



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2017 – 06:16 AM EST

PDB ID : 4WYB
Title : Structure of the Bud6 flank domain in complex with actin
Authors : Eck, M.J.; Park, E.; Zheng, W.
Deposited on : unknown
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

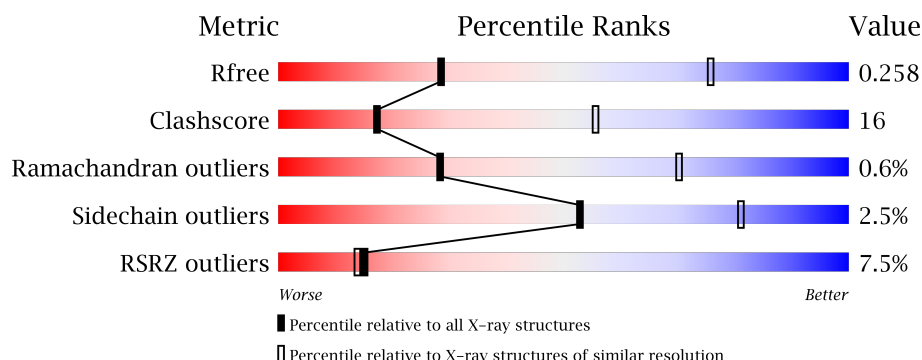
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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 ≥ 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>7%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
1	C	377	<div> <div>6%</div> <div>75%</div> <div>20%</div> <div>• 5%</div> </div>
1	E	377	<div> <div>7%</div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div>
1	G	377	<div> <div>8%</div> <div>69%</div> <div>23%</div> <div>• 6%</div> </div>
1	I	377	<div> <div>6%</div> <div>72%</div> <div>22%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	377	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	I	402	-	-	-	X
4	CA	M	402	-	-	-	X
4	CA	Q	402	-	-	-	X
4	CA	S	402	-	-	-	X
4	CA	X	402	-	-	-	X

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:

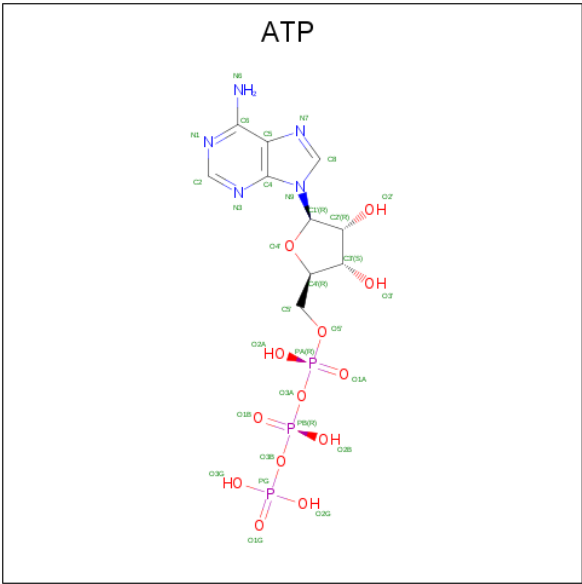
Chain	Residue	Modelled	Actual	Comment	Reference
B	697	GLY	-	expression tag	UNP P41697
B	698	SER	-	expression tag	UNP P41697
D	697	GLY	-	expression tag	UNP P41697
D	698	SER	-	expression tag	UNP P41697
F	697	GLY	-	expression tag	UNP P41697
F	698	SER	-	expression tag	UNP P41697
H	697	GLY	-	expression tag	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: C₁₀H₁₆N₅O₁₃P₃).



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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		

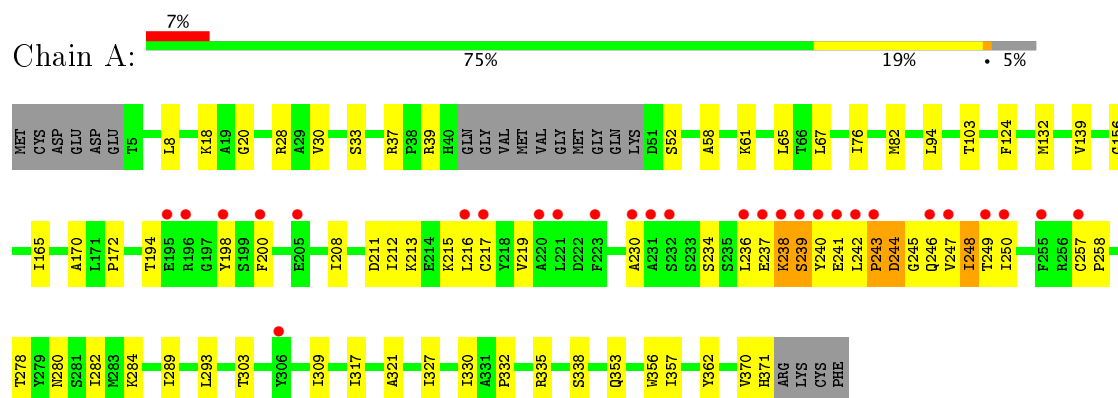
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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		

