0
			303	186	53	61	3			
2	P	37	Total	C	N	O	S	0	0	0
			303	186	53	61	3			
2	R	37	Total	C	N	O	S	0	0	0
			291	179	51	58	3			
2	T	38	Total	C	N	O	S	0	0	0
			314	192	57	62	3			
2	V	37	Total	C	N	O	S	0	0	0
			293	181	51	59	2			
2	Y	37	Total	C	N	O	S	0	0	0
			303	186	53	61	3			

There are 24 discrepancies between the modelled and reference sequences:

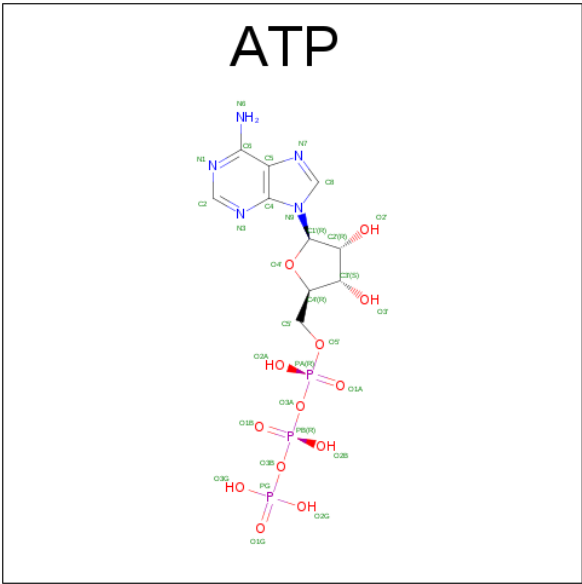
Chain	Residue	Modelled	Actual	Comment	Reference
B	697	GLY	-	expression tag	UNP P41697
B	698	SER	-	expression tag	UNP P41697
D	697	GLY	-	expression tag	UNP P41697
D	698	SER	-	expression tag	UNP P41697
F	697	GLY	-	expression tag	UNP P41697
F	698	SER	-	expression tag	UNP P41697
H	697	GLY	-	expression tag	UNP P41697
H	698	SER	-	expression tag	UNP P41697
J	697	GLY	-	expression tag	UNP P41697
J	698	SER	-	expression tag	UNP P41697
L	697	GLY	-	expression tag	UNP P41697
L	698	SER	-	expression tag	UNP P41697
N	697	GLY	-	expression tag	UNP P41697
N	698	SER	-	expression tag	UNP P41697
P	697	GLY	-	expression tag	UNP P41697
P	698	SER	-	expression tag	UNP P41697
R	697	GLY	-	expression tag	UNP P41697
R	698	SER	-	expression tag	UNP P41697
T	697	GLY	-	expression tag	UNP P41697

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Chain	Residue	Modelled	Actual	Comment	Reference
T	698	SER	-	expression tag	UNP P41697
V	697	GLY	-	expression tag	UNP P41697
V	698	SER	-	expression tag	UNP P41697
Y	697	GLY	-	expression tag	UNP P41697
Y	698	SER	-	expression tag	UNP P41697

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	O	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Q	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	U	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	X	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

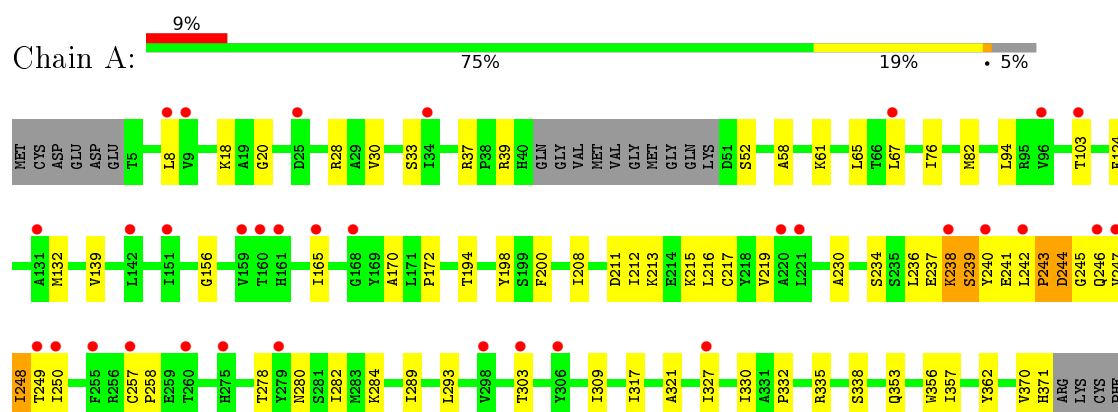
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	Q	1	Total	Ca	0	0
			1	1		
4	K	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	I	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	U	1	Total	Ca	0	0
			1	1		
4	X	1	Total	Ca	0	0
			1	1		
4	O	1	Total	Ca	0	0
			1	1		
4	S	1	Total	Ca	0	0
			1	1		
4	M	1	Total	Ca	0	0
			1	1		

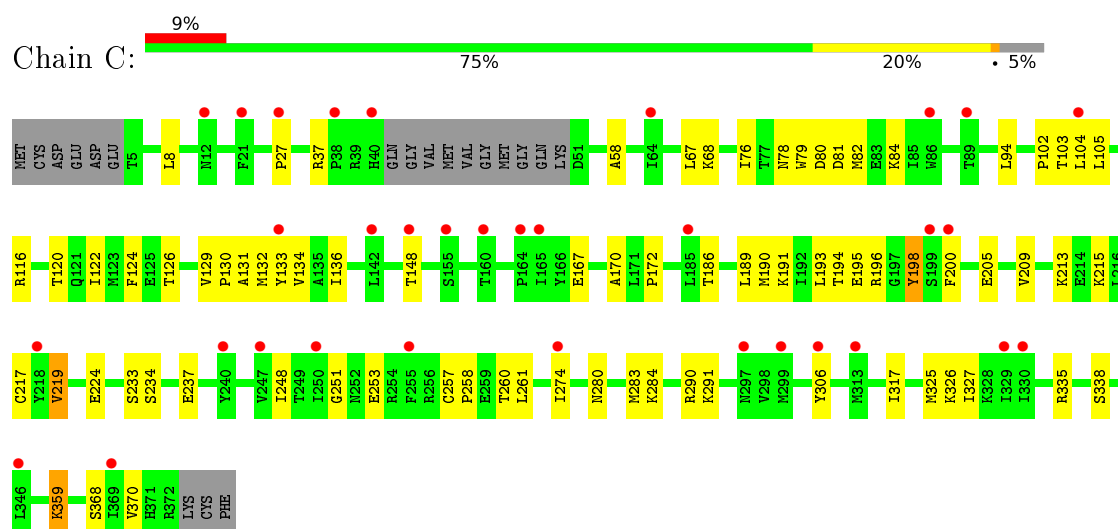
### 3 Residue-property plots [i](#)

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

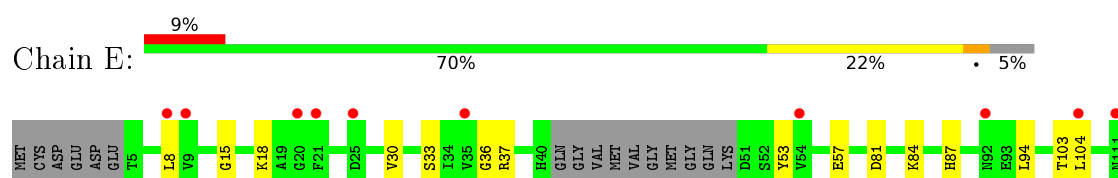
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

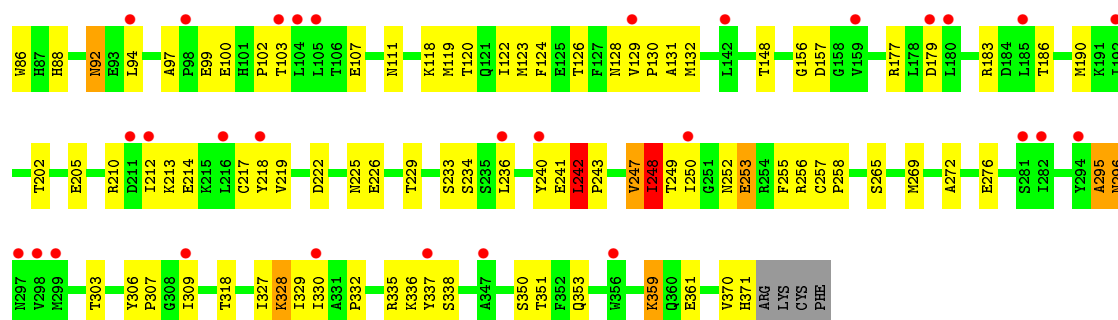


- Molecule 1: Actin, alpha skeletal muscle

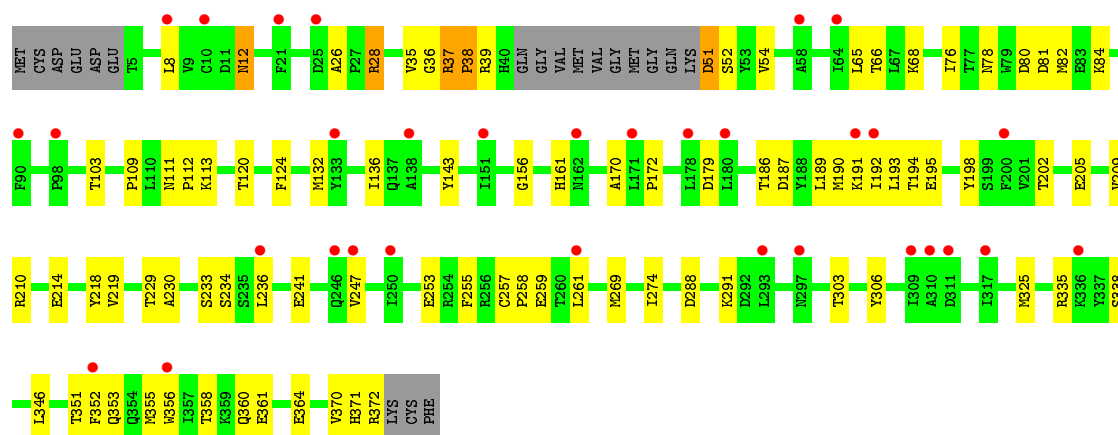
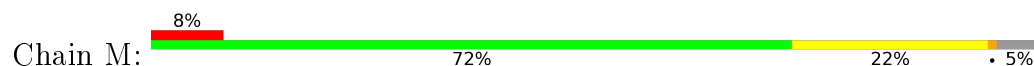




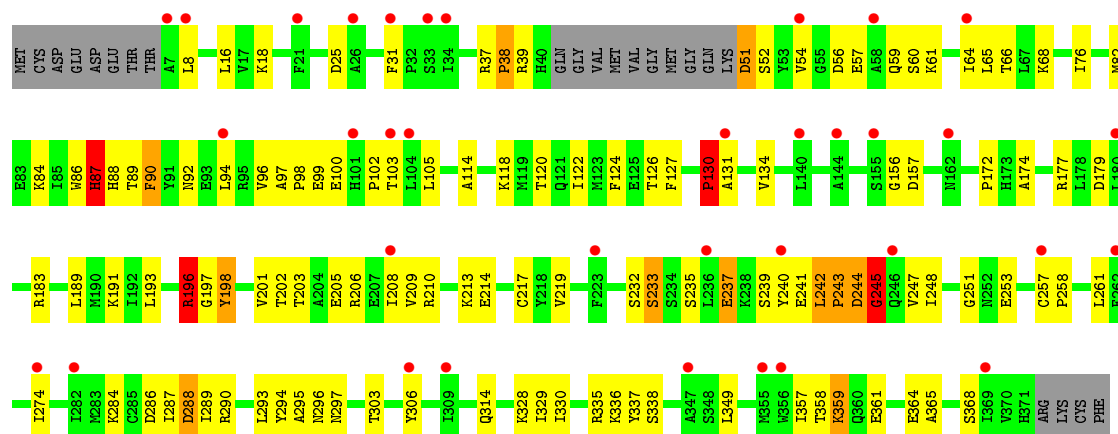




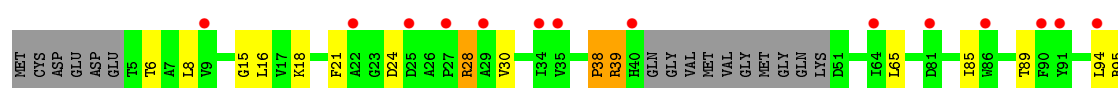
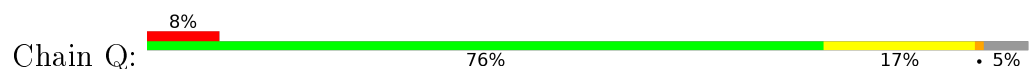
- Molecule 1: Actin, alpha skeletal muscle

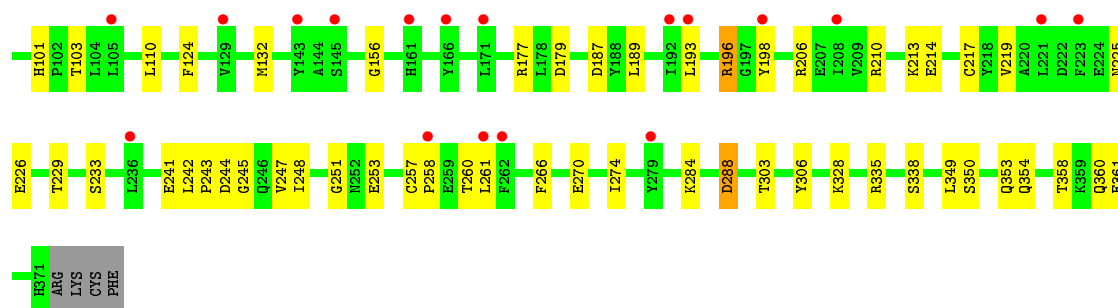


- Molecule 1: Actin, alpha skeletal muscle

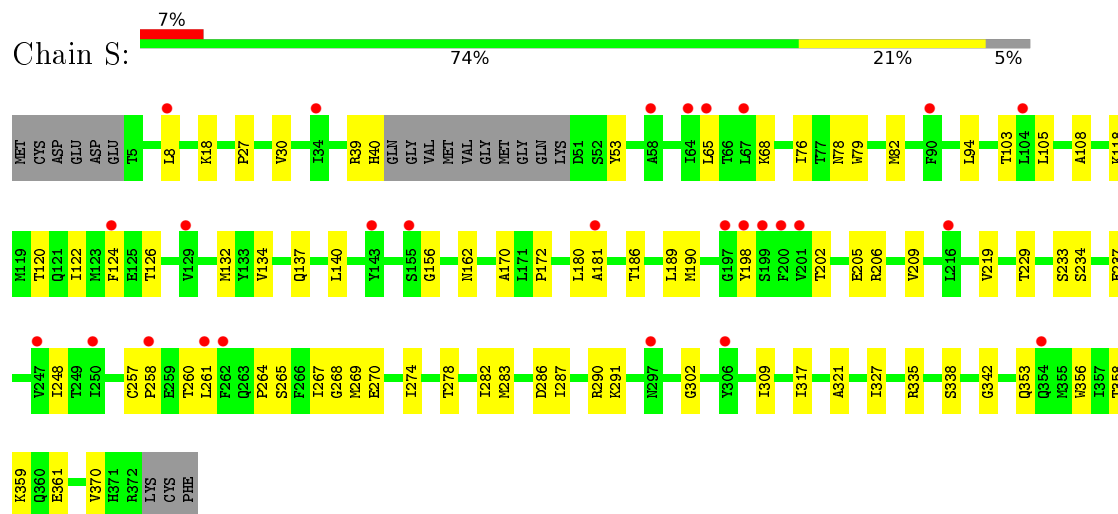


- Molecule 1: Actin, alpha skeletal muscle

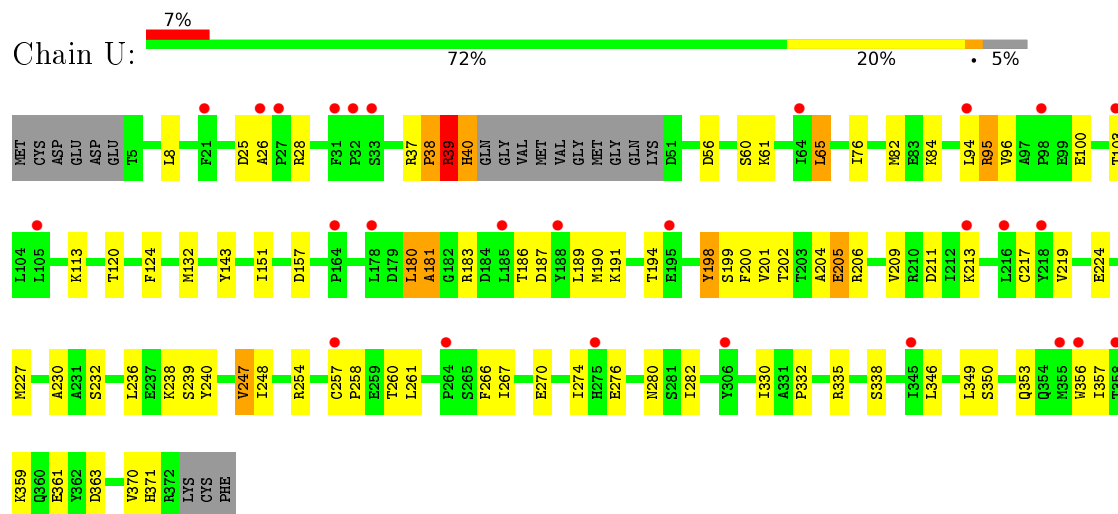




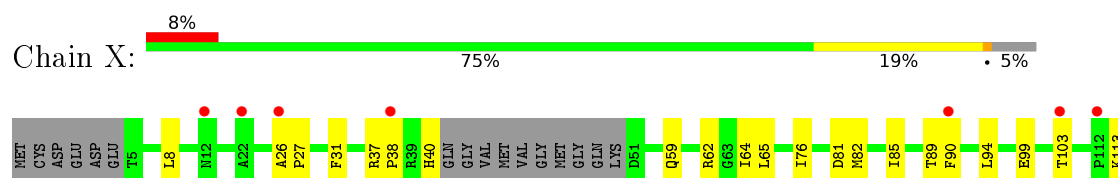
- Molecule 1: Actin, alpha skeletal muscle

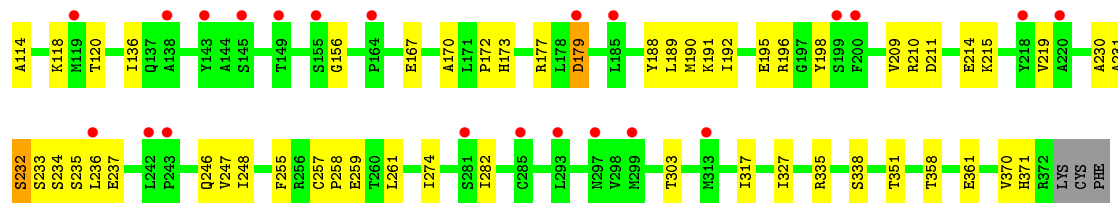


- Molecule 1: Actin, alpha skeletal muscle

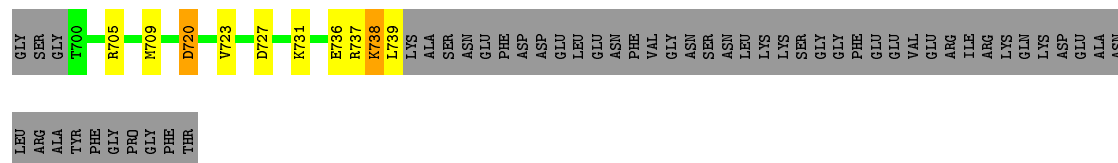


- Molecule 1: Actin, alpha skeletal muscle

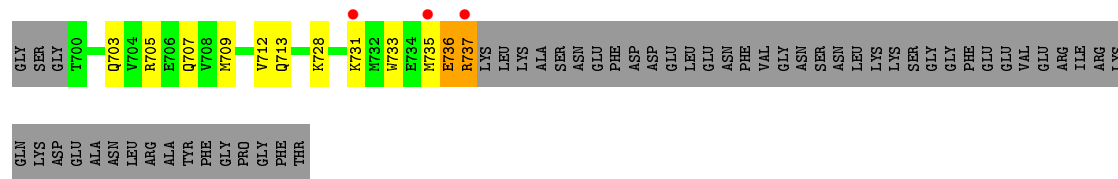




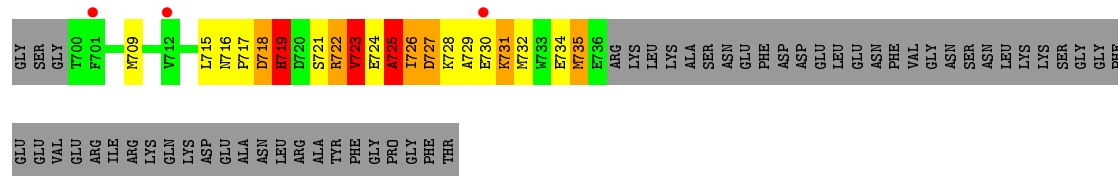
• Molecule 2: Bud site selection protein 6