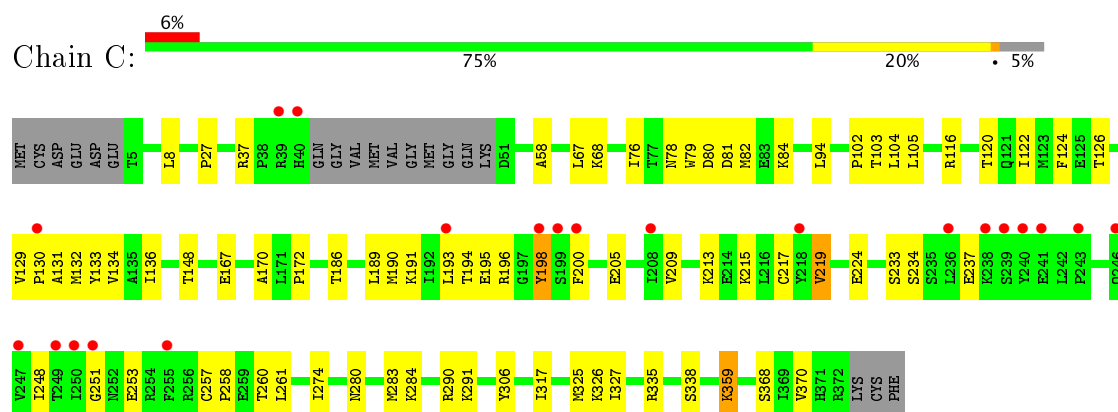
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

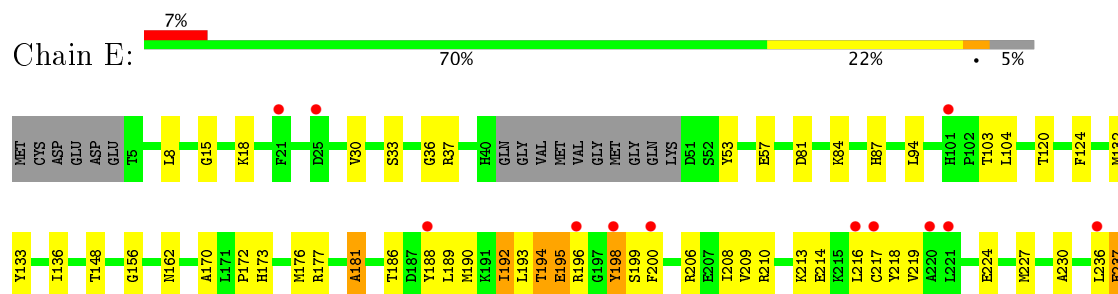
- Molecule 1: Actin, alpha skeletal muscle

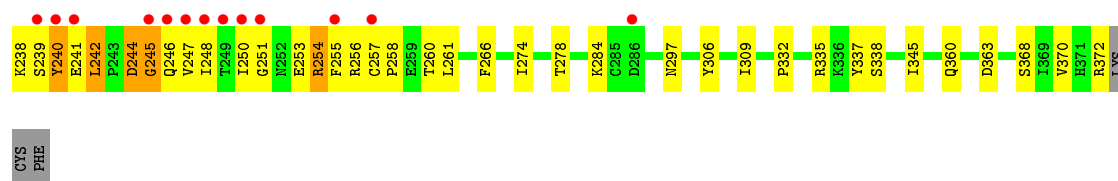


- Molecule 1: Actin, alpha skeletal muscle

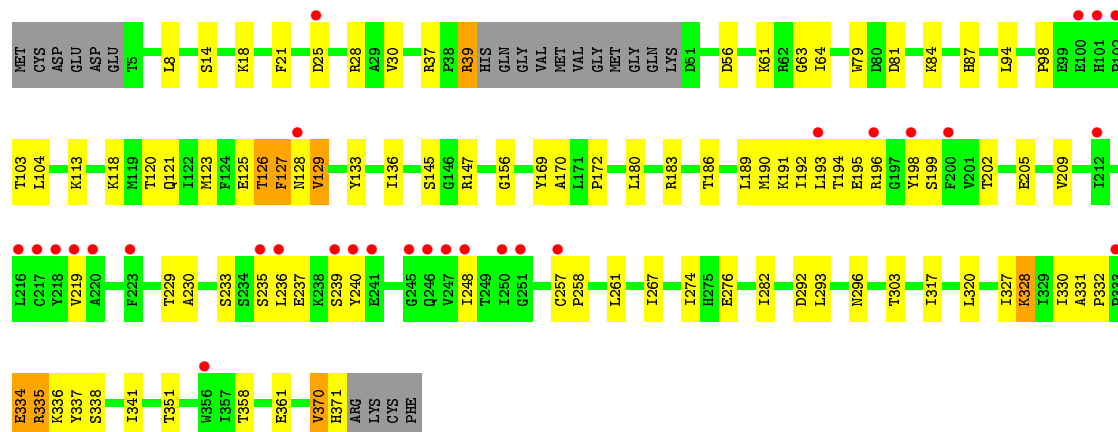


- Molecule 1: Actin, alpha skeletal muscle

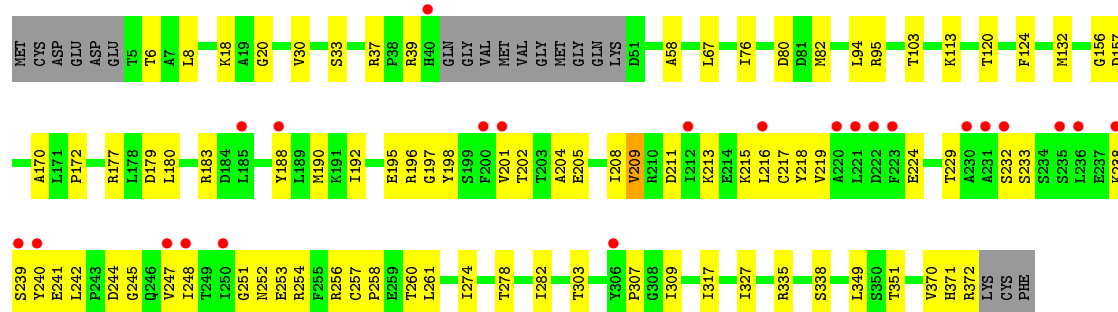




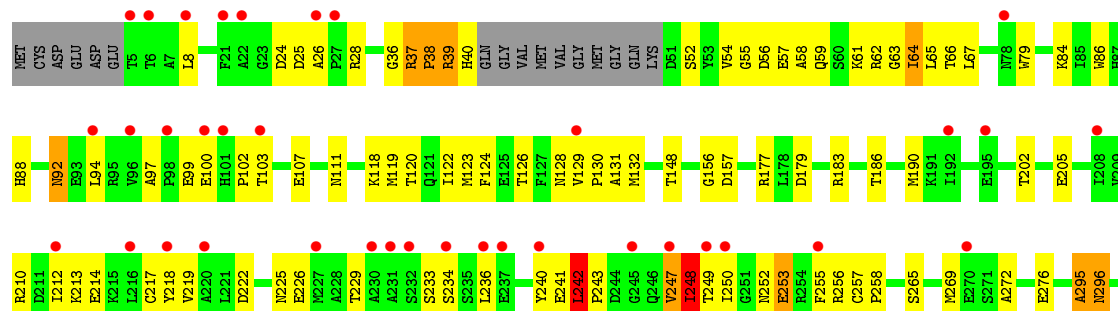
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