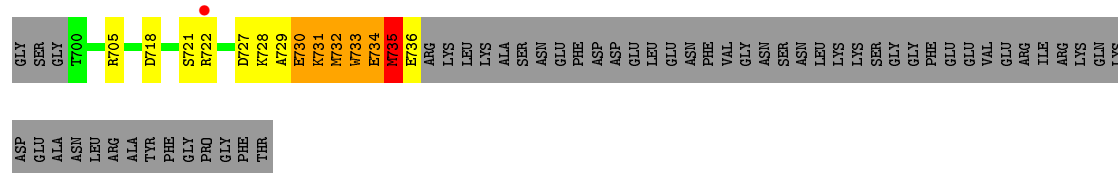
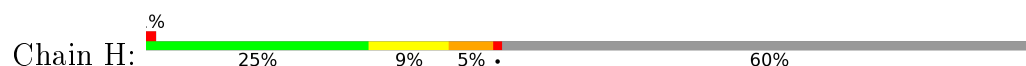
• Molecule 2: Bud site selection protein 6



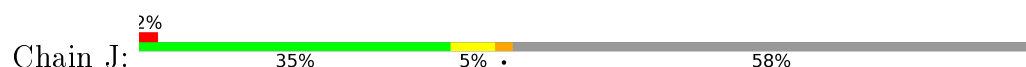
• Molecule 2: Bud site selection protein 6

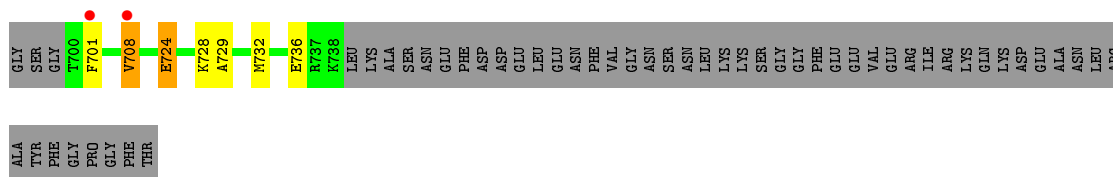


• Molecule 2: Bud site selection protein 6

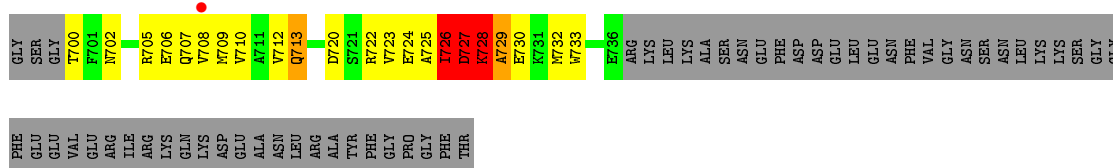


• Molecule 2: Bud site selection protein 6

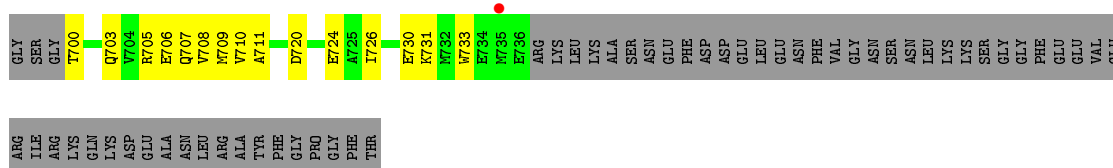




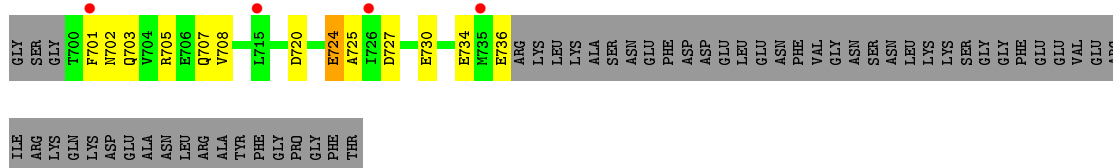
• Molecule 2: Bud site selection protein 6



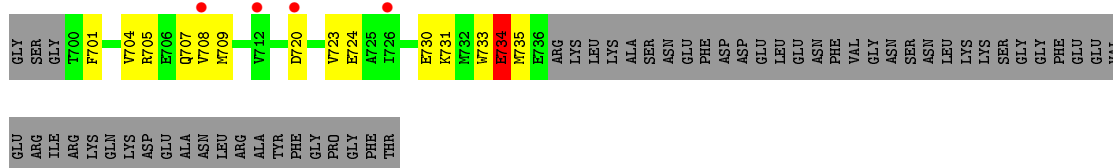
• Molecule 2: Bud site selection protein 6



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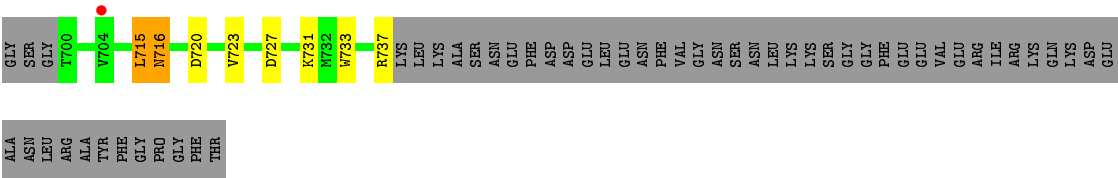


• Molecule 2: Bud site selection protein 6

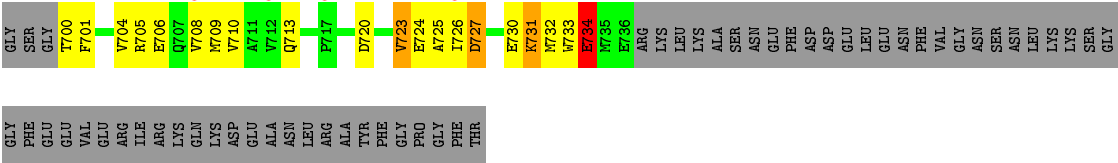


• Molecule 2: Bud site selection protein 6

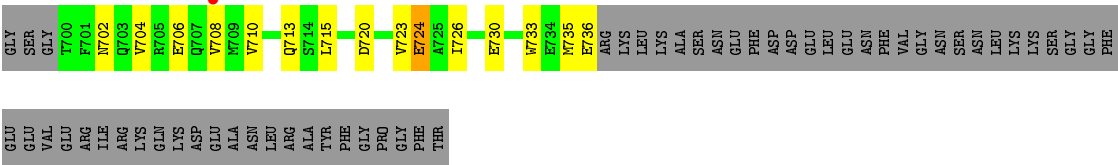




• Molecule 2: Bud site selection protein 6



• Molecule 2: Bud site selection protein 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.75Å 138.75Å 356.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.42 – 3.49 49.83 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.42-3.49) 93.1 (49.83-3.49)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.212 , 0.258 0.215 , 0.258	Depositor DCC
$R_{free}$ test set	1892 reflections (2.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l 0.428 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	37515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.27	0/2853	0.56	5/3870 (0.1%)
1	C	0.25	0/2864	0.45	0/3884
1	E	0.30	0/2858	0.61	6/3877 (0.2%)
1	G	0.27	0/2825	0.54	5/3835 (0.1%)
1	I	0.25	0/2864	0.46	0/3884
1	K	0.33	0/2843	0.62	7/3859 (0.2%)
1	M	0.27	0/2864	0.47	1/3884 (0.0%)
1	O	0.37	1/2829 (0.0%)	0.64	6/3839 (0.2%)
1	Q	0.25	0/2847	0.47	1/3862 (0.0%)
1	S	0.26	0/2854	0.52	3/3872 (0.1%)
1	U	0.26	0/2848	0.53	4/3866 (0.1%)
1	X	0.25	0/2857	0.54	4/3876 (0.1%)
2	B	0.36	0/335	0.64	0/449
2	D	0.43	0/318	0.61	0/427
2	F	0.49	0/307	1.15	5/413 (1.2%)
2	H	0.36	0/299	0.58	1/403 (0.2%)
2	J	0.27	0/313	0.48	0/423
2	L	0.51	0/300	1.23	4/406 (1.0%)
2	N	0.30	0/307	0.53	0/413
2	P	0.38	0/307	0.88	1/413 (0.2%)
2	R	0.35	0/295	0.66	0/399
2	T	0.36	0/318	0.67	0/427
2	V	0.51	0/297	1.00	3/401 (0.7%)
2	Y	0.28	0/307	0.54	0/413
All	All	0.29	1/37909 (0.0%)	0.57	56/51395 (0.1%)

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



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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	359	LYS	CD-CE	-5.10	1.38	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	196	ARG	CB-CA-C	-13.46	83.48	110.40
1	E	240	TYR	CB-CA-C	-11.91	86.59	110.40
2	L	726	ILE	N-CA-C	-11.31	80.45	111.00
1	X	231	ALA	CB-CA-C	-10.64	94.14	110.10
1	A	243	PRO	N-CA-C	-10.58	84.59	112.10
1	O	248	ILE	CB-CA-C	10.37	132.34	111.60
1	E	237	GLU	CB-CA-C	-10.20	90.00	110.40
1	E	242	LEU	CB-CA-C	-10.08	91.05	110.20
1	K	359	LYS	CB-CA-C	-9.75	90.90	110.40
2	L	729	ALA	CB-CA-C	9.57	124.45	110.10
1	X	231	ALA	N-CA-C	9.52	136.70	111.00
2	F	719	HIS	CB-CA-C	9.46	129.33	110.40
1	U	180	LEU	CB-CA-C	9.39	128.05	110.20
1	S	270	GLU	CB-CA-C	-9.09	92.21	110.40
1	G	196	ARG	CB-CA-C	-8.61	93.18	110.40
1	A	238	LYS	CB-CA-C	8.36	127.13	110.40
2	V	734	GLU	CB-CA-C	-8.09	94.22	110.40
1	G	336	LYS	N-CA-C	-8.03	89.32	111.00
1	S	268	GLY	N-CA-C	7.91	132.88	113.10
1	S	269	MET	CB-CA-C	7.88	126.15	110.40
1	G	334	GLU	CB-CA-C	-7.82	94.77	110.40
1	K	248	ILE	CB-CA-C	-7.78	96.04	111.60
2	F	723	VAL	CB-CA-C	7.58	125.80	111.40
1	A	238	LYS	N-CA-C	-7.30	91.30	111.00
1	E	245	GLY	N-CA-C	7.21	131.14	113.10
2	F	725	ALA	CB-CA-C	6.92	120.47	110.10
1	K	295	ALA	CB-CA-C	6.86	120.39	110.10
2	V	731	LYS	CB-CA-C	-6.80	96.79	110.40
1	K	361	GLU	CB-CA-C	6.77	123.94	110.40
1	A	245	GLY	N-CA-C	6.73	129.92	113.10
1	A	248	ILE	CB-CA-C	6.59	124.79	111.60
1	Q	28	ARG	NE-CZ-NH1	-6.53	117.04	120.30
2	V	727	ASP	CB-CG-OD1	-6.51	112.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	336	LYS	CB-CA-C	6.18	122.77	110.40
1	O	196	ARG	N-CA-C	6.05	127.33	111.00
1	K	242	LEU	CB-CA-C	5.89	121.39	110.20
1	U	180	LEU	N-CA-C	-5.88	95.12	111.00
2	F	718	ASP	N-CA-C	-5.84	95.23	111.00
2	L	728	LYS	CB-CA-C	5.67	121.73	110.40
1	O	244	ASP	N-CA-C	5.61	126.16	111.00
1	E	244	ASP	CB-CA-C	-5.57	99.26	110.40
1	O	242	LEU	CB-CA-C	-5.49	99.76	110.20
2	L	727	ASP	CB-CA-C	-5.43	99.53	110.40
1	X	233	SER	CB-CA-C	-5.42	99.79	110.10
1	E	181	ALA	CB-CA-C	-5.39	102.01	110.10
2	P	701	PHE	CB-CA-C	-5.30	99.79	110.40
2	H	733	TRP	CB-CA-C	-5.28	99.85	110.40
1	X	179	ASP	CB-CG-OD1	5.23	123.01	118.30
1	K	296	ASN	N-CA-C	5.22	125.09	111.00
1	O	237	GLU	CB-CA-C	-5.18	100.05	110.40
2	F	726	ILE	CB-CA-C	-5.13	101.35	111.60
1	M	37	ARG	C-N-CD	5.11	139.12	128.40
1	U	39	ARG	CB-CA-C	5.09	120.57	110.40
1	K	37	ARG	C-N-CD	5.08	139.07	128.40
1	U	65	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	G	126	THR	CB-CA-C	-5.04	97.98	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	245	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2753	93	0
1	C	2803	0	2769	62	0
1	E	2797	0	2758	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2765	0	2721	96	0
1	I	2803	0	2769	63	0
1	K	2782	0	2732	123	1
1	M	2803	0	2769	64	1
1	O	2768	0	2719	155	0
1	Q	2787	0	2751	57	0
1	S	2793	0	2754	50	0
1	U	2787	0	2736	63	0
1	X	2796	0	2756	54	0
2	B	331	0	325	7	0
2	D	314	0	301	9	0
2	F	303	0	287	47	0
2	H	295	0	278	21	0
2	J	309	0	281	10	0
2	L	296	0	270	37	0
2	N	303	0	288	8	0
2	P	303	0	288	10	0
2	R	291	0	267	17	0
2	T	314	0	301	12	0
2	V	293	0	271	16	0
2	Y	303	0	288	12	0
3	A	31	0	12	0	0
3	C	31	0	12	1	0
3	E	31	0	12	2	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
3	K	31	0	12	1	0
3	M	31	0	12	1	0
3	O	31	0	12	3	0
3	Q	31	0	12	1	0
3	S	31	0	12	1	0
3	U	31	0	12	0	0
3	X	31	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	1	0	0	0	0
4	U	1	0	0	0	0
4	X	1	0	0	0	0
All	All	37515	0	36576	1149	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 16.