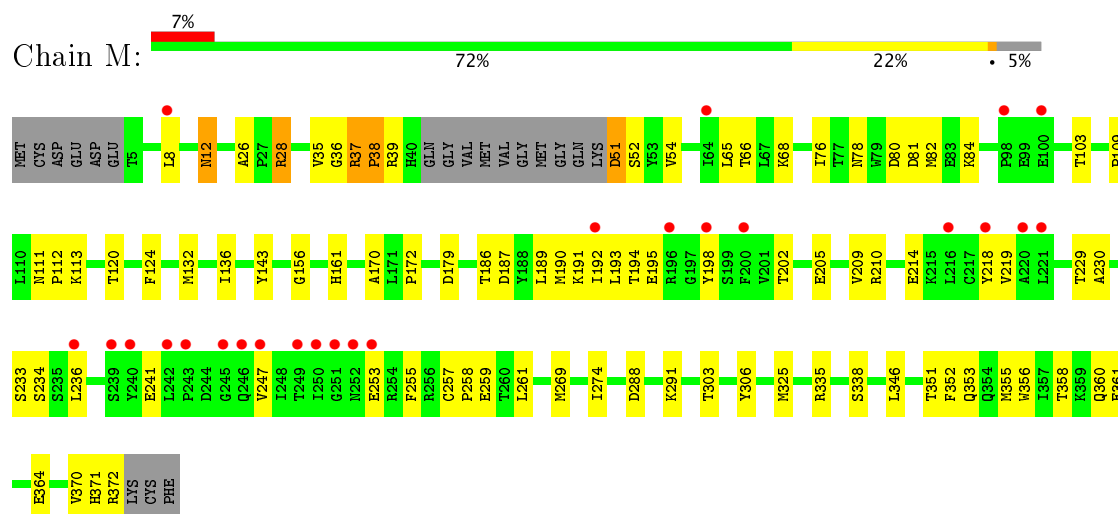


- Molecule 1: Actin, alpha skeletal muscle

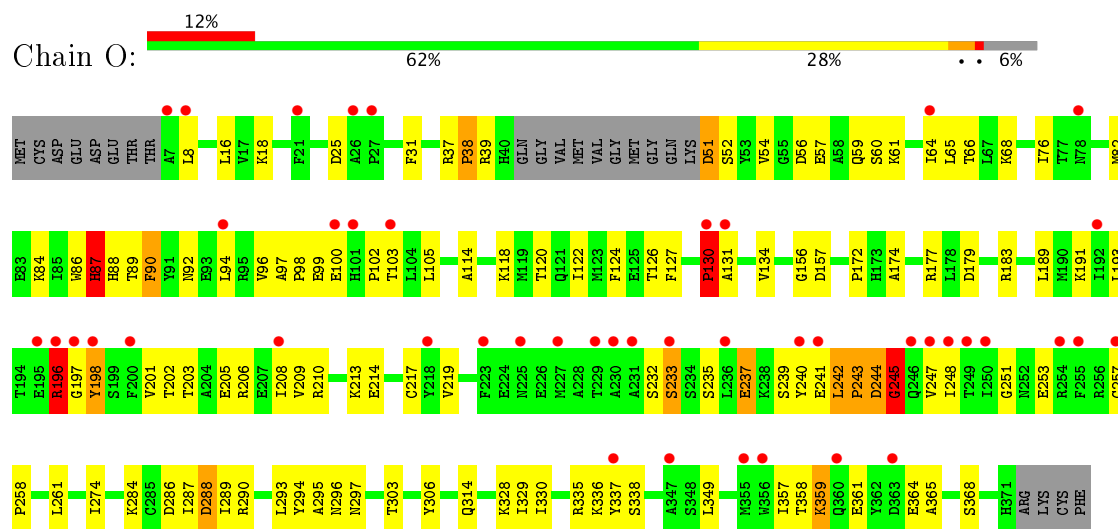




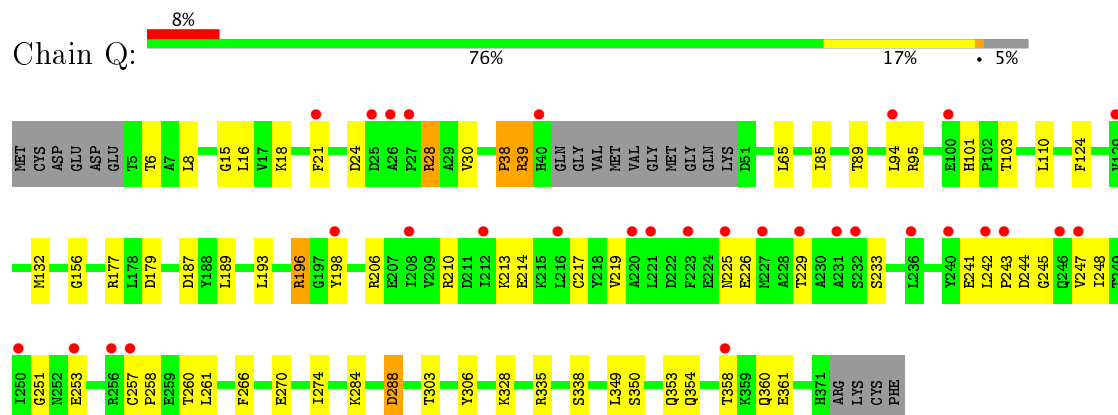
- Molecule 1: Actin, alpha skeletal muscle