All (1149) 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:K:240:TYR:CB	1:K:248:ILE:HG21	1.37	1.53
1:E:240:TYR:O	1:E:248:ILE:HG22	1.20	1.34
1:E:198:TYR:CE2	1:E:248:ILE:HG13	1.67	1.29
1:K:212:ILE:CG1	1:K:240:TYR:CE2	2.16	1.28
1:A:239:SER:CB	1:A:248:ILE:O	1.79	1.27
1:O:295:ALA:O	1:O:328:LYS:CD	1.82	1.26
1:O:90:PHE:CD2	1:O:98:PRO:HB3	1.72	1.24
2:H:735:MET:O	2:H:736:GLU:HG3	1.41	1.20
1:A:216:LEU:CD1	1:A:238:LYS:HG2	1.70	1.20
1:A:239:SER:HB3	1:A:248:ILE:O	1.05	1.19
1:X:234:SER:O	1:X:237:GLU:HG2	1.35	1.18
1:K:212:ILE:HG12	1:K:240:TYR:CD2	1.78	1.18
1:G:191:LYS:NZ	1:G:195:GLU:OE2	1.77	1.17
1:K:240:TYR:CB	1:K:248:ILE:CG2	2.23	1.17
1:G:198:TYR:OH	1:G:248:ILE:HG13	1.46	1.16
1:A:216:LEU:HD13	1:A:238:LYS:CG	1.76	1.16
1:O:241:GLU:OE2	1:O:245:GLY:O	1.64	1.15
2:L:709:MET:O	2:L:712:VAL:HG22	1.46	1.15
1:K:212:ILE:HG13	1:K:240:TYR:CE2	1.82	1.14
2:H:733:TRP:O	2:H:735:MET:N	1.77	1.14
1:K:212:ILE:HG12	1:K:240:TYR:CE2	1.80	1.14
1:O:296:ASN:OD1	1:O:328:LYS:NZ	1.81	1.13
1:K:240:TYR:N	1:K:248:ILE:HG22	1.64	1.13
1:K:240:TYR:HB2	1:K:248:ILE:HG21	1.17	1.12
1:K:240:TYR:H	1:K:248:ILE:HG22	1.12	1.12
1:K:240:TYR:HB3	1:K:248:ILE:HG21	1.15	1.12
1:K:247:VAL:HG12	1:K:248:ILE:H	0.99	1.11
1:O:296:ASN:HA	1:O:328:LYS:HD2	1.19	1.10
2:R:731:LYS:O	2:R:734:GLU:HB3	1.49	1.10
1:O:295:ALA:O	1:O:328:LYS:CG	1.99	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:724:GLU:CG	2:F:725:ALA:H	1.66	1.09
2:P:720:ASP:O	2:P:724:GLU:HG3	1.53	1.08
1:A:234:SER:HB2	1:A:237:GLU:HG2	1.30	1.08
1:K:240:TYR:HB3	1:K:248:ILE:CG2	1.78	1.08
1:E:198:TYR:HE2	1:E:248:ILE:CG1	1.66	1.08
2:L:727:ASP:O	2:L:730:GLU:O	1.69	1.08
1:O:208:ILE:HD13	1:O:242:LEU:HD22	1.37	1.07
1:G:334:GLU:OE1	1:G:334:GLU:N	1.88	1.05
1:O:208:ILE:CD1	1:O:242:LEU:HD22	1.86	1.04
1:G:193:LEU:O	1:G:198:TYR:HB2	1.54	1.04
1:A:216:LEU:HD22	1:A:238:LYS:HD3	1.36	1.04
1:G:332:PRO:HD2	1:G:335:ARG:HD2	1.35	1.04
2:B:737:ARG:O	2:B:738:LYS:O	1.76	1.04
1:A:208:ILE:HD12	1:A:242:LEU:CD2	1.85	1.04
1:A:234:SER:HB2	1:A:237:GLU:CG	1.90	1.02
1:K:240:TYR:CD2	1:K:248:ILE:HD13	1.94	1.02
1:O:208:ILE:HD12	1:O:242:LEU:CD2	1.89	1.02
1:E:198:TYR:CE2	1:E:248:ILE:CG1	2.42	1.01
1:G:127:PHE:O	1:G:129:VAL:N	1.92	1.01
1:G:198:TYR:OH	1:G:248:ILE:CG1	2.09	1.01
2:L:709:MET:O	2:L:712:VAL:CG2	2.08	1.00
1:A:208:ILE:HD12	1:A:242:LEU:HD23	1.40	1.00
2:H:733:TRP:C	2:H:735:MET:H	1.60	1.00
1:G:332:PRO:O	1:G:335:ARG:NH1	1.95	0.99
1:E:240:TYR:O	1:E:248:ILE:CG2	2.11	0.99
1:O:295:ALA:O	1:O:328:LYS:HD2	1.53	0.98
2:L:725:ALA:O	2:L:727:ASP:N	1.95	0.98
1:G:334:GLU:HG2	1:G:334:GLU:O	1.61	0.98
1:A:237:GLU:OE1	1:A:249:THR:HG21	1.62	0.98
1:K:61:LYS:O	1:K:64:ILE:CG2	2.10	0.98
1:O:208:ILE:CD1	1:O:242:LEU:CD2	2.43	0.97
1:A:198:TYR:CZ	1:A:248:ILE:HD11	2.02	0.95
1:A:198:TYR:CE1	1:A:248:ILE:HD11	2.02	0.95
1:O:241:GLU:CD	1:O:245:GLY:O	2.04	0.95
2:F:715:LEU:HD23	2:F:716:ASN:N	1.82	0.95
2:V:700:THR:O	2:V:704:VAL:HG13	1.66	0.95
1:O:296:ASN:CA	1:O:328:LYS:HD2	1.95	0.94
1:A:216:LEU:HD13	1:A:238:LYS:HG2	0.95	0.94
1:G:198:TYR:CE1	1:G:248:ILE:CG1	2.50	0.94
2:F:719:HIS:O	2:F:723:VAL:N	1.80	0.93
1:A:28:ARG:NH1	2:J:732:MET:SD	2.40	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:40:HIS:O	1:U:40:HIS:ND1	2.01	0.93
1:E:198:TYR:HE2	1:E:248:ILE:HG13	0.77	0.93
2:F:724:GLU:HG3	2:F:725:ALA:H	1.31	0.93
1:G:332:PRO:O	1:G:335:ARG:HD3	1.69	0.93
1:K:296:ASN:HA	1:K:328:LYS:HD2	1.51	0.93
1:G:193:LEU:HG	1:G:198:TYR:CD2	2.03	0.93
1:G:332:PRO:CD	1:G:335:ARG:HD2	2.00	0.92
1:K:212:ILE:CG1	1:K:240:TYR:CD2	2.44	0.92
1:O:61:LYS:HE2	1:O:64:ILE:HB	1.50	0.92
1:K:212:ILE:HG13	1:K:240:TYR:HE2	1.18	0.92
1:A:239:SER:CA	1:A:248:ILE:O	2.17	0.92
1:G:332:PRO:HD2	1:G:335:ARG:HB3	1.52	0.92
1:K:247:VAL:HG12	1:K:248:ILE:N	1.81	0.92
1:K:61:LYS:O	1:K:64:ILE:HG22	1.69	0.91
1:O:295:ALA:O	1:O:328:LYS:HG2	1.71	0.91
2:H:735:MET:O	2:H:736:GLU:CG	2.19	0.90
2:V:730:GLU:HA	2:V:733:TRP:CE3	2.06	0.90
1:O:90:PHE:HD2	1:O:98:PRO:HB3	1.18	0.90
2:F:725:ALA:O	2:F:728:LYS:N	2.03	0.90
1:G:123:MET:O	1:G:129:VAL:HG22	1.72	0.90
1:G:198:TYR:CE1	1:G:248:ILE:HG12	2.06	0.90
2:H:729:ALA:O	2:H:732:MET:N	2.05	0.90
2:F:724:GLU:CG	2:F:725:ALA:N	2.33	0.89
1:E:337:TYR:CD2	2:F:726:ILE:HD11	2.06	0.89
1:G:123:MET:HB3	1:G:129:VAL:HG21	1.53	0.89
2:L:723:VAL:O	2:L:726:ILE:O	1.90	0.89
2:F:724:GLU:HG3	2:F:725:ALA:N	1.86	0.88
1:E:208:ILE:CD1	1:E:242:LEU:CD2	2.51	0.88
1:X:234:SER:HB2	1:X:237:GLU:CD	1.93	0.88
1:A:37:ARG:CG	1:A:52:SER:HB3	2.03	0.87
1:E:337:TYR:CE2	2:F:726:ILE:HD11	2.09	0.87
1:E:208:ILE:HD12	1:E:242:LEU:HD23	1.57	0.86
1:K:240:TYR:HB3	1:K:248:ILE:CD1	2.05	0.86
1:Q:21:PHE:H	1:Q:28:ARG:HH12	1.20	0.86
2:T:727:ASP:O	2:T:731:LYS:HD3	1.75	0.86
1:O:295:ALA:C	1:O:328:LYS:CG	2.44	0.86
1:K:240:TYR:N	1:K:248:ILE:CG2	2.39	0.85
1:A:208:ILE:CD1	1:A:242:LEU:CD2	2.54	0.85
1:G:332:PRO:HD2	1:G:335:ARG:CD	2.05	0.85
1:A:37:ARG:HG3	1:A:52:SER:CB	2.04	0.85
1:G:198:TYR:HE1	1:G:248:ILE:CG1	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:736:GLU:O	2:D:737:ARG:O	1.95	0.85
1:G:335:ARG:HA	1:G:338:SER:OG	1.75	0.85
1:A:216:LEU:HD22	1:A:238:LYS:CD	2.05	0.85
1:E:216:LEU:O	1:E:254:ARG:NH1	2.10	0.85
1:E:189:LEU:O	1:E:192:ILE:HG13	1.75	0.84
1:X:234:SER:HB2	1:X:237:GLU:OE1	1.75	0.84
2:B:720:ASP:HA	2:B:723:VAL:HG12	1.60	0.84
2:F:724:GLU:O	2:F:726:ILE:HG22	1.76	0.84
1:A:37:ARG:HG2	1:A:52:SER:HB3	1.59	0.84
1:K:240:TYR:CD2	1:K:248:ILE:CD1	2.61	0.84
1:O:90:PHE:HD2	1:O:98:PRO:CB	1.90	0.84
1:K:240:TYR:HB3	1:K:248:ILE:CB	2.08	0.84
1:A:239:SER:HA	1:A:248:ILE:O	1.78	0.83
1:K:38:PRO:C	1:K:39:ARG:HG3	1.96	0.83
1:O:295:ALA:O	1:O:328:LYS:CE	2.27	0.83
2:V:724:GLU:HA	2:V:727:ASP:OD1	1.78	0.83
1:C:234:SER:OG	1:C:237:GLU:OE1	1.96	0.83
2:R:730:GLU:HA	2:R:733:TRP:CE3	2.13	0.83
1:O:241:GLU:CG	1:O:245:GLY:O	2.25	0.82
2:P:720:ASP:O	2:P:724:GLU:CG	2.27	0.82
1:G:198:TYR:CZ	1:G:248:ILE:HG13	2.14	0.82
1:K:240:TYR:HB3	1:K:248:ILE:HD13	1.60	0.82
1:E:194:THR:OG1	1:E:200:PHE:N	2.12	0.82
1:K:247:VAL:CG1	1:K:248:ILE:H	1.84	0.82
1:O:296:ASN:HA	1:O:328:LYS:CD	2.06	0.82
1:A:242:LEU:O	1:A:243:PRO:C	2.15	0.82
1:A:37:ARG:CG	1:A:52:SER:CB	2.58	0.82
1:K:240:TYR:CB	1:K:248:ILE:HD13	2.10	0.81
1:G:331:ALA:HB1	1:G:335:ARG:CZ	2.10	0.81
1:A:242:LEU:O	1:A:244:ASP:N	2.13	0.81
2:F:724:GLU:O	2:F:726:ILE:CG2	2.27	0.81
1:X:234:SER:CB	1:X:237:GLU:OE1	2.28	0.81
2:T:727:ASP:O	2:T:731:LYS:CD	2.29	0.81
1:C:189:LEU:O	1:C:193:LEU:HG	1.80	0.81
1:K:240:TYR:HD2	1:K:248:ILE:HD13	1.44	0.80
1:K:248:ILE:HG22	1:K:248:ILE:O	1.81	0.80
1:K:351:THR:HG21	2:L:707:GLN:HG3	1.63	0.80
1:G:198:TYR:CZ	1:G:248:ILE:CG1	2.65	0.80
1:O:102:PRO:HB3	1:O:131:ALA:HB3	1.62	0.80
1:E:216:LEU:HD22	1:E:238:LYS:HG2	1.62	0.80
2:R:730:GLU:HA	2:R:733:TRP:CZ3	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:ARG:O	2:B:738:LYS:C	2.20	0.79
1:E:198:TYR:HD1	1:E:198:TYR:H	1.31	0.79
1:O:241:GLU:HG3	1:O:245:GLY:O	1.82	0.79
1:C:194:THR:C	1:C:196:ARG:H	1.87	0.79
1:E:193:LEU:O	1:E:196:ARG:N	2.15	0.78
2:F:724:GLU:HG2	2:F:725:ALA:H	1.46	0.78
1:C:37:ARG:NH2	1:C:81:ASP:OD1	2.17	0.78
1:U:38:PRO:C	1:U:39:ARG:HG3	2.02	0.78
1:E:190:MET:SD	1:E:206:ARG:HB2	2.25	0.77
1:U:28:ARG:HH22	1:U:95:ARG:HH21	1.30	0.77
1:K:26:ALA:HB2	2:L:726:ILE:HD12	1.66	0.77
1:O:90:PHE:CE2	1:O:98:PRO:HB3	2.20	0.77
1:A:240:TYR:H	1:A:248:ILE:HG22	1.50	0.76
1:E:190:MET:HG2	1:E:209:VAL:HG11	1.67	0.76
1:A:208:ILE:CD1	1:A:242:LEU:HD22	2.14	0.76
2:F:722:ARG:O	2:F:724:GLU:N	2.18	0.76
1:E:208:ILE:CD1	1:E:242:LEU:HD23	2.14	0.76
1:E:241:GLU:HB2	1:E:246:GLN:O	1.85	0.76
2:H:727:ASP:OD1	2:H:731:LYS:HD3	1.85	0.76
1:Q:21:PHE:H	1:Q:28:ARG:NH1	1.84	0.76
1:I:335:ARG:HA	1:I:338:SER:HB2	1.66	0.76
1:K:248:ILE:CG2	1:K:248:ILE:O	2.32	0.76
1:O:202:THR:HG22	1:O:205:GLU:HG2	1.67	0.76
2:R:720:ASP:HA	2:R:723:VAL:HG12	1.68	0.76
2:H:735:MET:SD	2:H:736:GLU:N	2.59	0.76
1:K:240:TYR:CG	1:K:248:ILE:HD13	2.21	0.76
2:T:715:LEU:HD23	2:T:715:LEU:O	1.86	0.76
1:A:237:GLU:OE1	1:A:249:THR:CG2	2.34	0.75
1:E:217:CYS:HA	1:E:254:ARG:HG3	1.68	0.75
2:H:733:TRP:C	2:H:735:MET:N	2.29	0.75
1:A:37:ARG:HG3	1:A:52:SER:HB2	1.66	0.75
1:C:190:MET:HG2	1:C:209:VAL:HG11	1.69	0.75
1:O:90:PHE:CD2	1:O:98:PRO:CB	2.62	0.75
2:F:725:ALA:O	2:F:728:LYS:HB3	1.86	0.75
1:X:335:ARG:HA	1:X:338:SER:HB2	1.69	0.74
2:V:727:ASP:N	2:V:727:ASP:OD1	2.19	0.74
1:Q:177:ARG:NH2	1:Q:179:ASP:OD2	2.20	0.74
1:C:194:THR:C	1:C:196:ARG:N	2.38	0.74
1:K:212:ILE:CD1	1:K:240:TYR:CD2	2.71	0.74
1:G:193:LEU:O	1:G:198:TYR:CB	2.34	0.74
1:Q:241:GLU:HB2	1:Q:247:VAL:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:351:THR:CG2	2:L:707:GLN:HG3	2.18	0.73
1:E:337:TYR:CD2	2:F:726:ILE:CD1	2.70	0.73
1:A:240:TYR:O	1:A:247:VAL:HG13	1.89	0.73
2:F:724:GLU:O	2:F:727:ASP:N	2.21	0.73
1:C:129:VAL:HG23	1:C:359:LYS:HZ2	1.54	0.73
2:L:712:VAL:HG23	2:L:713:GLN:N	2.04	0.73
1:E:194:THR:HA	1:E:198:TYR:O	1.88	0.72
1:O:295:ALA:C	1:O:328:LYS:HD2	2.09	0.72
1:M:36:GLY:HA3	1:M:65:LEU:HD21	1.71	0.72
2:F:726:ILE:HG23	2:F:727:ASP:N	2.03	0.72
1:Q:187:ASP:OD1	1:Q:206:ARG:NH1	2.23	0.72
1:E:177:ARG:NH1	1:X:173:HIS:O	2.23	0.72
2:F:717:PRO:CG	2:F:719:HIS:HE1	2.03	0.72
2:Y:720:ASP:HA	2:Y:723:VAL:HG12	1.72	0.71
1:M:12:ASN:HD22	1:M:12:ASN:N	1.89	0.71
2:V:731:LYS:O	2:V:734:GLU:HG3	1.91	0.71
1:Q:21:PHE:N	1:Q:28:ARG:HH12	1.88	0.71
1:X:195:GLU:N	1:X:195:GLU:OE1	2.22	0.70
1:A:194:THR:HA	1:A:198:TYR:O	1.90	0.70
1:E:242:LEU:HB2	1:E:244:ASP:OD1	1.91	0.70
1:K:335:ARG:HA	1:K:338:SER:HB2	1.73	0.70
1:O:208:ILE:HD12	1:O:242:LEU:HD21	1.71	0.70
1:U:201:VAL:N	1:U:205:GLU:OE1	2.20	0.70
1:G:123:MET:O	1:G:129:VAL:CG2	2.39	0.70
1:K:61:LYS:O	1:K:64:ILE:HG23	1.92	0.70
1:Q:335:ARG:HA	1:Q:338:SER:HB2	1.73	0.70
1:A:234:SER:CB	1:A:237:GLU:HG2	2.17	0.70
1:O:54:VAL:HB	1:O:88:HIS:ND1	2.07	0.70
1:A:216:LEU:HD22	1:A:238:LYS:CG	2.22	0.70
1:E:244:ASP:OD1	1:E:245:GLY:N	2.25	0.69
1:G:145:SER:O	1:G:147:ARG:NH1	2.26	0.69
1:S:353:GLN:OE1	1:S:356:TRP:NE1	2.23	0.69
1:O:177:ARG:NH2	1:O:179:ASP:OD1	2.25	0.69
1:S:335:ARG:HA	1:S:338:SER:HB2	1.75	0.69
1:G:328:LYS:HE3	1:G:330:ILE:HG13	1.75	0.69
2:V:730:GLU:HA	2:V:733:TRP:CZ3	2.29	0.68
1:A:335:ARG:HA	1:A:338:SER:HB2	1.72	0.68
1:A:239:SER:HB2	1:A:247:VAL:HG12	1.74	0.68
2:F:718:ASP:O	2:F:722:ARG:HG3	1.94	0.68
1:O:156:GLY:O	1:O:303:THR:OG1	2.10	0.68
1:U:191:LYS:O	1:U:194:THR:OG1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:109:PRO:HG2	1:M:161:HIS:HD1	1.59	0.68
1:E:192:ILE:CG2	1:E:256:ARG:HH21	2.07	0.68
1:X:317:ILE:HG22	1:X:327:ILE:HD13	1.76	0.68
1:M:202:THR:HG22	1:M:205:GLU:HG3	1.74	0.68
1:K:212:ILE:CG1	1:K:240:TYR:HE2	1.79	0.68
1:K:25:ASP:O	2:L:726:ILE:HD11	1.94	0.68
1:G:331:ALA:HB1	1:G:335:ARG:NE	2.09	0.68
1:K:212:ILE:HD11	1:K:240:TYR:CD2	2.29	0.68
1:C:129:VAL:HG23	1:C:359:LYS:NZ	2.09	0.67
1:G:292:ASP:O	1:G:296:ASN:HB2	1.94	0.67
1:A:28:ARG:HH22	2:J:732:MET:HE3	1.58	0.67
1:M:36:GLY:CA	1:M:65:LEU:HD21	2.23	0.67
1:O:295:ALA:C	1:O:328:LYS:CD	2.63	0.67
1:C:78:ASN:ND2	1:C:81:ASP:OD2	2.28	0.67
1:I:202:THR:HG22	1:I:205:GLU:HG2	1.75	0.67
2:R:731:LYS:O	2:R:734:GLU:CB	2.37	0.67
1:G:198:TYR:CE1	1:G:248:ILE:HG13	2.30	0.67
1:K:59:GLN:HB2	1:K:62:ARG:HH21	1.58	0.67
1:K:92:ASN:N	1:K:92:ASN:OD1	2.28	0.67
1:O:335:ARG:HA	1:O:338:SER:HB2	1.77	0.66
1:G:198:TYR:HE1	1:G:248:ILE:CD1	2.08	0.66
1:O:358:THR:HG21	1:O:361:GLU:HG2	1.77	0.66
1:K:212:ILE:CD1	1:K:240:TYR:HD2	2.09	0.66
1:K:240:TYR:CA	1:K:248:ILE:CG2	2.73	0.66
1:E:188:TYR:O	1:E:192:ILE:HG12	1.96	0.66
1:Q:244:ASP:OD1	1:Q:245:GLY:N	2.29	0.66
1:A:219:VAL:HG12	1:A:258:PRO:HB2	1.79	0.65
1:A:28:ARG:NH2	2:J:732:MET:HE3	2.12	0.65
2:L:709:MET:C	2:L:712:VAL:HG22	2.16	0.65
1:A:216:LEU:CG	1:A:238:LYS:HG2	2.27	0.65
1:A:200:PHE:CZ	1:A:242:LEU:HD21	2.31	0.65
2:F:726:ILE:HG23	2:F:727:ASP:H	1.61	0.65
1:E:194:THR:OG1	1:E:199:SER:HA	1.96	0.65
1:E:198:TYR:CD2	1:E:248:ILE:HD11	2.32	0.64
1:K:54:VAL:HG12	1:K:55:GLY:N	2.12	0.64
2:V:732:MET:O	2:V:732:MET:HG2	1.96	0.64
2:Y:735:MET:O	2:Y:736:GLU:HG2	1.97	0.64
2:T:715:LEU:C	2:T:715:LEU:HD23	2.18	0.64
1:A:234:SER:O	1:A:237:GLU:HG2	1.98	0.64
2:B:731:LYS:HD3	1:I:6:THR:HG21	1.80	0.64
1:G:198:TYR:CZ	1:G:248:ILE:HG12	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:TYR:CZ	1:I:192:ILE:HD11	2.33	0.64
1:O:295:ALA:C	1:O:328:LYS:HG3	2.18	0.64
1:O:18:LYS:NZ	3:O:401:ATP:O2A	2.26	0.64
1:K:212:ILE:HD11	1:K:240:TYR:HD2	1.62	0.64
1:K:8:LEU:HB2	1:K:103:THR:HG22	1.78	0.64
2:L:727:ASP:O	2:L:730:GLU:C	2.36	0.64
1:M:28:ARG:O	1:M:28:ARG:HD2	1.98	0.64
1:E:186:THR:O	1:E:190:MET:HG3	1.98	0.63
1:O:241:GLU:OE2	1:O:245:GLY:C	2.36	0.63
1:G:240:TYR:HB3	1:G:248:ILE:HG22	1.79	0.63
2:L:709:MET:O	2:L:713:GLN:HG2	1.98	0.63
2:F:717:PRO:HG2	2:F:719:HIS:CE1	2.33	0.63
1:A:240:TYR:O	1:A:247:VAL:HA	1.98	0.63
2:L:720:ASP:HA	2:L:723:VAL:HG12	1.78	0.63
1:Q:270:GLU:N	1:Q:270:GLU:OE1	2.31	0.63
1:A:198:TYR:OH	1:A:248:ILE:HD11	1.98	0.63
2:F:722:ARG:O	2:F:723:VAL:C	2.37	0.63
1:X:8:LEU:HB2	1:X:103:THR:HG22	1.81	0.63
1:E:190:MET:CG	1:E:209:VAL:HG11	2.29	0.62
1:I:190:MET:HG2	1:I:209:VAL:HG11	1.80	0.62
1:K:156:GLY:O	1:K:303:THR:OG1	2.16	0.62
1:M:35:VAL:HB	1:M:68:LYS:HZ1	1.64	0.62
2:R:733:TRP:O	2:R:735:MET:N	2.33	0.62
1:S:219:VAL:HG12	1:S:258:PRO:HB2	1.81	0.62
2:H:731:LYS:N	2:H:731:LYS:HD2	2.13	0.62
1:K:38:PRO:O	1:K:39:ARG:HG3	1.98	0.62
1:G:123:MET:C	1:G:129:VAL:CG2	2.68	0.62
1:O:193:LEU:HG	1:O:196:ARG:NH2	2.15	0.62
1:Q:196:ARG:NH2	1:Q:253:GLU:OE1	2.30	0.62
1:I:202:THR:HG23	1:I:204:ALA:H	1.64	0.62
2:L:707:GLN:HA	2:L:710:VAL:HG22	1.79	0.62
1:M:12:ASN:ND2	1:M:12:ASN:N	2.47	0.62
1:G:198:TYR:HE1	1:G:248:ILE:HD11	1.63	0.62
1:X:234:SER:HB3	1:X:237:GLU:OE1	1.99	0.62
1:O:361:GLU:O	1:O:365:ALA:N	2.29	0.62
1:I:177:ARG:NH2	1:I:179:ASP:OD2	2.32	0.61
1:G:64:ILE:HG13	1:I:201:VAL:HG23	1.81	0.61
2:H:735:MET:C	2:H:736:GLU:HG3	2.20	0.61
1:U:38:PRO:N	1:U:65:LEU:HD21	2.15	0.61
1:A:216:LEU:HD12	1:A:250:ILE:HD11	1.81	0.61
1:A:239:SER:HB2	1:A:247:VAL:CG1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:8:LEU:HB2	1:M:103:THR:HG22	1.82	0.61
2:N:707:GLN:HA	2:N:710:VAL:HG22	1.83	0.61
1:A:216:LEU:CD1	1:A:238:LYS:CG	2.53	0.61
1:C:335:ARG:HA	1:C:338:SER:HB2	1.81	0.61
1:E:208:ILE:HD13	1:E:242:LEU:CD2	2.28	0.61
1:M:65:LEU:HD23	1:M:66:THR:N	2.16	0.60
1:Q:6:THR:HG22	1:Q:21:PHE:HB2	1.82	0.60
2:F:717:PRO:HB2	2:F:719:HIS:CE1	2.36	0.60
1:Q:38:PRO:HD3	1:Q:65:LEU:CD2	2.31	0.60
1:O:237:GLU:HG3	1:O:237:GLU:O	2.02	0.60
1:A:37:ARG:CG	1:A:52:SER:HB2	2.30	0.60
1:G:127:PHE:O	1:G:129:VAL:HG22	2.02	0.60
2:N:705:ARG:HA	2:N:708:VAL:HG12	1.84	0.60
2:T:731:LYS:N	2:T:731:LYS:HD2	2.17	0.60
1:E:192:ILE:HD12	1:E:253:GLU:HB3	1.84	0.60
2:F:715:LEU:HD23	2:F:716:ASN:C	2.22	0.60
1:Q:21:PHE:N	1:Q:28:ARG:HH22	1.99	0.60
1:E:173:HIS:O	1:X:177:ARG:NH2	2.28	0.59
1:K:100:GLU:C	1:K:130:PRO:HG3	2.21	0.59
1:A:353:GLN:HA	1:A:356:TRP:CD1	2.37	0.59
2:L:727:ASP:C	2:L:727:ASP:OD1	2.39	0.59
1:E:195:GLU:OE2	1:E:195:GLU:HA	2.01	0.59
2:H:730:GLU:HA	2:H:733:TRP:CE3	2.38	0.59
1:O:358:THR:HG22	1:O:361:GLU:H	1.67	0.59
1:U:359:LYS:NZ	1:U:363:ASP:OD2	2.32	0.59
1:E:230:ALA:HB2	1:E:236:LEU:HD12	1.85	0.59
1:E:242:LEU:C	1:E:244:ASP:H	2.05	0.59
1:G:190:MET:HG2	1:G:209:VAL:HG11	1.84	0.59
1:I:219:VAL:HG12	1:I:258:PRO:HB2	1.84	0.59
1:E:198:TYR:CD2	1:E:248:ILE:CG1	2.86	0.59
1:G:334:GLU:CG	1:G:334:GLU:O	2.29	0.59
1:O:61:LYS:HE2	1:O:64:ILE:CB	2.28	0.59
1:Q:24:ASP:OD2	1:Q:28:ARG:NH2	2.32	0.59
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.85	0.59
2:H:728:LYS:O	2:H:731:LYS:HB2	2.03	0.59
1:K:240:TYR:HD1	1:K:241:GLU:H	1.50	0.59
1:K:24:ASP:OD2	1:K:28:ARG:NH1	2.36	0.59
1:E:216:LEU:HB3	1:E:254:ARG:HD2	1.85	0.58
1:O:102:PRO:CB	1:O:131:ALA:HB3	2.33	0.58
1:G:189:LEU:O	1:G:193:LEU:N	2.28	0.58
1:I:244:ASP:OD1	1:I:245:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:233:SER:OG	1:M:234:SER:N	2.33	0.58
2:F:717:PRO:CG	2:F:719:HIS:CE1	2.85	0.58
1:Q:18:LYS:HG2	1:Q:30:VAL:HG22	1.83	0.58
1:C:283:MET:SD	1:C:290:ARG:NH1	2.77	0.58
1:E:198:TYR:CE2	1:E:248:ILE:CD1	2.85	0.58
1:G:18:LYS:HG2	1:G:30:VAL:HG22	1.85	0.58
1:A:246:GLN:HE21	1:A:248:ILE:HD13	1.66	0.58
2:F:731:LYS:O	2:F:735:MET:CG	2.51	0.58
1:A:317:ILE:HG22	1:A:327:ILE:HD13	1.84	0.58
1:G:219:VAL:HG12	1:G:258:PRO:HB2	1.86	0.58
1:I:8:LEU:HB2	1:I:103:THR:HG22	1.86	0.58
2:R:734:GLU:HG3	2:R:735:MET:HG3	1.85	0.58
1:X:234:SER:O	1:X:237:GLU:CG	2.31	0.58
1:U:202:THR:N	1:U:205:GLU:OE1	2.36	0.58
1:U:260:THR:HG22	1:U:266:PHE:HB2	1.86	0.58
1:C:131:ALA:N	1:C:359:LYS:HZ1	2.02	0.58
1:C:194:THR:O	1:C:196:ARG:N	2.36	0.58
1:S:190:MET:HG2	1:S:209:VAL:HG11	1.86	0.58
1:E:198:TYR:N	1:E:198:TYR:CD1	2.72	0.58
1:Q:38:PRO:HD3	1:Q:65:LEU:HD23	1.86	0.58
1:C:193:LEU:HD23	1:C:253:GLU:HG2	1.85	0.57
1:K:102:PRO:HB3	1:K:131:ALA:HB3	1.85	0.57
1:K:240:TYR:HB2	1:K:248:ILE:CG2	2.09	0.57
1:Q:8:LEU:HB2	1:Q:103:THR:HG22	1.85	0.57