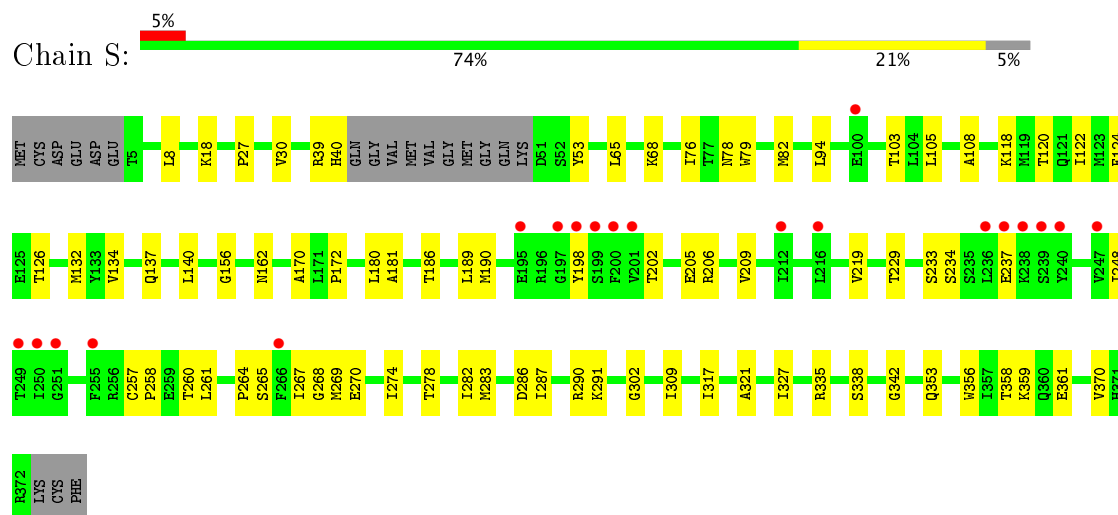
- Molecule 1: Actin, alpha skeletal muscle



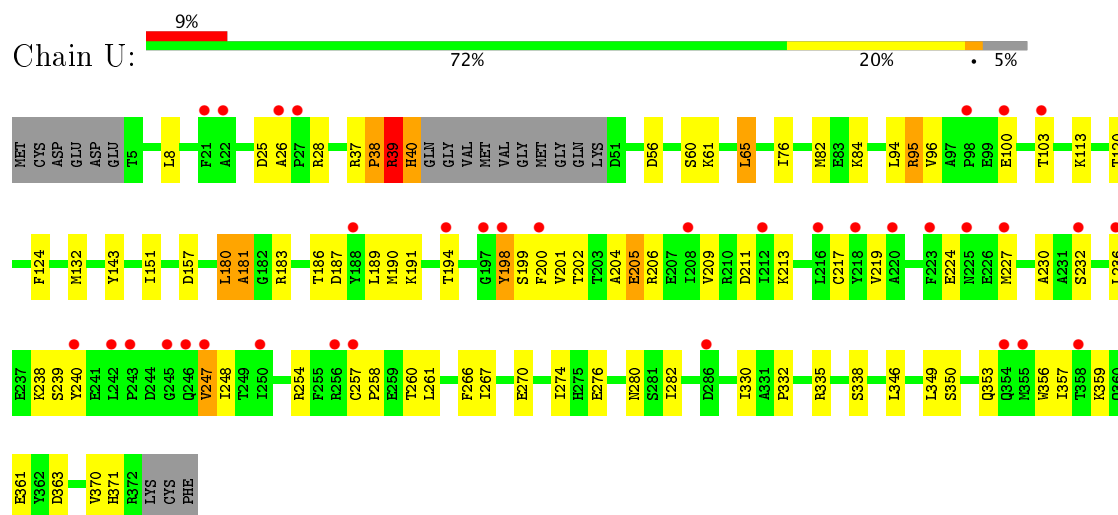
- Molecule 1: Actin, alpha skeletal muscle



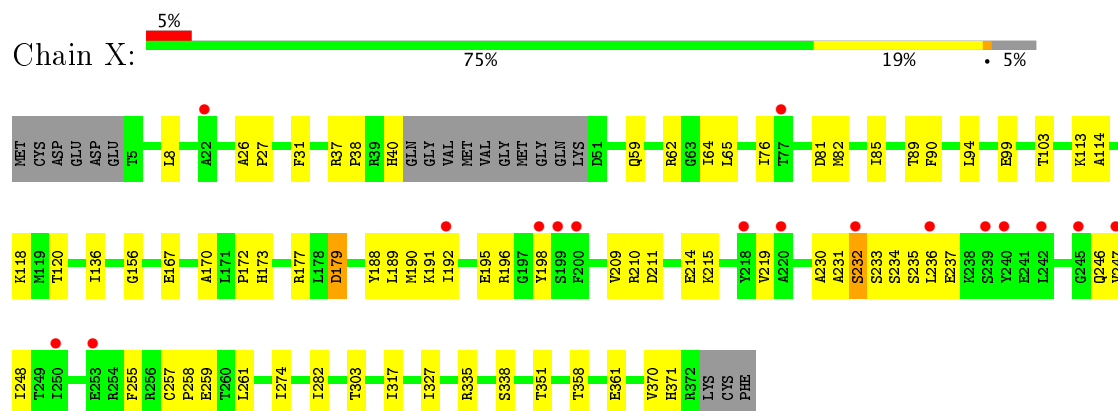
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