2:T:716:ASN:OD1	2:T:716:ASN:N	2.36	0.57
1:U:28:ARG:HH22	1:U:95:ARG:NH2	2.01	0.57
1:Q:219:VAL:HG12	1:Q:258:PRO:HB2	1.86	0.57
1:C:233:SER:OG	1:C:234:SER:N	2.35	0.57
2:D:731:LYS:HE2	2:D:735:MET:HE1	1.86	0.57
1:G:156:GLY:O	1:G:303:THR:OG1	2.22	0.57
1:K:242:LEU:HD23	1:K:243:PRO:HD2	1.85	0.57
2:P:727:ASP:O	2:P:730:GLU:HB3	2.04	0.57
1:S:180:LEU:HD11	1:S:260:THR:HG22	1.87	0.57
1:Q:196:ARG:HD2	1:Q:198:TYR:CZ	2.40	0.57
1:G:332:PRO:HD2	1:G:335:ARG:CB	2.28	0.57
1:O:90:PHE:N	1:O:90:PHE:HD1	2.03	0.57
2:L:725:ALA:C	2:L:727:ASP:N	2.50	0.57
1:A:8:LEU:HB2	1:A:103:THR:HG22	1.87	0.57
1:O:131:ALA:HA	1:O:359:LYS:CE	2.35	0.56
1:O:157:ASP:HB2	3:O:401:ATP:H5'1	1.87	0.56
1:Q:156:GLY:O	1:Q:303:THR:OG1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:240:TYR:CD1	1:K:241:GLU:N	2.73	0.56
1:O:97:ALA:HB1	1:O:99:GLU:HG3	1.87	0.56
1:U:194:THR:HG22	1:U:199:SER:HA	1.86	0.56
2:Y:735:MET:O	2:Y:736:GLU:CG	2.53	0.56
1:A:216:LEU:HD22	1:A:238:LYS:HG2	1.87	0.56
1:G:233:SER:HG	1:G:235:SER:HG	1.43	0.56
1:K:157:ASP:O	1:K:183:ARG:HG3	2.05	0.56
2:P:705:ARG:HG3	2:P:705:ARG:HH11	1.69	0.56
1:Q:229:THR:O	1:Q:233:SER:HB3	2.06	0.56
1:Q:358:THR:HG23	1:Q:360:GLN:H	1.71	0.56
1:E:368:SER:HB2	2:Y:702:ASN:OD1	2.06	0.56
1:X:210:ARG:O	1:X:214:GLU:HG3	2.05	0.56
2:L:705:ARG:O	2:L:708:VAL:HG22	2.04	0.56
1:O:193:LEU:C	1:O:196:ARG:HD2	2.25	0.56
1:U:37:ARG:HH22	1:U:84:LYS:NZ	2.04	0.56
1:A:241:GLU:HA	1:A:246:GLN:O	2.05	0.56
1:E:337:TYR:HD2	2:F:726:ILE:CD1	2.17	0.56
1:M:241:GLU:HA	1:M:247:VAL:HA	1.87	0.56
1:O:100:GLU:HA	1:O:130:PRO:HG3	1.86	0.56
1:A:216:LEU:CD2	1:A:238:LYS:HG2	2.36	0.56
1:G:328:LYS:HZ2	1:G:330:ILE:HD11	1.70	0.56
1:K:64:ILE:O	1:K:65:LEU:HD23	2.06	0.56
2:Y:710:VAL:HA	2:Y:713:GLN:OE1	2.04	0.56
1:A:240:TYR:CG	1:A:241:GLU:N	2.73	0.56
1:O:232:SER:OG	1:O:233:SER:N	2.38	0.56
1:O:357:ILE:O	1:O:359:LYS:NZ	2.24	0.56
2:L:727:ASP:OD1	2:L:728:LYS:N	2.39	0.55
1:O:208:ILE:CD1	1:O:242:LEU:HD21	2.32	0.55
1:X:37:ARG:NH1	1:X:81:ASP:OD1	2.39	0.55
1:A:240:TYR:N	1:A:248:ILE:HG22	2.20	0.55
1:K:219:VAL:HG12	1:K:258:PRO:HB2	1.88	0.55
1:C:189:LEU:HD13	1:C:257:CYS:HB2	1.88	0.55
1:I:317:ILE:HG22	1:I:327:ILE:HD13	1.87	0.55
1:K:350:SER:HA	1:K:353:GLN:HG2	1.87	0.55
2:F:725:ALA:O	2:F:728:LYS:CB	2.54	0.55
2:F:731:LYS:O	2:F:735:MET:HG2	2.06	0.55
1:O:157:ASP:OD2	1:O:183:ARG:NE	2.37	0.55
1:C:167:GLU:O	2:D:705:ARG:NH1	2.32	0.55
2:L:730:GLU:OE1	2:L:733:TRP:HB2	2.06	0.55
1:E:198:TYR:N	1:E:198:TYR:HD1	2.01	0.55
1:M:360:GLN:O	1:M:364:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:700:THR:HA	2:N:703:GLN:NE2	2.22	0.55
1:S:8:LEU:HD22	1:S:94:LEU:HD13	1.88	0.55
1:A:211:ASP:O	1:A:215:LYS:HG3	2.06	0.55
1:K:295:ALA:O	1:K:328:LYS:HG2	2.07	0.55
1:S:358:THR:HG23	1:S:361:GLU:H	1.72	0.55
1:U:219:VAL:HG12	1:U:258:PRO:HB2	1.89	0.54
1:C:219:VAL:HG12	1:C:258:PRO:HB2	1.89	0.54
1:G:334:GLU:CD	1:G:334:GLU:H	2.05	0.54
1:K:212:ILE:CD1	1:K:240:TYR:CE2	2.86	0.54
2:Y:720:ASP:O	2:Y:724:GLU:HB3	2.07	0.54
1:M:210:ARG:O	1:M:214:GLU:HG3	2.07	0.54
1:M:156:GLY:O	1:M:303:THR:OG1	2.25	0.54
1:U:38:PRO:CD	1:U:65:LEU:HD21	2.37	0.54
1:X:76:ILE:HD13	1:X:82:MET:HG2	1.88	0.54
1:G:230:ALA:HB2	1:G:236:LEU:HD12	1.90	0.54
2:L:706:GLU:O	2:L:710:VAL:HG13	2.08	0.54
1:M:219:VAL:HG12	1:M:258:PRO:HB2	1.90	0.54
1:U:187:ASP:OD1	1:U:206:ARG:NH1	2.40	0.54
2:V:709:MET:O	2:V:713:GLN:HG2	2.08	0.54
1:X:211:ASP:O	1:X:215:LYS:HG3	2.08	0.54
1:X:31:PHE:HZ	1:X:89:THR:HG22	1.72	0.54
1:A:200:PHE:HZ	1:A:242:LEU:HD21	1.71	0.54
1:O:219:VAL:HG12	1:O:258:PRO:HB2	1.88	0.54
2:P:705:ARG:HG3	2:P:705:ARG:NH1	2.23	0.54
1:C:104:LEU:HD12	1:C:133:TYR:HB3	1.90	0.54
1:C:257:CYS:O	1:C:260:THR:OG1	2.25	0.54
1:E:190:MET:O	1:E:194:THR:HB	2.08	0.54
1:M:194:THR:HA	1:M:198:TYR:O	2.08	0.54
1:A:124:PHE:HZ	1:A:132:MET:HG2	1.73	0.54
1:C:280:ASN:O	1:C:284:LYS:HG2	2.08	0.54
1:O:90:PHE:CD1	1:O:90:PHE:N	2.72	0.54
1:X:246:GLN:OE1	1:X:247:VAL:N	2.41	0.54
1:A:244:ASP:OD1	1:A:244:ASP:C	2.46	0.54
1:A:18:LYS:HG2	1:A:30:VAL:HG22	1.89	0.54
1:E:242:LEU:O	1:E:244:ASP:N	2.41	0.54
1:M:191:LYS:O	1:M:195:GLU:HG3	2.08	0.54
1:X:156:GLY:O	1:X:303:THR:OG1	2.25	0.54
2:H:734:GLU:O	2:H:735:MET:HB2	2.09	0.53
1:O:241:GLU:OE2	1:O:245:GLY:CA	2.57	0.53
1:Q:210:ARG:O	1:Q:214:GLU:HG3	2.08	0.53
1:U:28:ARG:HG2	1:U:28:ARG:HH11	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:31:PHE:HZ	1:O:89:THR:HG23	1.72	0.53
1:A:238:LYS:O	1:A:249:THR:HA	2.08	0.53
1:G:113:LYS:HB3	1:G:371:HIS:NE2	2.24	0.53
1:G:317:ILE:HG22	1:G:327:ILE:HD13	1.88	0.53
2:V:700:THR:O	2:V:704:VAL:CG1	2.50	0.53
1:O:295:ALA:O	1:O:328:LYS:HE3	2.07	0.53
1:O:8:LEU:HD22	1:O:94:LEU:HD13	1.91	0.53
1:C:189:LEU:HD23	1:C:209:VAL:HG12	1.90	0.53
1:E:8:LEU:HB2	1:E:103:THR:HG22	1.90	0.53
1:G:202:THR:HG23	1:G:205:GLU:H	1.74	0.53
1:G:332:PRO:CD	1:G:335:ARG:HB3	2.33	0.53
1:G:239:SER:HA	1:G:248:ILE:O	2.08	0.53
1:I:18:LYS:HG2	1:I:30:VAL:HG22	1.90	0.53
1:U:38:PRO:O	1:U:39:ARG:HG3	2.08	0.53
1:I:229:THR:O	1:I:232:SER:OG	2.27	0.53
1:Q:350:SER:HA	1:Q:353:GLN:HG2	1.91	0.53
2:N:720:ASP:O	2:N:724:GLU:HG3	2.08	0.53
2:T:737:ARG:HG2	2:T:737:ARG:HH11	1.74	0.53
1:U:202:THR:HG22	1:U:205:GLU:HG3	1.90	0.53
2:L:712:VAL:HG23	2:L:713:GLN:H	1.73	0.53
1:Q:196:ARG:HD2	1:Q:198:TYR:CE2	2.43	0.53
1:A:8:LEU:HD22	1:A:94:LEU:HD13	1.89	0.52
1:S:189:LEU:HD13	1:S:257:CYS:HB2	1.92	0.52
1:I:242:LEU:HD12	1:I:242:LEU:H	1.73	0.52
2:T:727:ASP:O	2:T:731:LYS:HD2	2.06	0.52
1:C:8:LEU:HD22	1:C:94:LEU:HD13	1.92	0.52
1:Q:242:LEU:HD12	1:Q:244:ASP:H	1.74	0.52
1:U:189:LEU:HD23	1:U:209:VAL:HG13	1.91	0.52
1:C:190:MET:CG	1:C:209:VAL:HG11	2.36	0.52
2:H:718:ASP:OD1	2:H:721:SER:N	2.38	0.52
1:K:233:SER:OG	1:K:234:SER:N	2.42	0.52
2:L:722:ARG:O	2:L:726:ILE:HD13	2.09	0.52
1:E:192:ILE:HG22	1:E:256:ARG:HH21	1.74	0.52
2:F:726:ILE:CG2	2:F:727:ASP:N	2.73	0.52
1:E:192:ILE:HG21	1:E:256:ARG:HH21	1.73	0.52
1:M:76:ILE:HD13	1:M:82:MET:HG2	1.92	0.52
1:O:251:GLY:N	1:O:253:GLU:OE1	2.43	0.52
2:L:726:ILE:O	2:L:727:ASP:CB	2.57	0.52
1:E:208:ILE:HD12	1:E:242:LEU:CD2	2.24	0.52
1:O:120:THR:HB	1:O:124:PHE:CE2	2.44	0.52
1:O:130:PRO:HA	1:O:359:LYS:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:242:LEU:HB2	1:O:244:ASP:OD1	2.10	0.52
1:U:224:GLU:OE1	1:U:224:GLU:N	2.29	0.52
1:A:353:GLN:N	1:A:353:GLN:OE1	2.42	0.52
1:E:216:LEU:HD22	1:E:238:LYS:CG	2.36	0.52
1:I:252:ASN:OD1	1:I:256:ARG:NH2	2.43	0.52
1:O:286:ASP:OD1	1:O:287:ILE:N	2.43	0.52
1:X:234:SER:HB2	1:X:237:GLU:CG	2.39	0.52
1:G:21:PHE:HE2	1:G:28:ARG:HD3	1.75	0.52
1:I:232:SER:OG	1:I:233:SER:N	2.43	0.52
1:K:52:SER:O	1:K:84:LYS:HE2	2.10	0.52
1:M:355:MET:O	1:M:372:ARG:NH1	2.41	0.52
1:O:100:GLU:C	1:O:130:PRO:HG3	2.29	0.52
1:O:241:GLU:HG2	1:O:242:LEU:O	2.10	0.52
1:U:183:ARG:HB3	1:U:206:ARG:HH22	1.75	0.52
1:K:54:VAL:CG1	1:K:55:GLY:N	2.72	0.51
1:O:359:LYS:HD3	1:O:359:LYS:N	2.23	0.51
2:R:734:GLU:HG3	2:R:735:MET:N	2.25	0.51
1:E:241:GLU:OE1	1:E:246:GLN:O	2.29	0.51
1:G:296:ASN:HA	1:G:328:LYS:CE	2.41	0.51
1:O:241:GLU:OE2	1:O:245:GLY:HA2	2.09	0.51
1:U:100:GLU:OE1	1:U:100:GLU:N	2.43	0.51
1:X:64:ILE:HB	1:X:65:LEU:HD12	1.92	0.51
1:A:156:GLY:O	1:A:303:THR:OG1	2.28	0.51
1:K:148:THR:HG22	2:L:712:VAL:HG21	1.91	0.51
1:M:190:MET:HG2	1:M:209:VAL:HG11	1.92	0.51
1:M:230:ALA:HB2	1:M:236:LEU:HD12	1.92	0.51
1:O:359:LYS:HZ2	1:O:359:LYS:N	2.08	0.51
1:O:90:PHE:HD2	1:O:98:PRO:CG	2.23	0.51
1:U:38:PRO:HD3	1:U:65:LEU:HD21	1.92	0.51
1:U:94:LEU:O	1:U:96:VAL:HG13	2.10	0.51
1:O:213:LYS:O	1:O:217:CYS:HB2	2.10	0.51
1:O:295:ALA:C	1:O:328:LYS:HG2	2.23	0.51
1:U:8:LEU:HB2	1:U:103:THR:HG22	1.92	0.51
1:C:205:GLU:O	1:C:209:VAL:HG23	2.10	0.51
1:C:76:ILE:HD13	1:C:82:MET:HG2	1.92	0.51
1:K:63:GLY:O	1:K:64:ILE:HB	2.11	0.51
1:U:330:ILE:HG22	1:U:332:PRO:HD3	1.92	0.51
1:X:120:THR:HG21	1:X:370:VAL:HB	1.92	0.51
1:C:291:LYS:HD3	1:C:325:MET:SD	2.51	0.51
1:G:126:THR:HG22	1:G:127:PHE:CD1	2.46	0.51
1:I:180:LEU:HD11	1:I:260:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:37:ARG:C	1:O:65:LEU:HD21	2.30	0.51
1:O:87:HIS:HB2	1:O:127:PHE:CE1	2.45	0.51
1:U:353:GLN:HA	1:U:356:TRP:CD1	2.46	0.51
1:C:124:PHE:CZ	1:C:132:MET:HG2	2.46	0.51
1:G:191:LYS:O	1:G:195:GLU:HG3	2.11	0.51
1:O:8:LEU:HB2	1:O:103:THR:HG22	1.93	0.51
1:K:210:ARG:O	1:K:214:GLU:HG3	2.11	0.51
1:K:52:SER:O	1:K:52:SER:OG	2.28	0.51
2:N:706:GLU:O	2:N:710:VAL:HG13	2.11	0.51
1:I:241:GLU:HB2	1:I:247:VAL:HG12	1.94	0.50
2:L:726:ILE:N	2:L:726:ILE:CD1	2.74	0.50
1:E:216:LEU:HB3	1:E:254:ARG:CD	2.40	0.50
1:X:190:MET:HG3	1:X:209:VAL:HG11	1.94	0.50
1:O:239:SER:OG	1:O:247:VAL:HG12	2.10	0.50
1:U:25:ASP:HB2	2:V:725:ALA:CB	2.41	0.50
1:A:124:PHE:HD2	1:A:362:TYR:CG	2.29	0.50
1:A:216:LEU:CD2	1:A:238:LYS:CG	2.89	0.50
1:C:186:THR:O	1:C:190:MET:HG3	2.11	0.50
2:N:730:GLU:HA	2:N:733:TRP:CE3	2.46	0.50
2:T:720:ASP:HA	2:T:723:VAL:HG12	1.93	0.50
1:U:113:LYS:HB3	1:U:371:HIS:CE1	2.46	0.50
1:I:39:ARG:HH11	1:I:39:ARG:HG2	1.77	0.50
1:K:213:LYS:O	1:K:217:CYS:HB2	2.11	0.50
1:K:359:LYS:O	1:K:359:LYS:HG2	2.11	0.50
1:O:157:ASP:O	1:O:183:ARG:HG3	2.12	0.50
1:S:39:ARG:O	1:S:39:ARG:HG2	2.11	0.50
1:O:130:PRO:C	1:O:359:LYS:HE2	2.31	0.50
1:Q:39:ARG:HA	1:Q:39:ARG:NE	2.26	0.50
1:E:15:GLY:O	1:E:33:SER:HB3	2.12	0.50
1:E:251:GLY:N	1:E:253:GLU:OE1	2.45	0.50
1:O:336:LYS:HE3	1:O:337:TYR:CE2	2.47	0.50
1:I:76:ILE:HD13	1:I:82:MET:HG2	1.94	0.50
1:S:202:THR:HG23	1:S:205:GLU:H	1.77	0.50
1:S:286:ASP:OD1	1:S:287:ILE:N	2.45	0.50
1:A:238:LYS:O	1:A:250:ILE:N	2.40	0.49
1:M:193:LEU:HD12	1:M:253:GLU:HG2	1.94	0.49
1:O:56:ASP:O	1:O:60:SER:OG	2.29	0.49
1:A:76:ILE:HD13	1:A:82:MET:HG2	1.94	0.49
1:E:208:ILE:HD13	1:E:242:LEU:HD22	1.93	0.49
1:G:79:TRP:CE2	1:G:118:LYS:HD2	2.47	0.49
1:O:131:ALA:HA	1:O:359:LYS:HE2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:205:GLU:HA	1:O:208:ILE:HG12	1.95	0.49
1:O:90:PHE:O	1:O:96:VAL:O	2.28	0.49
1:C:8:LEU:HB2	1:C:103:THR:HG22	1.94	0.49
1:M:288:ASP:HB3	1:S:291:LYS:HD3	1.93	0.49
1:A:216:LEU:HD13	1:A:238:LYS:CB	2.41	0.49
2:D:703:GLN:O	2:D:707:GLN:HG3	2.12	0.49
1:I:239:SER:HA	1:I:248:ILE:O	2.13	0.49
1:M:37:ARG:HG3	1:M:68:LYS:HE3	1.94	0.49
1:O:202:THR:HG22	1:O:205:GLU:CG	2.41	0.49
1:Q:257:CYS:O	1:Q:260:THR:OG1	2.30	0.49
1:X:219:VAL:HG12	1:X:258:PRO:HB2	1.93	0.49
2:H:718:ASP:OD1	2:H:721:SER:OG	2.29	0.49
1:Q:21:PHE:H	1:Q:28:ARG:CZ	2.25	0.49
2:R:734:GLU:OE2	2:R:735:MET:HG3	2.12	0.49
1:E:260:THR:HG22	1:E:266:PHE:HB2	1.94	0.49
2:F:715:LEU:HD23	2:F:716:ASN:H	1.68	0.49
1:G:169:TYR:CZ	2:H:705:ARG:NH1	2.80	0.49
1:O:88:HIS:CD2	1:O:92:ASN:HB2	2.47	0.49
1:U:120:THR:HG21	1:U:370:VAL:HB	1.95	0.49
1:X:230:ALA:HA	1:X:236:LEU:HD12	1.95	0.49
1:A:198:TYR:CZ	1:A:248:ILE:CD1	2.87	0.49
2:F:730:GLU:O	2:F:734:GLU:HG3	2.12	0.49
1:M:26:ALA:HB2	2:N:726:ILE:HD12	1.95	0.49
1:O:76:ILE:HD12	1:O:82:MET:HG2	1.93	0.49
2:F:717:PRO:CB	2:F:719:HIS:CE1	2.96	0.49
1:M:306:TYR:CZ	3:M:401:ATP:H2	2.31	0.49
1:O:31:PHE:CZ	1:O:89:THR:CG2	2.96	0.49
1:Q:196:ARG:HH21	1:Q:253:GLU:CD	2.14	0.49
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.95	0.48
1:C:78:ASN:OD1	1:C:79:TRP:N	2.45	0.48
2:F:718:ASP:O	2:F:722:ARG:CG	2.60	0.48
1:M:261:LEU:HB3	1:M:274:ILE:HD13	1.95	0.48
1:O:57:GLU:N	1:O:57:GLU:OE1	2.42	0.48
1:S:257:CYS:HB3	1:S:258:PRO:HD3	1.94	0.48
2:T:727:ASP:C	2:T:731:LYS:HD3	2.33	0.48
2:V:705:ARG:HA	2:V:708:VAL:HG12	1.95	0.48
1:K:240:TYR:H	1:K:248:ILE:CG2	2.01	0.48
1:K:328:LYS:O	1:K:329:ILE:HG13	2.13	0.48
1:O:189:LEU:O	1:O:193:LEU:N	2.44	0.48
1:U:270:GLU:N	1:U:270:GLU:OE1	2.45	0.48
1:U:276:GLU:O	1:U:280:ASN:ND2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG22	1:A:293:LEU:HG	1.96	0.48
1:C:58:ALA:HB1	1:C:67:LEU:HD22	1.94	0.48
1:K:218:TYR:OH	1:K:236:LEU:HD13	2.12	0.48
1:M:189:LEU:HD12	1:M:192:ILE:HD11	1.93	0.48
1:U:200:PHE:HD1	1:U:205:GLU:HB3	1.78	0.48
1:E:15:GLY:O	1:E:33:SER:N	2.29	0.48
2:F:731:LYS:O	2:F:735:MET:SD	2.71	0.48
1:G:121:GLN:O	1:G:125:GLU:HB2	2.12	0.48
1:G:98:PRO:CG	1:G:127:PHE:HB3	2.44	0.48
1:G:189:LEU:HA	1:G:192:ILE:HG12	1.94	0.48
1:G:120:THR:HG21	1:G:370:VAL:HB	1.96	0.48
1:S:358:THR:OG1	1:S:359:LYS:N	2.46	0.48
1:K:336:LYS:HE3	1:K:337:TYR:CE1	2.48	0.48
1:A:280:ASN:O	1:A:284:LYS:HG3	2.13	0.48
1:E:335:ARG:HA	1:E:338:SER:HB3	1.96	0.48
1:G:257:CYS:HB3	1:G:258:PRO:HD3	1.95	0.48
1:K:306:TYR:CE1	3:K:401:ATP:H2	2.31	0.48
1:O:368:SER:HG	2:R:701:PHE:HD2	1.62	0.48
1:C:198:TYR:CE1	1:C:248:ILE:HD11	2.48	0.48
1:G:233:SER:OG	1:G:235:SER:OG	2.24	0.48
1:K:351:THR:HB	2:L:708:VAL:HG12	1.96	0.48
1:Q:196:ARG:NH2	1:Q:251:GLY:H	2.12	0.48
1:M:202:THR:N	1:M:205:GLU:OE2	2.36	0.48
1:M:291:LYS:HG3	1:M:325:MET:SD	2.53	0.48
1:Q:193:LEU:HD12	1:Q:253:GLU:HG2	1.94	0.48
1:Q:21:PHE:H	1:Q:28:ARG:HH22	1.59	0.48
1:Q:21:PHE:H	1:Q:28:ARG:NH2	2.12	0.48
1:C:257:CYS:HB3	1:C:258:PRO:HD3	1.96	0.48
1:M:136:ILE:H	1:M:136:ILE:HD12	1.78	0.48
1:M:358:THR:OG1	1:M:361:GLU:OE1	2.30	0.48
1:O:25:ASP:HB2	2:P:725:ALA:CB	2.44	0.48
1:Q:349:LEU:HD23	2:R:708:VAL:HG23	1.96	0.48
1:E:372:ARG:HH22	1:X:113:LYS:NZ	2.12	0.48
2:F:718:ASP:HB3	2:F:721:SER:HB2	1.94	0.48
1:K:296:ASN:HA	1:K:328:LYS:CD	2.35	0.48
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.95	0.47
1:G:104:LEU:HD12	1:G:133:TYR:HB3	1.96	0.47
1:A:237:GLU:CD	1:A:249:THR:CG2	2.82	0.47
1:O:54:VAL:HB	1:O:88:HIS:CE1	2.49	0.47
1:U:61:LYS:O	1:U:65:LEU:HB2	2.15	0.47
1:G:123:MET:O	1:G:127:PHE:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:TYR:O	1:G:341:ILE:HG13	2.15	0.47
1:I:120:THR:HG21	1:I:370:VAL:HB	1.95	0.47
1:K:226:GLU:HA	1:K:229:THR:HB	1.95	0.47
1:O:296:ASN:N	1:O:328:LYS:HD2	2.28	0.47
1:C:291:LYS:HE3	1:C:326:LYS:HB3	1.96	0.47
1:E:210:ARG:O	1:E:214:GLU:HG3	2.14	0.47
1:E:53:TYR:HB3	1:E:57:GLU:HG3	1.95	0.47
1:G:37:ARG:NH2	1:G:81:ASP:OD1	2.47	0.47
1:I:202:THR:HG22	1:I:205:GLU:CG	2.44	0.47
1:M:143:TYR:HD2	1:M:346:LEU:HD12	1.78	0.47
1:S:317:ILE:HG22	1:S:327:ILE:HD13	1.96	0.47
1:S:68:LYS:HE3	1:S:78:ASN:HD21	1.79	0.47
1:E:261:LEU:HB3	1:E:274:ILE:HD13	1.97	0.47
1:I:251:GLY:O	1:I:254:ARG:HG3	2.15	0.47
1:O:105:LEU:HB2	1:O:134:VAL:HG12	1.96	0.47
1:O:177:ARG:NH2	1:Q:284:LYS:HE2	2.29	0.47
1:O:31:PHE:HZ	1:O:89:THR:CG2	2.28	0.47
1:U:151:ILE:HG21	1:U:282:ILE:HD11	1.95	0.47
1:E:241:GLU:HB3	1:E:247:VAL:HA	1.95	0.47
1:E:120:THR:HG21	1:E:370:VAL:HB	1.97	0.47
1:G:189:LEU:HD13	1:G:257:CYS:HB2	1.96	0.47
2:L:712:VAL:CG2	2:L:713:GLN:N	2.73	0.47
2:L:724:GLU:O	2:L:727:ASP:HB3	2.13	0.47
1:S:321:ALA:HB3	1:S:327:ILE:HD11	1.96	0.47
1:U:180:LEU:HD12	1:U:267:ILE:HD11	1.97	0.47
1:E:104:LEU:HD12	1:E:133:TYR:HB3	1.96	0.47
1:K:148:THR:CG2	2:L:712:VAL:HG21	2.45	0.47
1:K:240:TYR:CG	1:K:248:ILE:CD1	2.91	0.47
1:S:108:ALA:HA	1:S:137:GLN:HE21	1.79	0.47
1:X:40:HIS:ND1	1:X:40:HIS:O	2.48	0.47
1:X:85:ILE:O	1:X:89:THR:HG23	2.15	0.47
1:E:219:VAL:HG11	1:E:309:ILE:HA	1.96	0.47
1:G:189:LEU:O	1:G:193:LEU:HB2	2.14	0.47
1:I:198:TYR:CD2	1:I:248:ILE:HD11	2.49	0.47
1:K:8:LEU:HD22	1:K:94:LEU:HD13	1.96	0.47
1:U:202:THR:HG23	1:U:204:ALA:H	1.80	0.47
1:U:198:TYR:CE1	1:U:248:ILE:HD11	2.49	0.47
1:U:65:LEU:HA	1:U:65:LEU:HD23	1.44	0.47
1:A:61:LYS:HB2	1:A:65:LEU:HD12	1.97	0.47
1:C:261:LEU:HB3	1:C:274:ILE:HD13	1.96	0.47
1:G:14:SER:O	1:G:183:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:59:GLN:HG3	1:X:62:ARG:CZ	2.44	0.47
1:E:162:ASN:HB2	1:E:176:MET:HB2	1.95	0.47
1:E:188:TYR:O	1:E:192:ILE:CG1	2.61	0.47
1:K:250:ILE:HG13	1:K:253:GLU:HG3	1.97	0.47
1:M:143:TYR:CD2	1:M:346:LEU:HD12	2.49	0.47
1:O:88:HIS:HD2	1:O:92:ASN:HB2	1.80	0.47
1:E:198:TYR:CD2	1:E:248:ILE:CD1	2.98	0.47
1:E:37:ARG:NH2	1:E:81:ASP:OD1	2.48	0.47
1:Q:85:ILE:O	1:Q:89:THR:OG1	2.28	0.47
1:X:230:ALA:CA	1:X:236:LEU:HD12	2.45	0.47
2:Y:730:GLU:HA	2:Y:733:TRP:CE3	2.50	0.47
1:C:148:THR:HG23	2:D:713:GLN:HG3	1.97	0.46
1:G:193:LEU:HG	1:G:198:TYR:CE2	2.45	0.46
2:B:736:GLU:OE1	1:I:95:ARG:NH2	2.49	0.46
1:I:372:ARG:HE	2:J:701:PHE:HZ	1.61	0.46
1:M:189:LEU:HD13	1:M:257:CYS:HB2	1.96	0.46
2:P:703:GLN:O	2:P:707:GLN:HG3	2.14	0.46
1:S:40:HIS:CG	1:S:40:HIS:O	2.68	0.46
1:U:357:ILE:HD13	1:U:370:VAL:HA	1.98	0.46
1:X:189:LEU:HD23	1:X:209:VAL:HG13	1.96	0.46
1:G:180:LEU:HD12	1:G:267:ILE:HD11	1.97	0.46
1:K:222:ASP:OD2	1:K:225:ASN:HB2	2.15	0.46
1:O:242:LEU:HB3	1:O:243:PRO:CD	2.45	0.46
2:R:733:TRP:O	2:R:734:GLU:C	2.54	0.46
1:C:80:ASP:O	1:C:84:LYS:HG3	2.15	0.46
1:I:213:LYS:O	1:I:217:CYS:HB2	2.15	0.46
1:M:113:LYS:HB3	1:M:371:HIS:CE1	2.50	0.46
1:M:229:THR:O	1:M:233:SER:HB3	2.15	0.46
1:U:190:MET:HG3	1:U:209:VAL:HG11	1.97	0.46
1:K:240:TYR:HB3	1:K:248:ILE:CG1	2.45	0.46
1:K:318:THR:HA	1:K:327:ILE:HD13	1.96	0.46
1:O:201:VAL:H	1:O:205:GLU:CD	2.18	0.46
1:Q:242:LEU:HB2	1:Q:243:PRO:HD2	1.96	0.46
1:A:170:ALA:O	1:A:172:PRO:HD3	2.15	0.46
1:A:20:GLY:HA2	1:A:94:LEU:HD21	1.97	0.46
2:B:705:ARG:O	2:B:709:MET:HG3	2.15	0.46
1:O:196:ARG:HD3	1:O:198:TYR:H	1.79	0.46
1:O:208:ILE:HG13	1:O:209:VAL:N	2.29	0.46
1:S:261:LEU:HB3	1:S:274:ILE:HD13	1.97	0.46