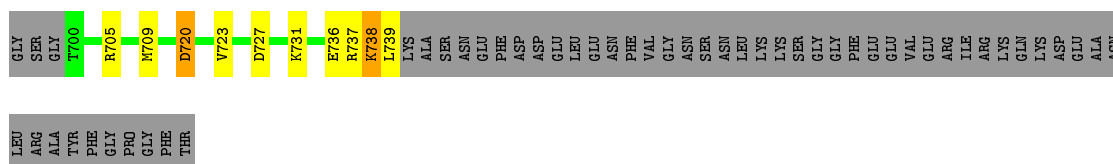


- Molecule 1: Actin, alpha skeletal muscle

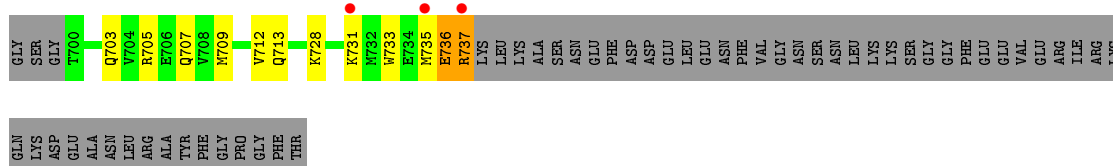


- Molecule 2: Bud site selection protein 6

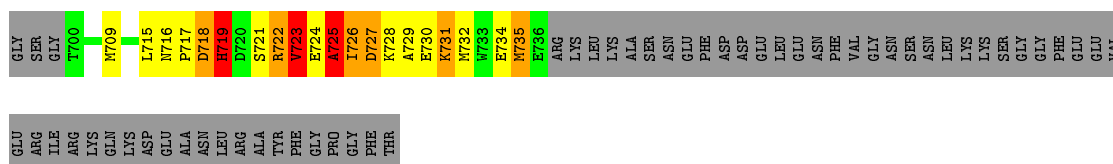




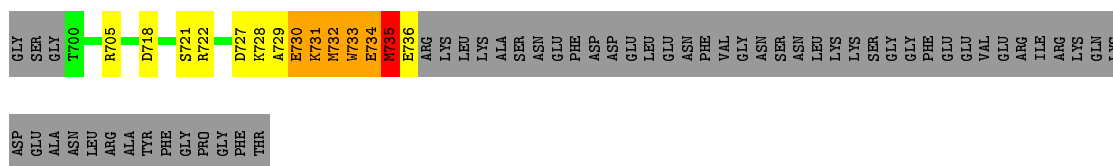
• Molecule 2: Bud site selection protein 6



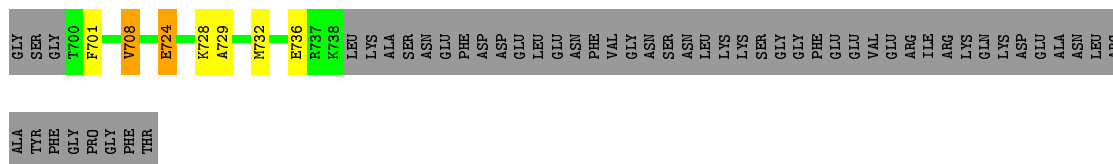
• Molecule 2: Bud site selection protein 6



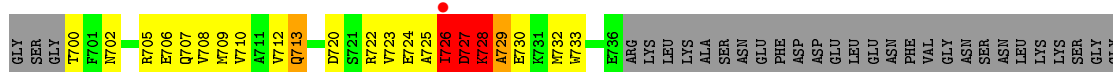
• Molecule 2: Bud site selection protein 6



• Molecule 2: Bud site selection protein 6



• Molecule 2: Bud site selection protein 6



PHE
GLU
GLU
VAL
GLU
ARG
ILE
ARG
LYS
GLN
LYS
ASP
GLU
ALA
ASN
LEU
ARG
ALA
TYR
PHE
GLY
PRO
GLY
PHE
THR

• Molecule 2: Bud site selection protein 6

Chain N: 24% 16% 60%

GLY SER GLY T700 Q703 N704 R705 E706 Q707 V708 M709 V710 A711 D720 E724 A725 I726 E730 K731 M732 M733 E736 ARG LYS LEU LYS LYS ALA SER ASN GLU PHE ASP ASP GLU LEU LEU ASN PHE VAL GLY ASN SER ASN LEU LYS LYS SER GLY PHE GLU VAL GLU ARG

ILE ARG LYS GLN LYS ASP GLU ALA ASN LEU ARG ALA TYR PHE GLY PRO PHE THR

• Molecule 2: Bud site selection protein 6

Chain P: 10% 26% 13% 60%

GLY SER GLY T700 F701 N702 Q703 R704 E705 Q707 V708 M709 H719 D720 S721 R722 V723 E724 A725 I726 D727 E730 E734 M735 E736 ARG LYS LYS LEU LYS ALA SER ASN GLU PHE ASP ASP GLU LEU LEU ASN PHE VAL GLY ASN SER ASN LEU LYS LYS SER GLY PHE GLU VAL GLU

ARG ILE ARG LYS GLN LYS ASP GLU ALA ASN LEU ARG ALA TYR PHE GLY PRO PHE THR

• Molecule 2: Bud site selection protein 6

Chain R: .% 25% 14% 60%

GLY SER GLY T700 F701 N704 R705 E706 Q707 M709 D720 V723 E724 E730 K731 M732 M733 E734 M735 E736 ARG LYS LEU LYS ALA SER ASN GLU PHE ASP ASP GLU LEU LEU ASN PHE VAL GLY ASN SER ASN LEU LYS LYS SER GLY PHE GLU VAL GLU ARG ILE ARG

LYS GLN LYS ASP GLU ALA ASN LEU ARG ALA TYR PHE GLY PRO PHE THR

• Molecule 2: Bud site selection protein 6

Chain T: 33% 7% 59%

GLY SER GLY T700 L715 N716 D720 V723 D727 K731 M732 M733 R737 LYS LEU LYS LYS ALA ALA SER ASN GLU PHE ASP ASP GLU LEU LEU ASN VAL PHE GLY ASN SER ASN LEU LYS LYS SER GLY PHE VAL GLU VAL GLU ARG ARG ARG LYS LYS LYS ASP GLU ILE ARG ASN

LEU ARG ALA TYR PHE GLY PRO PHE THR

• Molecule 2: Bud site selection protein 6

Chain V: 2% 18% 17% 60%

GLY SER GLY T700 F701 V704 R705 E706 Q707 M709 V710 Q713 D720 V723 E724 A725 I726 D727 E730 K731 M732 M733 E734 M735 E736 ARG LYS LYS LYS ALA SER ASN GLU PHE ASP ASP GLU LEU LEU ASN VAL PHE GLY ASN SER ASN LEU LYS LYS SER GLY PHE VAL GLU VAL GLU ARG ARG ARG LYS LYS LYS ASP GLY PHE GLU

GLU	VAL	GLU	ARG	ILE	ARG	LYS	GLN	LYS	ASP	GLU	ALA	ASN	LEU	ARG	ALA	TYR	PHE	GLY	PRO	GLY	PHE	THR
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● Molecule 2: Bud site selection protein 6



GLY	SER	GLY	T700	N701	N702	Q703	R704	R705	E706	Q707	V708	N709	V710	Q713	S714	L715	D720	V723	E724	A725	I726	E730	W733	E734	M735	E736	ARG	LYS	LEU	LYS	LYS	ALA	SER	ASN	GLU	PHE	ASP	ASP	GLU	LEU	GLU	ASN	PHE	VAL	GLY	ASN	SER	ASN	LEU	LYS	LYS	SER	GLY	PHE
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GLU	GLU	VAL	GLU	ARG	ILE	ARG	LYS	GLN	LYS	ASP	GLU	ALA	ASN	LEU	ARG	ALA	TYR	PHE	GLY	PRO	GLY	PHE	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.48Å)	Xtriage
Refinement program	PHENIX 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 ²)	86.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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	0.91	EDS
Total number of atoms	37515	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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%)	44	80
1	C	354/377 (94%)	334 (94%)	19 (5%)	1 (0%)	44	80
1	E	354/377 (94%)	325 (92%)	29 (8%)	0	100	100
1	G	352/377 (93%)	326 (93%)	24 (7%)	2 (1%)	28	70
1	I	354/377 (94%)	333 (94%)	20 (6%)	1 (0%)	44	80
1	K	353/377 (94%)	329 (93%)	20 (6%)	4 (1%)	17	59
1	M	354/377 (94%)	337 (95%)	15 (4%)	2 (1%)	28	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	351/377 (93%)	322 (92%)	24 (7%)	5 (1%)	13	53
1	Q	353/377 (94%)	340 (96%)	12 (3%)	1 (0%)	44	80
1	S	354/377 (94%)	334 (94%)	20 (6%)	0	100	100
1	U	354/377 (94%)	338 (96%)	14 (4%)	2 (1%)	28	70
1	X	354/377 (94%)	335 (95%)	17 (5%)	2 (1%)	28	70
2	B	38/92 (41%)	35 (92%)	2 (5%)	1 (3%)	6	40
2	D	36/92 (39%)	33 (92%)	3 (8%)	0	100	100
2	F	35/92 (38%)	30 (86%)	3 (9%)	2 (6%)	2	21
2	H	35/92 (38%)	29 (83%)	3 (9%)	3 (9%)	1	11
2	J	37/92 (40%)	36 (97%)	1 (3%)	0	100	100
2	L	35/92 (38%)	25 (71%)	9 (26%)	1 (3%)	5	38
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%)	5	38
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%)	28	70