1:U:157:ASP:O	1:U:183:ARG:HG3	2.15	0.46
1:C:189:LEU:HG	1:C:193:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:LEU:HD21	1:E:250:ILE:HG22	1.96	0.46
2:H:730:GLU:HA	2:H:733:TRP:CZ3	2.50	0.46
1:G:39:ARG:NH2	1:I:179:ASP:O	2.47	0.46
1:O:31:PHE:CZ	1:O:89:THR:HG23	2.50	0.46
1:S:274:ILE:O	1:S:278:THR:HG23	2.15	0.46
1:A:219:VAL:HG21	1:A:309:ILE:HA	1.97	0.46
1:E:194:THR:HG1	1:E:200:PHE:N	2.10	0.46
2:L:708:VAL:O	2:L:712:VAL:HG13	2.16	0.46
1:O:31:PHE:CE1	1:O:89:THR:HG22	2.51	0.46
1:Q:95:ARG:HB2	1:Q:95:ARG:HE	1.29	0.46
1:S:105:LEU:HB2	1:S:134:VAL:HG12	1.98	0.46
1:I:113:LYS:HB3	1:I:371:HIS:CE1	2.51	0.46
1:M:335:ARG:HA	1:M:338:SER:OG	2.15	0.46
1:A:248:ILE:HA	1:A:248:ILE:HD12	1.77	0.46
1:E:278:THR:HG21	1:E:297:ASN:HD21	1.80	0.46
1:E:8:LEU:HD22	1:E:94:LEU:HD13	1.97	0.46
1:O:86:TRP:C	1:O:88:HIS:N	2.69	0.46
1:Q:189:LEU:HD13	1:Q:257:CYS:HB2	1.98	0.46
1:S:198:TYR:CE2	1:S:248:ILE:HD11	2.50	0.46
1:S:302:GLY:HA3	3:S:401:ATP:H5'2	1.96	0.46
1:X:31:PHE:CZ	1:X:89:THR:HG22	2.50	0.46
1:C:306:TYR:CZ	3:C:401:ATP:H2	2.34	0.46
1:E:18:LYS:HG2	1:E:30:VAL:HG22	1.98	0.46
1:E:214:GLU:OE2	3:E:401:ATP:H2'	2.16	0.46
1:E:84:LYS:HA	1:E:87:HIS:HB3	1.98	0.46
1:G:8:LEU:HB2	1:G:103:THR:HG22	1.98	0.46
1:I:218:TYR:HE2	1:I:254:ARG:NH2	2.14	0.46
1:K:229:THR:O	1:K:233:SER:HB3	2.16	0.46
1:O:38:PRO:N	1:O:65:LEU:HD21	2.32	0.46
1:O:61:LYS:CE	1:O:64:ILE:HB	2.34	0.46
1:S:53:TYR:HD2	1:S:65:LEU:HD11	1.79	0.46
1:U:56:ASP:O	1:U:60:SER:OG	2.33	0.46
1:X:190:MET:CG	1:X:209:VAL:HG11	2.46	0.45
1:A:33:SER:OG	1:A:33:SER:O	2.32	0.45
1:C:124:PHE:HE1	1:C:132:MET:HB3	1.81	0.45
1:C:78:ASN:ND2	1:C:81:ASP:CG	2.69	0.45
1:G:25:ASP:HB3	2:H:722:ARG:HG2	1.97	0.45
1:O:122:ILE:O	1:O:126:THR:HB	2.16	0.45
1:S:122:ILE:O	1:S:126:THR:HB	2.17	0.45
1:S:229:THR:O	1:S:233:SER:HB3	2.16	0.45
2:T:737:ARG:HG3	2:T:737:ARG:H	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ILE:H	1:E:136:ILE:HD12	1.81	0.45
1:E:360:GLN:O	1:E:363:ASP:HB2	2.16	0.45
1:I:261:LEU:HB3	1:I:274:ILE:HD13	1.97	0.45
1:K:257:CYS:HB3	1:K:258:PRO:HD3	1.98	0.45
2:L:728:LYS:HB3	2:L:728:LYS:HE3	1.70	0.45
1:O:86:TRP:O	1:O:88:HIS:N	2.49	0.45
2:P:702:ASN:O	2:P:705:ARG:HB3	2.16	0.45
1:E:196:ARG:O	1:E:198:TYR:HD1	2.00	0.45
1:E:216:LEU:HD13	1:E:250:ILE:HD11	1.98	0.45
1:G:170:ALA:O	1:G:172:PRO:HD3	2.16	0.45
1:I:216:LEU:O	1:I:254:ARG:HB3	2.16	0.45
1:K:79:TRP:CE2	1:K:118:LYS:HD2	2.51	0.45
1:O:183:ARG:HB3	1:O:206:ARG:HH22	1.80	0.45
1:Q:213:LYS:O	1:Q:217:CYS:HB2	2.16	0.45
2:R:705:ARG:O	2:R:709:MET:HG3	2.16	0.45
2:V:701:PHE:HA	2:V:704:VAL:HG22	1.98	0.45
1:A:213:LYS:O	1:A:217:CYS:HB2	2.16	0.45
1:E:213:LYS:O	1:E:217:CYS:HB2	2.16	0.45
1:K:202:THR:HG23	1:K:205:GLU:H	1.82	0.45
1:K:55:GLY:O	1:K:57:GLU:N	2.50	0.45
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.99	0.45
1:C:191:LYS:O	1:C:195:GLU:HG3	2.16	0.45
1:G:296:ASN:HA	1:G:328:LYS:NZ	2.32	0.45
1:K:63:GLY:C	1:K:64:ILE:HG22	2.37	0.45
2:L:700:THR:O	2:L:700:THR:OG1	2.32	0.45
1:Q:306:TYR:CZ	3:Q:401:ATP:H2	2.35	0.45
1:S:186:THR:O	1:S:190:MET:HG3	2.16	0.45
1:S:180:LEU:HD12	1:S:267:ILE:HD11	1.97	0.45
1:S:283:MET:SD	1:S:290:ARG:NH1	2.89	0.45
1:X:114:ALA:O	1:X:118:LYS:HG3	2.17	0.45
1:E:306:TYR:CZ	3:E:401:ATP:H2	2.34	0.45
1:I:124:PHE:CZ	1:I:132:MET:HG2	2.52	0.45
1:S:267:ILE:HG13	1:S:267:ILE:O	2.15	0.45
1:K:240:TYR:HB3	1:K:248:ILE:HB	1.93	0.45
1:O:174:ALA:HA	1:O:284:LYS:HG2	1.99	0.45
1:S:260:THR:HG21	1:S:267:ILE:HD13	1.98	0.45
1:X:188:TYR:HA	1:X:191:LYS:HB2	1.99	0.45
1:X:198:TYR:CE1	1:X:248:ILE:HD11	2.52	0.45
1:X:257:CYS:HB3	1:X:258:PRO:HD3	1.99	0.45
1:A:321:ALA:HB3	1:A:327:ILE:HD11	1.99	0.45
2:F:717:PRO:CB	2:F:719:HIS:HE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:188:TYR:O	1:I:192:ILE:HG12	2.17	0.45
1:O:328:LYS:HD3	1:O:330:ILE:HD11	1.99	0.45
1:O:358:THR:HG22	1:O:361:GLU:N	2.31	0.45
1:Q:8:LEU:HD22	1:Q:94:LEU:HD13	1.98	0.45
1:X:8:LEU:HD22	1:X:94:LEU:HD13	1.99	0.45
1:E:170:ALA:O	1:E:172:PRO:HD3	2.17	0.45
1:O:177:ARG:NH1	1:O:179:ASP:OD2	2.50	0.45
1:O:235:SER:HA	1:O:237:GLU:HG2	1.99	0.45
1:O:358:THR:C	1:O:359:LYS:HZ2	2.20	0.45
1:G:296:ASN:HA	1:G:328:LYS:HZ3	1.82	0.44
1:K:63:GLY:O	1:K:64:ILE:CB	2.65	0.44
1:Q:358:THR:HG22	1:Q:361:GLU:CD	2.37	0.44
1:S:8:LEU:HB2	1:S:103:THR:HG22	1.98	0.44
2:Y:704:VAL:O	2:Y:708:VAL:HG23	2.16	0.44
1:C:148:THR:HB	2:D:709:MET:HE3	1.99	0.44
1:K:58:ALA:HB1	1:K:67:LEU:HD22	1.98	0.44
1:M:255:PHE:O	1:M:259:GLU:HB2	2.18	0.44
1:O:210:ARG:O	1:O:214:GLU:HG3	2.18	0.44
1:O:88:HIS:O	1:O:88:HIS:CD2	2.70	0.44
1:A:124:PHE:CZ	1:A:132:MET:HG2	2.53	0.44
1:G:358:THR:OG1	1:G:361:GLU:HG3	2.18	0.44
1:I:20:GLY:HA2	1:I:94:LEU:HD21	2.00	0.44
1:M:36:GLY:C	1:M:65:LEU:HD21	2.37	0.44
1:E:218:TYR:CE1	1:E:255:PHE:HB3	2.52	0.44
2:F:718:ASP:O	2:F:719:HIS:C	2.55	0.44
1:E:345:ILE:HD11	2:F:722:ARG:NH2	2.31	0.44
1:I:170:ALA:O	1:I:172:PRO:HD3	2.17	0.44
1:K:296:ASN:CA	1:K:328:LYS:HD2	2.35	0.44
1:M:355:MET:C	1:M:372:ARG:HH12	2.20	0.44
1:S:76:ILE:HD13	1:S:82:MET:HG2	1.98	0.44
1:X:261:LEU:HB3	1:X:274:ILE:HD13	1.99	0.44
1:A:28:ARG:HH22	2:J:732:MET:CE	2.28	0.44
1:C:120:THR:HG21	1:C:370:VAL:HB	1.99	0.44
1:G:63:GLY:HA3	1:I:201:VAL:O	2.18	0.44
1:G:8:LEU:HD22	1:G:94:LEU:HD13	1.99	0.44
1:K:240:TYR:HD2	1:K:248:ILE:CD1	2.15	0.44
1:K:250:ILE:HG13	1:K:253:GLU:HB2	1.98	0.44
1:M:109:PRO:HG2	1:M:161:HIS:ND1	2.29	0.44
2:N:709:MET:O	2:N:711:ALA:N	2.50	0.44
1:O:288:ASP:N	1:O:288:ASP:OD1	2.50	0.44
1:O:65:LEU:CD2	1:O:66:THR:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:726:ILE:HG22	2:V:727:ASP:N	2.33	0.44
1:X:136:ILE:H	1:X:136:ILE:HD12	1.82	0.44
1:X:196:ARG:C	1:X:196:ARG:HD3	2.37	0.44
1:I:211:ASP:O	1:I:215:LYS:HG2	2.18	0.44
1:M:186:THR:O	1:M:190:MET:HG3	2.16	0.44
1:U:143:TYR:HD2	1:U:346:LEU:HD12	1.82	0.44
2:V:706:GLU:O	2:V:710:VAL:HG13	2.17	0.44
1:A:208:ILE:HD11	1:A:242:LEU:HD22	1.96	0.44
1:K:122:ILE:O	1:K:126:THR:HB	2.18	0.44
1:M:218:TYR:O	1:M:255:PHE:HA	2.18	0.44
1:M:81:ASP:OD1	1:M:81:ASP:N	2.49	0.44
1:U:180:LEU:O	1:U:181:ALA:HB2	2.18	0.44
1:X:26:ALA:HB2	2:Y:726:ILE:HD12	1.98	0.44
1:C:170:ALA:O	1:C:172:PRO:HD3	2.18	0.44
1:G:186:THR:O	1:G:190:MET:HG3	2.18	0.44
2:J:729:ALA:HA	2:J:732:MET:HE1	1.99	0.44
1:Q:260:THR:HG22	1:Q:266:PHE:HB2	2.00	0.44
1:X:196:ARG:O	1:X:196:ARG:HD3	2.18	0.44
1:A:230:ALA:HB2	1:A:236:LEU:HD12	2.00	0.44
1:C:27:PRO:HG2	2:D:733:TRP:HH2	1.83	0.44
1:I:216:LEU:HD11	1:I:240:TYR:HB2	1.98	0.44
1:K:218:TYR:HB3	1:K:307:PRO:HG2	1.99	0.44
2:D:709:MET:HA	2:D:712:VAL:HG22	2.00	0.43
1:K:120:THR:HG21	1:K:370:VAL:HB	2.00	0.43
1:O:82:MET:HE3	1:O:86:TRP:NE1	2.33	0.43
1:S:124:PHE:CZ	1:S:132:MET:HG2	2.53	0.43
1:S:27:PRO:HG2	2:T:733:TRP:HH2	1.83	0.43
1:U:211:ASP:OD2	1:U:240:TYR:OH	2.28	0.43
1:X:189:LEU:HA	1:X:192:ILE:HG12	1.99	0.43
1:G:237:GLU:N	1:G:237:GLU:OE1	2.50	0.43
1:S:233:SER:OG	1:S:234:SER:N	2.51	0.43
1:U:335:ARG:HA	1:U:338:SER:HB3	2.00	0.43
2:D:728:LYS:HE3	2:D:728:LYS:HB3	1.61	0.43
1:O:196:ARG:CZ	1:O:198:TYR:CD2	3.02	0.43
1:O:31:PHE:HE1	1:O:89:THR:HG22	1.83	0.43
1:U:143:TYR:CD2	1:U:346:LEU:HD12	2.54	0.43
1:M:205:GLU:O	1:M:209:VAL:HG23	2.18	0.43
1:O:289:ILE:HG22	1:O:293:LEU:HG	1.98	0.43
1:Q:124:PHE:CZ	1:Q:132:MET:HG2	2.53	0.43
1:I:201:VAL:N	1:I:205:GLU:OE2	2.33	0.43
1:O:261:LEU:HB3	1:O:274:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LYS:HD2	1:C:68:LYS:HA	1.69	0.43
1:C:317:ILE:HG22	1:C:327:ILE:HD13	1.99	0.43
1:E:124:PHE:CZ	1:E:132:MET:HG2	2.54	0.43
1:I:195:GLU:C	1:I:197:GLY:N	2.72	0.43
1:I:218:TYR:HB3	1:I:307:PRO:HG2	2.01	0.43
1:I:238:LYS:HE3	1:I:238:LYS:HA	2.00	0.43
1:I:240:TYR:O	1:I:248:ILE:N	2.51	0.43
2:P:734:GLU:C	2:P:736:GLU:H	2.21	0.43
1:U:261:LEU:HB3	1:U:274:ILE:HD13	2.00	0.43
1:A:240:TYR:HB3	1:A:248:ILE:HG22	2.00	0.43
1:E:216:LEU:C	1:E:254:ARG:HD2	2.39	0.43
2:F:726:ILE:CG2	2:F:727:ASP:H	2.29	0.43
1:G:61:LYS:HG2	1:I:201:VAL:HG21	2.01	0.43
1:K:54:VAL:HB	1:K:88:HIS:ND1	2.33	0.43
1:M:124:PHE:CZ	1:M:132:MET:HG2	2.53	0.43
1:O:257:CYS:HB3	1:O:258:PRO:HD3	2.01	0.43
1:O:361:GLU:HA	1:O:364:GLU:HB3	2.00	0.43
2:R:731:LYS:HG3	2:R:731:LYS:O	2.18	0.43
1:U:213:LYS:O	1:U:217:CYS:HB2	2.18	0.43
1:U:76:ILE:HD13	1:U:82:MET:HG2	2.00	0.43
2:V:720:ASP:HA	2:V:723:VAL:HB	2.01	0.43
1:E:196:ARG:HG3	1:E:196:ARG:O	2.19	0.43
1:E:332:PRO:O	1:E:335:ARG:NH1	2.51	0.43
1:I:211:ASP:OD2	1:I:240:TYR:OH	2.26	0.43
1:I:349:LEU:HD23	2:J:708:VAL:HG23	2.01	0.43
1:M:38:PRO:HB2	1:M:39:ARG:H	1.72	0.43
1:S:265:SER:C	1:S:267:ILE:N	2.70	0.43
2:F:719:HIS:HB3	2:F:723:VAL:HG12	1.91	0.43
1:G:136:ILE:H	1:G:136:ILE:HD12	1.83	0.43
1:I:257:CYS:HB3	1:I:258:PRO:HD3	2.00	0.43
2:L:702:ASN:HA	2:L:705:ARG:HB3	2.01	0.43
1:M:35:VAL:HG22	1:M:54:VAL:HG22	2.00	0.43
1:O:253:GLU:N	1:O:253:GLU:OE1	2.29	0.43
1:O:290:ARG:O	1:O:294:TYR:HD2	2.01	0.43
1:Q:358:THR:HG22	1:Q:361:GLU:OE2	2.19	0.43
1:Q:6:THR:O	1:Q:101:HIS:ND1	2.52	0.43
1:S:120:THR:HG21	1:S:370:VAL:HB	2.01	0.43
1:I:205:GLU:H	1:I:205:GLU:HG2	1.58	0.42
1:K:330:ILE:HG22	1:K:332:PRO:HD3	2.01	0.42
1:O:84:LYS:O	1:O:88:HIS:HB2	2.17	0.42
1:Q:288:ASP:OD1	1:Q:288:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:GLY:O	1:E:181:ALA:HB1	2.19	0.42
1:K:36:GLY:HA3	1:K:67:LEU:HD23	2.00	0.42
1:O:358:THR:C	1:O:359:LYS:HD3	2.39	0.42
1:E:196:ARG:O	1:E:198:TYR:CD1	2.72	0.42
1:K:107:GLU:HB2	1:K:111:ASN:HD22	1.84	0.42
1:O:295:ALA:C	1:O:296:ASN:ND2	2.73	0.42
1:U:232:SER:OG	1:U:232:SER:O	2.27	0.42
1:C:116:ARG:HG2	1:C:370:VAL:HG21	2.00	0.42
1:E:238:LYS:HD2	1:E:238:LYS:HA	1.94	0.42
1:G:84:LYS:HA	1:G:87:HIS:HB3	2.01	0.42
2:J:736:GLU:OE1	2:J:736:GLU:N	2.52	0.42
1:K:240:TYR:CB	1:K:248:ILE:CD1	2.79	0.42
1:O:68:LYS:HA	1:O:68:LYS:HD2	1.73	0.42
1:O:87:HIS:C	1:O:87:HIS:ND1	2.73	0.42
1:S:278:THR:O	1:S:282:ILE:HD12	2.19	0.42
1:E:224:GLU:HA	1:E:227:MET:HB2	1.99	0.42
1:E:242:LEU:C	1:E:244:ASP:N	2.71	0.42
1:K:124:PHE:CZ	1:K:132:MET:HG2	2.55	0.42
1:K:328:LYS:HZ1	1:K:330:ILE:HD12	1.84	0.42
1:O:124:PHE:HE1	1:O:359:LYS:CD	2.33	0.42
1:O:51:ASP:HB2	1:O:52:SER:H	1.68	0.42
1:S:156:GLY:O	1:S:181:ALA:HB1	2.18	0.42
1:U:189:LEU:HD22	1:U:213:LYS:HB2	2.02	0.42
1:E:198:TYR:CE2	1:E:248:ILE:HD11	2.53	0.42
1:K:272:ALA:HB1	1:K:276:GLU:HB2	2.01	0.42
1:O:100:GLU:CA	1:O:130:PRO:HG3	2.49	0.42
1:O:131:ALA:CA	1:O:359:LYS:HE2	2.49	0.42
1:S:170:ALA:O	1:S:172:PRO:HD3	2.20	0.42
1:U:124:PHE:CZ	1:U:132:MET:HG2	2.54	0.42
1:X:27:PRO:HG2	2:Y:733:TRP:HH2	1.84	0.42
1:X:282:ILE:HG13	1:X:282:ILE:H	1.74	0.42
1:C:122:ILE:O	1:C:126:THR:HB	2.20	0.42
1:E:216:LEU:CD2	1:E:238:LYS:HZ1	2.33	0.42
1:C:136:ILE:HD12	1:C:136:ILE:H	1.85	0.42
2:F:729:ALA:C	2:F:732:MET:H	2.23	0.42
1:I:192:ILE:HG21	1:I:253:GLU:HG3	2.00	0.42
1:I:8:LEU:HD22	1:I:94:LEU:HD13	2.01	0.42
1:M:35:VAL:HB	1:M:68:LYS:NZ	2.33	0.42
1:O:114:ALA:O	1:O:118:LYS:HG3	2.20	0.42
1:O:102:PRO:HA	1:O:131:ALA:O	2.20	0.42
1:O:16:LEU:HD11	1:O:210:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:306:TYR:CE1	3:O:401:ATP:H2	2.38	0.42
1:U:239:SER:HB3	1:U:247:VAL:CG2	2.50	0.42
1:U:248:ILE:HD12	1:U:248:ILE:HA	1.93	0.42
1:U:26:ALA:HB2	2:V:726:ILE:HD12	2.01	0.42
1:X:113:LYS:HB3	1:X:371:HIS:CE1	2.54	0.42
1:C:215:LYS:HD2	1:C:215:LYS:HA	1.67	0.42
1:E:337:TYR:CD2	2:F:726:ILE:HD12	2.53	0.42
1:K:86:TRP:HH2	1:K:119:MET:HG3	1.84	0.42
1:K:100:GLU:O	1:K:130:PRO:HG3	2.20	0.42
1:K:186:THR:O	1:K:190:MET:HG3	2.20	0.42
1:X:358:THR:HG23	1:X:361:GLU:HG2	2.00	0.42
1:E:36:GLY:N	1:E:53:TYR:O	2.44	0.42
1:E:37:ARG:NH1	1:E:81:ASP:OD1	2.53	0.42
1:I:58:ALA:HB1	1:I:67:LEU:HD22	2.01	0.42
1:O:65:LEU:HD23	1:O:65:LEU:HA	1.64	0.42
1:Q:198:TYR:CE1	1:Q:248:ILE:HD11	2.55	0.42
1:U:8:LEU:HD22	1:U:94:LEU:HD13	2.01	0.42
2:Y:713:GLN:C	2:Y:715:LEU:H	2.22	0.42
2:J:724:GLU:O	2:J:728:LYS:HG3	2.20	0.41
1:K:219:VAL:HG21	1:K:309:ILE:HA	2.02	0.41
1:M:190:MET:O	1:M:194:THR:HG23	2.19	0.41
1:M:68:LYS:HD2	1:M:81:ASP:OD2	2.19	0.41
1:O:191:LYS:HE2	1:O:191:LYS:HB2	1.52	0.41
2:B:738:LYS:HB2	2:B:739:LEU:H	1.56	0.41
1:G:341:ILE:HG21	2:H:722:ARG:HD3	2.00	0.41
1:I:219:VAL:HG21	1:I:309:ILE:HA	2.01	0.41
1:K:99:GLU:HA	1:K:128:ASN:O	2.20	0.41
1:M:111:ASN:HA	1:M:112:PRO:HD3	1.93	0.41
1:M:78:ASN:ND2	1:M:81:ASP:OD2	2.53	0.41
1:O:189:LEU:HD13	1:O:257:CYS:HB2	2.01	0.41
1:U:230:ALA:HA	1:U:236:LEU:HD12	2.02	0.41
1:E:189:LEU:HD12	1:E:189:LEU:HA	1.84	0.41
1:G:276:GLU:HG2	1:G:320:LEU:HD21	2.01	0.41
1:M:120:THR:HG21	1:M:370:VAL:HB	2.03	0.41
1:S:180:LEU:HD13	1:S:264:PRO:HB3	2.01	0.41
1:X:179:ASP:OD1	1:X:179:ASP:O	2.38	0.41
1:A:58:ALA:HB1	1:A:67:LEU:HD22	2.02	0.41
1:C:198:TYR:CZ	1:C:248:ILE:HD11	2.55	0.41
1:G:240:TYR:O	1:G:248:ILE:N	2.54	0.41
1:K:265:SER:HA	1:K:269:MET:O	2.20	0.41
1:M:51:ASP:HB2	1:M:52:SER:H	1.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:HIS:HB2	1:O:127:PHE:HE1	1.85	0.41
2:R:731:LYS:NZ	2:R:734:GLU:OE1	2.47	0.41
1:X:170:ALA:O	1:X:172:PRO:HD3	2.20	0.41
1:X:234:SER:HB2	1:X:237:GLU:HG2	2.01	0.41
1:C:200:PHE:HD1	1:C:205:GLU:HB3	1.85	0.41
2:F:732:MET:O	2:F:732:MET:HG3	2.20	0.41
1:G:192:ILE:C	1:G:194:THR:N	2.74	0.41
1:I:195:GLU:O	1:I:197:GLY:N	2.53	0.41
1:K:222:ASP:O	1:K:226:GLU:HG3	2.20	0.41
1:M:353:GLN:HA	1:M:356:TRP:CD1	2.56	0.41
1:Q:28:ARG:HH11	1:Q:28:ARG:HD2	1.59	0.41
1:Q:354:GLN:OE1	2:R:704:VAL:HG13	2.21	0.41
1:A:139:VAL:HA	1:A:165:ILE:HD13	2.01	0.41
1:E:208:ILE:CD1	1:E:242:LEU:HD21	2.48	0.41
1:E:148:THR:HG21	2:F:709:MET:HB3	2.02	0.41
1:I:157:ASP:O	1:I:183:ARG:HG3	2.21	0.41
1:K:252:ASN:HA	1:K:255:PHE:CE2	2.56	0.41
1:U:189:LEU:HD13	1:U:257:CYS:HB2	2.01	0.41
1:A:208:ILE:O	1:A:212:ILE:HG13	2.20	0.41
1:C:213:LYS:O	1:C:217:CYS:HB2	2.20	0.41
1:C:248:ILE:HD12	1:C:248:ILE:HA	1.87	0.41
1:E:370:VAL:C	1:E:372:ARG:H	2.24	0.41
2:F:722:ARG:C	2:F:724:GLU:N	2.72	0.41
1:K:252:ASN:O	1:K:256:ARG:HB2	2.20	0.41
1:O:196:ARG:HG3	1:O:197:GLY:N	2.36	0.41
1:O:202:THR:CG2	1:O:205:GLU:HG2	2.45	0.41
1:Q:261:LEU:HB3	1:Q:274:ILE:HD13	2.03	0.41
1:X:255:PHE:O	1:X:259:GLU:HB2	2.20	0.41
1:A:257:CYS:HB3	1:A:258:PRO:HD3	2.02	0.41
1:C:196:ARG:HH12	1:C:251:GLY:H	1.69	0.41
1:E:193:LEU:C	1:E:195:GLU:N	2.73	0.41
1:E:37:ARG:HD2	1:E:37:ARG:HH11	1.74	0.41
1:I:33:SER:OG	1:I:33:SER:O	2.27	0.41
1:K:123:MET:SD	1:K:129:VAL:HG21	2.61	0.41
2:L:709:MET:O	2:L:712:VAL:HG23	2.08	0.41
1:M:80:ASP:OD1	1:M:84:LYS:NZ	2.47	0.41
1:M:37:ARG:NH2	1:M:84:LYS:HE2	2.36	0.41
1:O:131:ALA:N	1:O:359:LYS:HE2	2.36	0.41
1:Q:15:GLY:C	1:Q:16:LEU:HD12	2.41	0.41
1:U:202:THR:HG22	1:U:205:GLU:CD	2.41	0.41
1:G:261:LEU:HB3	1:G:274:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:727:ASP:O	2:H:731:LYS:HD3	2.21	0.41
1:K:97:ALA:HB1	1:K:99:GLU:CG	2.50	0.41
2:L:730:GLU:C	2:L:732:MET:H	2.23	0.41
1:O:172:PRO:HB2	1:Q:110:LEU:HB3	2.01	0.41
1:Q:248:ILE:HD12	1:Q:248:ILE:HA	1.87	0.41
1:X:89:THR:OG1	1:X:90:PHE:N	2.53	0.41
1:A:357:ILE:HD12	1:A:370:VAL:HG23	2.03	0.41
1:E:218:TYR:O	1:E:255:PHE:HA	2.21	0.41
1:E:284:LYS:HA	1:E:284:LYS:HD2	1.90	0.41
1:E:244:ASP:CG	1:E:245:GLY:N	2.73	0.41
2:F:724:GLU:C	2:F:726:ILE:HG22	2.38	0.41
1:G:282:ILE:HG23	1:G:293:LEU:HD12	2.03	0.41
1:I:156:GLY:O	1:I:303:THR:OG1	2.37	0.41
1:M:288:ASP:OD1	1:M:288:ASP:N	2.53	0.41
1:M:65:LEU:C	1:M:65:LEU:HD23	2.41	0.41
1:O:86:TRP:C	1:O:88:HIS:H	2.23	0.41
1:S:358:THR:CG2	1:S:361:GLU:HG3	2.51	0.41
1:A:278:THR:O	1:A:282:ILE:HG13	2.21	0.40
1:C:105:LEU:HB2	1:C:134:VAL:HG12	2.03	0.40
1:E:216:LEU:CD2	1:E:238:LYS:NZ	2.84	0.40
1:I:224:GLU:HG2	1:I:224:GLU:H	1.54	0.40
1:I:37:ARG:NH2	1:I:80:ASP:OD2	2.26	0.40
2:L:725:ALA:O	2:L:729:ALA:HB3	2.21	0.40
1:O:241:GLU:HB2	1:O:247:VAL:HG22	2.02	0.40
1:O:87:HIS:O	1:O:87:HIS:ND1	2.54	0.40
1:E:241:GLU:CB	1:E:246:GLN:O	2.64	0.40
1:I:205:GLU:HA	1:I:208:ILE:HG12	2.03	0.40
1:I:278:THR:O	1:I:282:ILE:HG12	2.21	0.40
2:J:729:ALA:HA	2:J:732:MET:CE	2.51	0.40
1:K:359:LYS:O	1:K:359:LYS:CG	2.66	0.40
1:M:352:PHE:CD1	1:M:355:MET:HB2	2.55	0.40
1:O:235:SER:CA	1:O:237:GLU:HG2	2.51	0.40
1:O:314:GLN:HB2	1:O:329:ILE:HD12	2.02	0.40
2:R:720:ASP:O	2:R:724:GLU:HG2	2.21	0.40
1:S:206:ARG:HA	1:S:209:VAL:HG12	2.03	0.40
1:X:189:LEU:HD13	1:X:257:CYS:HB2	2.03	0.40
1:G:229:THR:O	1:G:233:SER:HB3	2.21	0.40
1:K:177:ARG:NH2	1:K:179:ASP:OD1	2.55	0.40
1:O:349:LEU:HD23	2:P:708:VAL:HG23	2.03	0.40
1:S:140:LEU:O	1:S:342:GLY:HA3	2.21	0.40
2:Y:706:GLU:O	2:Y:710:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:THR:HG22	1:C:132:MET:SD	2.61	0.40
1:G:192:ILE:C	1:G:194:THR:H	2.25	0.40
1:S:162:ASN:ND2	1:S:278:THR:HG22	2.37	0.40
1:S:79:TRP:CE2	1:S:118:LYS:HD2	2.56	0.40
1:U:186:THR:O	1:U:190:MET:HG3	2.21	0.40
1:U:238:LYS:HG3	1:U:254:ARG:NH1	2.36	0.40
2:H:729:ALA:O	2:H:731:LYS:N	2.55	0.40
1:K:247:VAL:CG1	1:K:248:ILE:N	2.54	0.40
1:M:170:ALA:O	1:M:172:PRO:HD3	2.20	0.40
1:Q:225:ASN:OD1	1:Q:226:GLU:N	2.54	0.40
1:S:18:LYS:HG2	1:S:30:VAL:HG22	2.03	0.40
1:S:219:VAL:HG21	1:S:309:ILE:HA	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:K:39:ARG:NH1	1:M:187:ASP:OD2[3_755]	1.82	0.38

## 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	353/377 (94%)	339 (96%)	13 (4%)	1 (0%)	46	84
1	C	354/377 (94%)	334 (94%)	19 (5%)	1 (0%)	46	84
1	E	354/377 (94%)	325 (92%)	29 (8%)	0	100	100
1	G	352/377 (93%)	326 (93%)	24 (7%)	2 (1%)	30	75
1	I	354/377 (94%)	333 (94%)	20 (6%)	1 (0%)	46	84
1	K	353/377 (94%)	329 (93%)	20 (6%)	4 (1%)	17	63
1	M	354/377 (94%)	337 (95%)	15 (4%)	2 (1%)	30	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	351/377 (93%)	322 (92%)	24 (7%)	5 (1%)	14	58
1	Q	353/377 (94%)	340 (96%)	12 (3%)	1 (0%)	46	84
1	S	354/377 (94%)	334 (94%)	20 (6%)	0	100	100
1	U	354/377 (94%)	338 (96%)	14 (4%)	2 (1%)	30	75
1	X	354/377 (94%)	335 (95%)	17 (5%)	2 (1%)	30	75
2	B	38/92 (41%)	35 (92%)	2 (5%)	1 (3%)	7	45
2	D	36/92 (39%)	33 (92%)	3 (8%)	0	100	100
2	F	35/92 (38%)	30 (86%)	3 (9%)	2 (6%)	2	23
2	H	35/92 (38%)	29 (83%)	3 (9%)	3 (9%)	1	12
2	J	37/92 (40%)	36 (97%)	1 (3%)	0	100	100
2	L	35/92 (38%)	25 (71%)	9 (26%)	1 (3%)	6	42
2	N	35/92 (38%)	31 (89%)	4 (11%)	0	100	100
2	P	35/92 (38%)	32 (91%)	3 (9%)	0	100	100
2	R	35/92 (38%)	32 (91%)	2 (6%)	1 (3%)	6	42
2	T	36/92 (39%)	34 (94%)	2 (6%)	0	100	100
2	V	35/92 (38%)	31 (89%)	4 (11%)	0	100	100
2	Y	35/92 (38%)	34 (97%)	1 (3%)	0	100	100
All	All	4667/5628 (83%)	4374 (94%)	264 (6%)	29 (1%)	30	75

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ASP
2	B	738	LYS
2	F	723	VAL
2	F	725	ALA
1	G	128	ASN
2	H	734	GLU
1	K	38	PRO
1	K	64	ILE
2	L	727	ASP
2	R	734	GLU
1	M	38	PRO
1	U	38	PRO
2	H	735	MET
1	Q	38	PRO

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Mol	Chain	Res	Type
1	X	232	SER
1	I	196	ARG
1	K	56	ASP
1	M	179	ASP
1	U	181	ALA
1	O	196	ARG
2	H	730	GLU
1	O	87	HIS
1	O	130	PRO
1	C	130	PRO
1	K	247	VAL
1	O	38	PRO
1	G	370	VAL
1	X	38	PRO
1	O	245	GLY

### 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	303/320 (95%)	300 (99%)	3 (1%)	82	93
1	C	304/320 (95%)	299 (98%)	5 (2%)	70	89
1	E	303/320 (95%)	296 (98%)	7 (2%)	58	85
1	G	298/320 (93%)	290 (97%)	8 (3%)	52	83
1	I	304/320 (95%)	302 (99%)	2 (1%)	88	96
1	K	301/320 (94%)	290 (96%)	11 (4%)	41	76
1	M	304/320 (95%)	299 (98%)	5 (2%)	70	89
1	O	299/320 (93%)	286 (96%)	13 (4%)	35	74
1	Q	302/320 (94%)	298 (99%)	4 (1%)	76	91
1	S	302/320 (94%)	301 (100%)	1 (0%)	94	99
1	U	301/320 (94%)	291 (97%)	10 (3%)	45	79
1	X	302/320 (94%)	297 (98%)	5 (2%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	37/79 (47%)	35 (95%)	2 (5%)	27	67
2	D	35/79 (44%)	33 (94%)	2 (6%)	25	66
2	F	34/79 (43%)	29 (85%)	5 (15%)	4	22
2	H	32/79 (40%)	29 (91%)	3 (9%)	11	44
2	J	33/79 (42%)	31 (94%)	2 (6%)	23	64
2	L	32/79 (40%)	29 (91%)	3 (9%)	11	44
2	N	34/79 (43%)	33 (97%)	1 (3%)	50	81
2	P	34/79 (43%)	33 (97%)	1 (3%)	50	81
2	R	31/79 (39%)	29 (94%)	2 (6%)	21	62
2	T	35/79 (44%)	33 (94%)	2 (6%)	25	66
2	V	31/79 (39%)	29 (94%)	2 (6%)	21	62
2	Y	34/79 (43%)	33 (97%)	1 (3%)	50	81
All	All	4025/4788 (84%)	3925 (98%)	100 (2%)	55	84

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	239	SER
1	A	371	HIS
2	B	720	ASP
2	B	727	ASP
1	C	198	TYR
1	C	219	VAL
1	C	224	GLU
1	C	359	LYS
1	C	368	SER
2	D	736	GLU
2	D	737	ARG
1	E	192	ILE
1	E	194	THR
1	E	195	GLU
1	E	198	TYR
1	E	237	GLU
1	E	239	SER
1	E	254	ARG
2	F	719	HIS
2	F	722	ARG

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Mol	Chain	Res	Type
2	F	727	ASP
2	F	731	LYS
2	F	735	MET
1	G	39	ARG
1	G	56	ASP
1	G	127	PHE
1	G	129	VAL
1	G	199	SER
1	G	328	LYS
1	G	335	ARG
1	G	351	THR
2	H	731	LYS
2	H	732	MET
2	H	735	MET
1	I	209	VAL
1	I	351	THR
2	J	708	VAL
2	J	724	GLU
1	K	37	ARG
1	K	39	ARG
1	K	40	HIS
1	K	66	THR
1	K	92	ASN
1	K	242	LEU
1	K	248	ILE
1	K	249	THR
1	K	253	GLU
1	K	328	LYS
1	K	371	HIS
2	L	713	GLN
2	L	726	ILE
2	L	728	LYS
1	M	12	ASN
1	M	28	ARG
1	M	51	ASP
1	M	269	MET
1	M	351	THR
2	N	731	LYS
1	O	39	ARG
1	O	51	ASP
1	O	59	GLN
1	O	87	HIS

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Mol	Chain	Res	Type
1	O	90	PHE
1	O	130	PRO
1	O	198	TYR
1	O	203	THR
1	O	233	SER
1	O	240	TYR
1	O	243	PRO
1	O	288	ASP
1	O	297	ASN
2	P	724	GLU
1	Q	39	ARG
1	Q	196	ARG
1	Q	288	ASP
1	Q	328	LYS
2	R	707	GLN
2	R	734	GLU
1	S	237	GLU
2	T	715	LEU
2	T	716	ASN
1	U	39	ARG
1	U	40	HIS
1	U	95	ARG
1	U	198	TYR
1	U	205	GLU
1	U	227	MET
1	U	247	VAL
1	U	349	LEU
1	U	350	SER
1	U	361	GLU
2	V	723	VAL
2	V	734	GLU
1	X	99	GLU
1	X	167	GLU
1	X	232	SER
1	X	235	SER
1	X	351	THR
2	Y	724	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	719	HIS

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Mol	Chain	Res	Type
1	M	12	ASN
1	M	40	HIS
2	P	702	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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
3	ATP	A	401	4	26,33,33	4.46	9 (34%)	26,52,52	3.67	4 (15%)
3	ATP	C	401	4	26,33,33	4.43	9 (34%)	26,52,52	3.68	4 (15%)
3	ATP	E	401	4	26,33,33	4.44	9 (34%)	26,52,52	3.62	4 (15%)
3	ATP	G	401	4	26,33,33	4.44	9 (34%)	26,52,52	3.70	4 (15%)
3	ATP	I	401	4	26,33,33	4.42	9 (34%)	26,52,52	3.68	4 (15%)
3	ATP	K	401	4	26,33,33	4.42	9 (34%)	26,52,52	3.74	4 (15%)
3	ATP	M	401	4	26,33,33	4.46	9 (34%)	26,52,52	3.65	4 (15%)
3	ATP	O	401	4	26,33,33	4.39	9 (34%)	26,52,52	4.00	4 (15%)
3	ATP	Q	401	4	26,33,33	4.46	9 (34%)	26,52,52	3.70	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	S	401	4	26,33,33	4.44	9 (34%)	26,52,52	3.72	4 (15%)
3	ATP	U	401	4	26,33,33	4.44	9 (34%)	26,52,52	3.67	4 (15%)
3	ATP	X	401	4	26,33,33	4.41	9 (34%)	26,52,52	3.70	4 (15%)

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
3	ATP	A	401	4	-	0/18/38/38	0/3/3/3
3	ATP	C	401	4	-	0/18/38/38	0/3/3/3
3	ATP	E	401	4	-	0/18/38/38	0/3/3/3
3	ATP	G	401	4	-	0/18/38/38	0/3/3/3
3	ATP	I	401	4	-	0/18/38/38	0/3/3/3
3	ATP	K	401	4	-	0/18/38/38	0/3/3/3
3	ATP	M	401	4	-	0/18/38/38	0/3/3/3
3	ATP	O	401	4	-	0/18/38/38	0/3/3/3
3	ATP	Q	401	4	-	0/18/38/38	0/3/3/3
3	ATP	S	401	4	-	0/18/38/38	0/3/3/3
3	ATP	U	401	4	-	0/18/38/38	0/3/3/3
3	ATP	X	401	4	-	0/18/38/38	0/3/3/3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	401	ATP	C2'-C1'	-15.34	1.29	1.53
3	C	401	ATP	C2'-C1'	-15.34	1.29	1.53
3	U	401	ATP	C2'-C1'	-15.31	1.29	1.53
3	M	401	ATP	C2'-C1'	-15.31	1.29	1.53
3	I	401	ATP	C2'-C1'	-15.28	1.29	1.53
3	G	401	ATP	C2'-C1'	-15.28	1.29	1.53
3	A	401	ATP	C2'-C1'	-15.28	1.29	1.53
3	X	401	ATP	C2'-C1'	-15.26	1.29	1.53
3	K	401	ATP	C2'-C1'	-15.26	1.29	1.53
3	E	401	ATP	C2'-C1'	-15.20	1.29	1.53
3	S	401	ATP	C2'-C1'	-15.15	1.29	1.53
3	O	401	ATP	C2'-C1'	-14.99	1.29	1.53
3	O	401	ATP	C3'-C4'	-9.42	1.27	1.53
3	S	401	ATP	C3'-C4'	-9.38	1.27	1.53
3	K	401	ATP	C3'-C4'	-9.30	1.28	1.53
3	I	401	ATP	C3'-C4'	-9.27	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	401	ATP	C3'-C4'	-9.27	1.28	1.53
3	A	401	ATP	C3'-C4'	-9.23	1.28	1.53
3	X	401	ATP	C3'-C4'	-9.22	1.28	1.53
3	G	401	ATP	C3'-C4'	-9.22	1.28	1.53
3	C	401	ATP	C3'-C4'	-9.20	1.28	1.53
3	U	401	ATP	C3'-C4'	-9.19	1.28	1.53
3	E	401	ATP	C3'-C4'	-9.19	1.28	1.53
3	M	401	ATP	C3'-C4'	-9.16	1.28	1.53
3	O	401	ATP	C5-C4	-2.52	1.34	1.40
3	G	401	ATP	C5-C4	-2.49	1.34	1.40
3	K	401	ATP	C5-C4	-2.47	1.34	1.40
3	S	401	ATP	C5-C4	-2.46	1.34	1.40
3	X	401	ATP	C5-C4	-2.46	1.35	1.40
3	U	401	ATP	C5-C4	-2.45	1.35	1.40
3	Q	401	ATP	C5-C4	-2.45	1.35	1.40
3	A	401	ATP	C5-C4	-2.45	1.35	1.40
3	M	401	ATP	C5-C4	-2.44	1.35	1.40
3	I	401	ATP	C5-C4	-2.43	1.35	1.40
3	C	401	ATP	C5-C4	-2.40	1.35	1.40
3	E	401	ATP	C5-C4	-2.38	1.35	1.40
3	O	401	ATP	PA-O5'	2.31	1.69	1.59
3	X	401	ATP	PA-O5'	2.38	1.69	1.59
3	I	401	ATP	PA-O5'	2.40	1.69	1.59
3	M	401	ATP	PA-O5'	2.43	1.69	1.59
3	C	401	ATP	PA-O5'	2.43	1.69	1.59
3	A	401	ATP	PA-O5'	2.43	1.69	1.59
3	G	401	ATP	PA-O5'	2.43	1.69	1.59
3	E	401	ATP	PA-O5'	2.44	1.69	1.59
3	Q	401	ATP	PA-O5'	2.44	1.69	1.59
3	U	401	ATP	PA-O5'	2.45	1.69	1.59
3	X	401	ATP	O3'-C3'	2.45	1.48	1.43
3	E	401	ATP	O3'-C3'	2.48	1.48	1.43
3	S	401	ATP	O3'-C3'	2.48	1.48	1.43
3	O	401	ATP	O3'-C3'	2.48	1.48	1.43
3	A	401	ATP	O3'-C3'	2.49	1.48	1.43
3	G	401	ATP	O3'-C3'	2.50	1.48	1.43
3	U	401	ATP	O3'-C3'	2.50	1.48	1.43
3	K	401	ATP	O3'-C3'	2.50	1.48	1.43
3	I	401	ATP	O3'-C3'	2.50	1.48	1.43
3	K	401	ATP	PA-O5'	2.50	1.69	1.59
3	Q	401	ATP	O3'-C3'	2.51	1.48	1.43
3	M	401	ATP	O3'-C3'	2.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	401	ATP	PA-O5'	2.52	1.69	1.59
3	C	401	ATP	O3'-C3'	2.53	1.48	1.43
3	Q	401	ATP	C6-N6	3.78	1.49	1.34
3	I	401	ATP	C6-N6	3.79	1.49	1.34
3	G	401	ATP	C6-N6	3.79	1.49	1.34
3	X	401	ATP	C6-N6	3.80	1.49	1.34
3	C	401	ATP	C6-N6	3.80	1.49	1.34
3	K	401	ATP	C6-N6	3.80	1.49	1.34
3	S	401	ATP	C6-N6	3.80	1.49	1.34
3	E	401	ATP	C6-N6	3.80	1.49	1.34
3	A	401	ATP	C6-N6	3.81	1.49	1.34
3	M	401	ATP	C6-N6	3.81	1.49	1.34
3	O	401	ATP	C6-N6	3.81	1.49	1.34
3	U	401	ATP	C6-N6	3.81	1.49	1.34
3	A	401	ATP	C2'-C3'	4.29	1.65	1.53
3	I	401	ATP	C2'-C3'	4.30	1.65	1.53
3	S	401	ATP	C2'-C3'	4.31	1.65	1.53
3	Q	401	ATP	C2'-C3'	4.31	1.65	1.53
3	K	401	ATP	C2'-C3'	4.31	1.65	1.53
3	G	401	ATP	C2'-C3'	4.31	1.65	1.53
3	X	401	ATP	C2'-C3'	4.32	1.65	1.53
3	M	401	ATP	C2'-C3'	4.33	1.65	1.53
3	U	401	ATP	C2'-C3'	4.33	1.65	1.53
3	C	401	ATP	C2'-C3'	4.35	1.65	1.53
3	E	401	ATP	C2'-C3'	4.38	1.65	1.53
3	O	401	ATP	C2'-C3'	4.46	1.65	1.53
3	O	401	ATP	O4'-C4'	4.72	1.55	1.45
3	S	401	ATP	O4'-C4'	4.88	1.56	1.45
3	K	401	ATP	O4'-C4'	4.94	1.56	1.45
3	Q	401	ATP	O4'-C4'	5.00	1.56	1.45
3	U	401	ATP	O4'-C4'	5.00	1.56	1.45
3	X	401	ATP	O4'-C4'	5.00	1.56	1.45
3	G	401	ATP	O4'-C4'	5.01	1.56	1.45
3	I	401	ATP	O4'-C4'	5.02	1.56	1.45
3	A	401	ATP	O4'-C4'	5.03	1.56	1.45
3	C	401	ATP	O4'-C4'	5.04	1.56	1.45
3	E	401	ATP	O4'-C4'	5.09	1.56	1.45
3	M	401	ATP	O4'-C4'	5.09	1.56	1.45
3	O	401	ATP	O4'-C1'	9.37	1.54	1.41
3	E	401	ATP	O4'-C1'	9.63	1.55	1.41
3	I	401	ATP	O4'-C1'	9.66	1.55	1.41
3	X	401	ATP	O4'-C1'	9.66	1.55	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	401	ATP	O4'-C1'	9.69	1.55	1.41
3	G	401	ATP	O4'-C1'	9.69	1.55	1.41
3	Q	401	ATP	O4'-C1'	9.72	1.55	1.41
3	S	401	ATP	O4'-C1'	9.72	1.55	1.41
3	A	401	ATP	O4'-C1'	9.72	1.55	1.41
3	C	401	ATP	O4'-C1'	9.73	1.55	1.41
3	K	401	ATP	O4'-C1'	9.73	1.55	1.41
3	M	401	ATP	O4'-C1'	9.75	1.55	1.41

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	401	ATP	C1'-N9-C4	-12.59	112.75	126.81
3	K	401	ATP	C1'-N9-C4	-12.10	113.30	126.81
3	S	401	ATP	C1'-N9-C4	-11.92	113.51	126.81
3	C	401	ATP	C1'-N9-C4	-11.74	113.70	126.81
3	Q	401	ATP	C1'-N9-C4	-11.73	113.72	126.81
3	G	401	ATP	C1'-N9-C4	-11.69	113.76	126.81
3	I	401	ATP	C1'-N9-C4	-11.63	113.83	126.81
3	X	401	ATP	C1'-N9-C4	-11.62	113.83	126.81
3	U	401	ATP	C1'-N9-C4	-11.58	113.88	126.81
3	M	401	ATP	C1'-N9-C4	-11.55	113.92	126.81
3	E	401	ATP	C1'-N9-C4	-11.45	114.02	126.81
3	A	401	ATP	C1'-N9-C4	-11.45	114.03	126.81
3	X	401	ATP	N3-C2-N1	-11.36	119.94	128.87
3	A	401	ATP	N3-C2-N1	-11.32	119.98	128.87
3	Q	401	ATP	N3-C2-N1	-11.27	120.02	128.87
3	O	401	ATP	N3-C2-N1	-11.27	120.02	128.87
3	G	401	ATP	N3-C2-N1	-11.25	120.03	128.87
3	I	401	ATP	N3-C2-N1	-11.25	120.03	128.87
3	U	401	ATP	N3-C2-N1	-11.24	120.04	128.87
3	S	401	ATP	N3-C2-N1	-11.11	120.15	128.87
3	K	401	ATP	N3-C2-N1	-11.10	120.15	128.87
3	M	401	ATP	N3-C2-N1	-11.02	120.22	128.87
3	C	401	ATP	N3-C2-N1	-11.01	120.22	128.87
3	E	401	ATP	N3-C2-N1	-10.91	120.30	128.87
3	E	401	ATP	N6-C6-N1	-8.13	104.87	118.52
3	O	401	ATP	N6-C6-N1	-8.11	104.90	118.52
3	K	401	ATP	N6-C6-N1	-8.05	105.01	118.52
3	X	401	ATP	N6-C6-N1	-8.02	105.06	118.52
3	C	401	ATP	N6-C6-N1	-8.01	105.08	118.52
3	S	401	ATP	N6-C6-N1	-8.01	105.08	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	I	401	ATP	N6-C6-N1	-8.00	105.10	118.52
3	M	401	ATP	N6-C6-N1	-8.00	105.10	118.52
3	U	401	ATP	N6-C6-N1	-7.98	105.12	118.52
3	A	401	ATP	N6-C6-N1	-7.98	105.12	118.52
3	G	401	ATP	N6-C6-N1	-7.98	105.13	118.52
3	Q	401	ATP	N6-C6-N1	-7.98	105.13	118.52
3	O	401	ATP	C4'-O4'-C1'	-7.18	102.03	109.64
3	S	401	ATP	C4'-O4'-C1'	-4.49	104.88	109.64
3	Q	401	ATP	C4'-O4'-C1'	-3.98	105.42	109.64
3	K	401	ATP	C4'-O4'-C1'	-3.91	105.50	109.64
3	G	401	ATP	C4'-O4'-C1'	-3.87	105.54	109.64
3	X	401	ATP	C4'-O4'-C1'	-3.85	105.56	109.64
3	I	401	ATP	C4'-O4'-C1'	-3.78	105.64	109.64
3	C	401	ATP	C4'-O4'-C1'	-3.74	105.68	109.64
3	M	401	ATP	C4'-O4'-C1'	-3.69	105.73	109.64
3	A	401	ATP	C4'-O4'-C1'	-3.68	105.74	109.64
3	U	401	ATP	C4'-O4'-C1'	-3.66	105.76	109.64
3	E	401	ATP	C4'-O4'-C1'	-3.52	105.91	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ATP	1	0
3	E	401	ATP	2	0
3	K	401	ATP	1	0
3	M	401	ATP	1	0
3	O	401	ATP	3	0
3	Q	401	ATP	1	0
3	S	401	ATP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	357/377 (94%)	0.86	33 (9%)	11 10	47, 76, 125, 154	0
1	C	358/377 (94%)	0.80	33 (9%)	11 10	50, 79, 125, 174	0
1	E	358/377 (94%)	0.83	34 (9%)	10 10	57, 89, 133, 161	0
1	G	356/377 (94%)	0.91	43 (12%)	6 6	57, 89, 130, 155	0
1	I	358/377 (94%)	0.82	29 (8%)	15 12	48, 76, 125, 168	0
1	K	357/377 (94%)	0.92	36 (10%)	9 9	62, 94, 144, 169	0
1	M	358/377 (94%)	0.85	32 (8%)	12 10	53, 79, 121, 171	0
1	O	355/377 (94%)	0.85	35 (9%)	9 9	61, 95, 144, 161	0
1	Q	357/377 (94%)	0.83	32 (8%)	12 10	59, 87, 126, 171	0
1	S	358/377 (94%)	0.77	27 (7%)	17 14	53, 78, 123, 172	0
1	U	358/377 (94%)	0.78	27 (7%)	17 14	57, 87, 123, 167	0
1	X	358/377 (94%)	0.84	29 (8%)	15 12	52, 78, 125, 168	0
2	B	40/92 (43%)	0.28	0	100 100	69, 85, 119, 129	0
2	D	38/92 (41%)	0.67	3 (7%)	15 13	71, 92, 129, 151	0
2	F	37/92 (40%)	0.34	3 (8%)	15 12	95, 108, 133, 149	0
2	H	37/92 (40%)	0.34	1 (2%)	58 47	24, 103, 125, 131	0
2	J	39/92 (42%)	0.26	2 (5%)	32 24	68, 83, 102, 113	0
2	L	37/92 (40%)	0.19	1 (2%)	58 47	95, 121, 165, 173	0
2	N	37/92 (40%)	0.46	1 (2%)	58 47	78, 97, 111, 118	0
2	P	37/92 (40%)	0.67	4 (10%)	8 7	98, 115, 158, 172	0
2	R	37/92 (40%)	0.51	4 (10%)	8 7	87, 108, 127, 135	0
2	T	38/92 (41%)	0.44	1 (2%)	59 49	73, 88, 116, 122	0
2	V	37/92 (40%)	0.54	4 (10%)	8 7	92, 113, 126, 130	0
2	Y	37/92 (40%)	0.29	1 (2%)	58 47	79, 93, 107, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4739/5628 (84%)	0.80	415 (8%) 12 11	24, 86, 130, 174	0

All (415) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199	SER	5.5
1	M	236	LEU	5.4
1	S	198	TYR	4.8
2	P	726	ILE	4.6
1	X	218	TYR	4.3
1	K	250	ILE	4.3
1	A	250	ILE	4.3
1	I	200	PHE	4.2
1	C	250	ILE	4.2
1	C	255	PHE	4.2
1	X	22	ALA	4.1
1	G	101	HIS	4.1
1	I	38	PRO	4.0
1	U	27	PRO	3.9
1	Q	40	HIS	3.9
1	K	356	TRP	3.9
1	M	250	ILE	3.9
1	O	208	ILE	3.8
1	U	33	SER	3.8
1	O	54	VAL	3.8
1	S	297	ASN	3.7
1	E	240	TYR	3.7
1	Q	208	ILE	3.7
1	O	8	LEU	3.6
1	K	103	THR	3.6
1	C	40	HIS	3.6
1	K	10	CYS	3.6
1	E	356	TRP	3.6
1	C	200	PHE	3.6
1	O	64	ILE	3.6
1	K	129	VAL	3.6
1	E	200	PHE	3.5
1	G	198	TYR	3.5
1	A	247	VAL	3.5
2	P	701	PHE	3.5
1	E	220	ALA	3.5
1	S	247	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	216	LEU	3.4
1	S	67	LEU	3.4
1	Q	129	VAL	3.4
1	K	236	LEU	3.4
1	S	200	PHE	3.4
1	I	58	ALA	3.4
1	O	33	SER	3.4
1	O	236	LEU	3.3
2	D	731	LYS	3.3
1	Q	34	ILE	3.3
1	E	330	ILE	3.3
1	E	21	PHE	3.3
1	I	201	VAL	3.3
1	E	236	LEU	3.2
1	U	103	THR	3.2
1	A	238	LYS	3.2
1	E	250	ILE	3.2
1	O	34	ILE	3.2
1	O	246	GLN	3.2
1	M	10	CYS	3.2
1	X	200	PHE	3.2
1	K	240	TYR	3.2
1	X	243	PRO	3.2
1	I	185	LEU	3.2
1	C	38	PRO	3.1
1	G	218	TYR	3.1
1	O	274	ILE	3.1
2	R	720	ASP	3.1
1	I	40	HIS	3.1
1	M	58	ALA	3.1
1	K	212	ILE	3.1
1	G	236	LEU	3.1
1	G	257	CYS	3.1
1	O	355	MET	3.1
2	V	726	ILE	3.0
1	E	9	VAL	3.0
1	Q	25	ASP	3.0
1	U	257	CYS	3.0
1	E	281	SER	3.0
1	E	277	THR	3.0
1	M	293	LEU	3.0
1	M	8	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	U	355	MET	3.0
1	M	21	PHE	3.0
1	U	218	TYR	3.0
1	G	282	ILE	3.0
1	A	160	THR	3.0
1	U	98	PRO	3.0
1	K	35	VAL	2.9
1	X	155	SER	2.9
1	S	34	ILE	2.9
1	C	313	MET	2.9
1	A	161	HIS	2.9
1	A	240	TYR	2.9
1	C	165	ILE	2.9
1	S	64	ILE	2.9
1	X	236	LEU	2.9
1	O	21	PHE	2.9
1	G	162	ASN	2.9
1	Q	145	SER	2.9
1	A	249	THR	2.9
1	A	142	LEU	2.9
1	O	101	HIS	2.9
1	O	31	PHE	2.8
1	S	8	LEU	2.8
1	X	299	MET	2.8
1	X	185	LEU	2.8
1	I	356	TRP	2.8
1	G	274	ILE	2.8
1	K	211	ASP	2.8
1	C	297	ASN	2.8
1	O	356	TRP	2.8
1	S	250	ILE	2.8
1	E	25	ASP	2.8
1	G	240	TYR	2.8
1	Q	262	PHE	2.7
1	K	98	PRO	2.7
1	G	53	TYR	2.7
1	G	100	GLU	2.7
1	I	8	LEU	2.7
1	S	199	SER	2.7
1	M	356	TRP	2.7
2	V	708	VAL	2.7
1	E	143	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	U	94	LEU	2.7
1	Q	193	LEU	2.6
1	U	21	PHE	2.6
1	K	27	PRO	2.6
1	E	132	MET	2.6
1	Q	261	LEU	2.6
1	X	12	ASN	2.6
2	D	737	ARG	2.6
1	Q	143	TYR	2.6
1	O	140	LEU	2.6
1	X	242	LEU	2.6
1	C	164	PRO	2.6
1	A	168	GLY	2.6
1	S	65	LEU	2.6
1	G	262	PHE	2.6
1	S	262	PHE	2.6
1	G	160	THR	2.6
2	L	708	VAL	2.6
1	A	220	ALA	2.6
1	G	33	SER	2.6
1	G	102	PRO	2.6
1	Q	86	TRP	2.6
1	E	54	VAL	2.6
1	M	247	VAL	2.6
1	M	171	LEU	2.6
1	G	21	PHE	2.6
1	M	317	ILE	2.6
1	Q	64	ILE	2.6
1	Q	81	ASP	2.5
1	S	143	TYR	2.5
1	G	124	PHE	2.5
1	M	200	PHE	2.5
2	D	735	MET	2.5
1	I	53	TYR	2.5
1	E	104	LEU	2.5
1	K	142	LEU	2.5
2	P	735	MET	2.5
2	H	722	ARG	2.5
1	C	299	MET	2.5
2	J	701	PHE	2.5
1	M	98	PRO	2.5
1	M	162	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	U	26	ALA	2.5
1	Q	171	LEU	2.5
1	A	327	ILE	2.5
1	K	309	ILE	2.5
1	E	155	SER	2.5
1	G	243	PRO	2.5
1	O	180	LEU	2.5
1	U	185	LEU	2.5
1	E	272	ALA	2.5
1	K	298	VAL	2.5
2	N	735	MET	2.5
1	I	143	TYR	2.5
1	X	220	ALA	2.5
1	S	201	VAL	2.5
1	C	369	ILE	2.5
1	S	197	GLY	2.5
1	O	223	PHE	2.5
1	I	57	GLU	2.5
1	C	142	LEU	2.4
1	K	180	LEU	2.4
1	M	178	LEU	2.4
1	G	245	GLY	2.4
1	K	216	LEU	2.4
1	A	303	THR	2.4
1	G	159	VAL	2.4
1	G	347	ALA	2.4
1	O	162	ASN	2.4
1	U	264	PRO	2.4
1	A	159	VAL	2.4
1	X	293	LEU	2.4
1	S	181	ALA	2.4
1	M	310	ALA	2.4
1	X	143	TYR	2.4
1	I	309	ILE	2.4
1	I	223	PHE	2.4
1	I	306	TYR	2.4
1	E	274	ILE	2.4
1	C	104	LEU	2.4
1	A	260	THR	2.4
1	A	298	VAL	2.4
1	C	12	ASN	2.4
1	M	25	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	S	58	ALA	2.4
1	K	330	ILE	2.4
2	R	712	VAL	2.4
1	X	297	ASN	2.4
1	I	101	HIS	2.4
1	G	25	ASP	2.4
1	G	185	LEU	2.4
1	A	165	ILE	2.4
1	M	64	ILE	2.4
1	O	103	THR	2.4
1	G	352	PHE	2.4
1	Q	279	TYR	2.4
1	X	38	PRO	2.4
1	E	162	ASN	2.4
1	I	274	ILE	2.4
1	M	297	ASN	2.4
1	U	275	HIS	2.4
1	Q	35	VAL	2.3
1	C	247	VAL	2.3
1	A	34	ILE	2.3
1	G	217	CYS	2.3
1	K	297	ASN	2.3
1	Q	9	VAL	2.3
1	M	191	LYS	2.3
1	U	356	TRP	2.3
1	C	218	TYR	2.3
1	Q	22	ALA	2.3
1	C	160	THR	2.3
1	S	261	LEU	2.3
1	O	262	PHE	2.3
1	S	124	PHE	2.3
1	G	132	MET	2.3
1	G	51	ASP	2.3
1	K	104	LEU	2.3
1	O	347	ALA	2.3
1	Q	221	LEU	2.3
1	K	281	SER	2.3
1	G	241	GLU	2.3
1	O	155	SER	2.3
1	I	359	LYS	2.3
1	Q	161	HIS	2.3
1	E	35	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	219	VAL	2.3
1	C	133	TYR	2.3
1	U	345	ILE	2.3
1	U	195	GLU	2.3
1	I	102	PRO	2.3
1	C	240	TYR	2.3
1	K	218	TYR	2.3
1	A	246	GLN	2.3
1	M	133	TYR	2.3
1	Q	90	PHE	2.3
2	J	708	VAL	2.3
1	A	67	LEU	2.3
1	K	94	LEU	2.3
1	O	104	LEU	2.3
1	X	164	PRO	2.3
1	E	282	ILE	2.3
1	M	151	ILE	2.3
1	O	94	LEU	2.2
1	C	27	PRO	2.2
1	C	306	TYR	2.2
1	O	58	ALA	2.2
1	C	346	LEU	2.2
1	K	105	LEU	2.2
1	X	90	PHE	2.2
1	X	112	PRO	2.2
1	A	279	TYR	2.2
1	C	86	TRP	2.2
1	C	185	LEU	2.2
1	E	293	LEU	2.2
1	K	185	LEU	2.2
1	Q	258	PRO	2.2
1	U	358	THR	2.2
1	Q	91	TYR	2.2
1	G	8	LEU	2.2
1	K	299	MET	2.2
1	G	299	MET	2.2
1	A	25	ASP	2.2
1	G	98	PRO	2.2
1	O	7	ALA	2.2
1	A	242	LEU	2.2
1	I	262	PHE	2.2
1	U	213	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	27	PRO	2.2
1	E	8	LEU	2.2
1	C	21	PHE	2.2
1	Q	29	ALA	2.2
1	U	32	PRO	2.2
1	G	90	PHE	2.2
1	G	356	TRP	2.2
1	K	159	VAL	2.2
1	I	221	LEU	2.2
1	M	336	LYS	2.2
1	A	151	ILE	2.2
1	M	309	ILE	2.2
1	G	28	ARG	2.2
1	M	138	ALA	2.2
1	M	180	LEU	2.2
1	O	257	CYS	2.2
1	C	329	ILE	2.2
1	X	149	THR	2.2
2	R	708	VAL	2.2
1	E	185	LEU	2.2
1	X	285	CYS	2.2
2	F	730	GLU	2.2
1	I	278	THR	2.2
1	X	103	THR	2.2
1	M	246	GLN	2.1
1	G	250	ILE	2.1
1	Q	27	PRO	2.1
1	S	258	PRO	2.1
1	U	164	PRO	2.1
1	X	313	MET	2.1
2	V	712	VAL	2.1
1	E	20	GLY	2.1
1	E	92	ASN	2.1
1	S	216	LEU	2.1
1	U	216	LEU	2.1
1	A	306	TYR	2.1
1	Q	198	TYR	2.1
1	U	64	ILE	2.1
1	X	281	SER	2.1
1	A	221	LEU	2.1
1	K	53	TYR	2.1
1	K	294	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	90	PHE	2.1
1	Q	166	TYR	2.1
1	U	188	TYR	2.1
1	U	306	TYR	2.1
1	E	186	THR	2.1
1	A	96	VAL	2.1
1	S	129	VAL	2.1
1	M	261	LEU	2.1
1	Q	236	LEU	2.1
1	K	22	ALA	2.1
1	A	9	VAL	2.1
1	A	103	THR	2.1
1	C	89	THR	2.1
1	E	111	ASN	2.1
1	A	257	CYS	2.1
1	A	8	LEU	2.1
1	E	171	LEU	2.1
1	I	293	LEU	2.1
1	X	179	ASP	2.1
1	O	309	ILE	2.1
1	C	155	SER	2.1
1	X	199	SER	2.1
2	F	701	PHE	2.1
1	O	131	ALA	2.1
1	Q	192	ILE	2.1
1	S	104	LEU	2.1
1	U	105	LEU	2.1
1	A	255	PHE	2.1
1	G	220	ALA	2.1
1	I	54	VAL	2.1
2	T	704	VAL	2.1
1	S	354	GLN	2.1
1	G	200	PHE	2.1
1	M	352	PHE	2.1
1	K	347	ALA	2.1
1	G	64	ILE	2.1
1	Q	105	LEU	2.1
1	X	119	MET	2.1
1	S	90	PHE	2.1
1	E	247	VAL	2.1
1	O	26	ALA	2.1
2	Y	708	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	37	ARG	2.1
1	I	303	THR	2.1
1	G	32	PRO	2.1
1	K	282	ILE	2.1
2	R	726	ILE	2.1
1	A	275	HIS	2.1
1	K	179	ASP	2.1
1	U	31	PHE	2.0
1	X	138	ALA	2.0
1	C	330	ILE	2.0
1	I	355	MET	2.0
1	S	155	SER	2.0
1	K	337	TYR	2.0
1	O	144	ALA	2.0
1	C	274	ILE	2.0
1	E	140	LEU	2.0
1	G	261	LEU	2.0
1	M	192	ILE	2.0
2	P	715	LEU	2.0
1	Q	223	PHE	2.0
1	M	311	ASP	2.0
1	X	145	SER	2.0
1	A	131	ALA	2.0
1	O	240	TYR	2.0
1	E	216	LEU	2.0
1	I	105	LEU	2.0
1	K	192	ILE	2.0
1	X	26	ALA	2.0
2	V	717	PRO	2.0
1	I	163	VAL	2.0
2	F	712	VAL	2.0
1	O	369	ILE	2.0
1	Q	94	LEU	2.0
1	E	305	MET	2.0
1	I	194	THR	2.0
1	K	33	SER	2.0
1	S	306	TYR	2.0
1	C	64	ILE	2.0
1	O	282	ILE	2.0
1	C	148	THR	2.0
1	O	306	TYR	2.0
1	U	178	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	S	402	1/1	0.97	0.31	1.12	66,66,66,66	0
4	CA	X	402	1/1	0.98	0.27	0.05	70,70,70,70	0
4	CA	Q	402	1/1	0.96	0.27	-0.17	68,68,68,68	0
3	ATP	I	401	31/31	0.95	0.28	-0.27	62,81,88,92	0
3	ATP	A	401	31/31	0.95	0.29	-0.34	66,77,85,89	0
3	ATP	U	401	31/31	0.95	0.25	-0.48	69,90,98,108	0
3	ATP	G	401	31/31	0.94	0.28	-0.48	75,91,100,102	0
3	ATP	Q	401	31/31	0.95	0.26	-0.51	69,88,94,95	0
4	CA	A	402	1/1	0.93	0.28	-0.57	62,62,62,62	0
3	ATP	X	401	31/31	0.96	0.24	-0.62	73,81,87,89	0
3	ATP	O	401	31/31	0.94	0.25	-0.65	81,94,104,111	0
4	CA	I	402	1/1	0.93	0.25	-0.67	72,72,72,72	0
4	CA	U	402	1/1	0.93	0.23	-0.71	67,67,67,67	0
3	ATP	M	401	31/31	0.96	0.21	-0.95	75,83,94,99	0
3	ATP	K	401	31/31	0.94	0.23	-0.95	83,97,101,105	0
3	ATP	C	401	31/31	0.95	0.22	-0.97	72,82,91,95	0
3	ATP	S	401	31/31	0.95	0.22	-0.97	72,78,88,90	0
3	ATP	E	401	31/31	0.94	0.24	-0.99	76,91,107,118	0
4	CA	M	402	1/1	0.97	0.22	-1.39	67,67,67,67	0
4	CA	E	402	1/1	0.96	0.20	-2.35	73,73,73,73	0
4	CA	G	402	1/1	0.93	0.22	-	80,80,80,80	0
4	CA	O	402	1/1	0.94	0.20	-	73,73,73,73	0
4	CA	C	402	1/1	0.97	0.21	-	65,65,65,65	0
4	CA	K	402	1/1	0.92	0.23	-	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.