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%)	80	91
1	C	304/320 (95%)	299 (98%)	5 (2%)	68	87
1	E	303/320 (95%)	296 (98%)	7 (2%)	56	82
1	G	298/320 (93%)	290 (97%)	8 (3%)	50	80
1	I	304/320 (95%)	302 (99%)	2 (1%)	87	95
1	K	301/320 (94%)	290 (96%)	11 (4%)	39	73
1	M	304/320 (95%)	299 (98%)	5 (2%)	68	87
1	O	299/320 (93%)	286 (96%)	13 (4%)	33	70
1	Q	302/320 (94%)	298 (99%)	4 (1%)	73	90
1	S	302/320 (94%)	301 (100%)	1 (0%)	94	98
1	U	301/320 (94%)	291 (97%)	10 (3%)	43	76
1	X	302/320 (94%)	297 (98%)	5 (2%)	66	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	37/79 (47%)	35 (95%)	2 (5%)	26	63
2	D	35/79 (44%)	33 (94%)	2 (6%)	24	61
2	F	34/79 (43%)	29 (85%)	5 (15%)	3	20
2	H	32/79 (40%)	29 (91%)	3 (9%)	10	40
2	J	33/79 (42%)	31 (94%)	2 (6%)	22	60
2	L	32/79 (40%)	29 (91%)	3 (9%)	10	40
2	N	34/79 (43%)	33 (97%)	1 (3%)	48	78
2	P	34/79 (43%)	33 (97%)	1 (3%)	48	78
2	R	31/79 (39%)	29 (94%)	2 (6%)	20	58
2	T	35/79 (44%)	33 (94%)	2 (6%)	24	61
2	V	31/79 (39%)	29 (94%)	2 (6%)	20	58
2	Y	34/79 (43%)	33 (97%)	1 (3%)	48	78
All	All	4025/4788 (84%)	3925 (98%)	100 (2%)	53	81

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	27,33,33	4.54	10 (37%)	25,52,52	3.34	5 (20%)
3	ATP	C	401	4	27,33,33	4.53	10 (37%)	25,52,52	3.34	6 (24%)
3	ATP	E	401	4	27,33,33	4.53	10 (37%)	25,52,52	3.32	6 (24%)
3	ATP	G	401	4	27,33,33	4.53	10 (37%)	25,52,52	3.35	5 (20%)
3	ATP	I	401	4	27,33,33	4.51	10 (37%)	25,52,52	3.34	5 (20%)
3	ATP	K	401	4	27,33,33	4.51	10 (37%)	25,52,52	3.37	5 (20%)
3	ATP	M	401	4	27,33,33	4.55	10 (37%)	25,52,52	3.32	6 (24%)
3	ATP	O	401	4	27,33,33	4.48	10 (37%)	25,52,52	3.64	5 (20%)
3	ATP	Q	401	4	27,33,33	4.55	10 (37%)	25,52,52	3.36	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	S	401	4	27,33,33	4.54	10 (37%)	25,52,52	3.38	5 (20%)
3	ATP	U	401	4	27,33,33	4.53	10 (37%)	25,52,52	3.34	5 (20%)
3	ATP	X	401	4	27,33,33	4.51	10 (37%)	25,52,52	3.36	5 (20%)

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 (120) 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'	-9.65	1.27	1.53
3	S	401	ATP	C3'-C4'	-9.61	1.27	1.53
3	K	401	ATP	C3'-C4'	-9.53	1.28	1.53
3	I	401	ATP	C3'-C4'	-9.50	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	401	ATP	C3'-C4'	-9.49	1.28	1.53
3	A	401	ATP	C3'-C4'	-9.45	1.28	1.53
3	X	401	ATP	C3'-C4'	-9.44	1.28	1.53
3	G	401	ATP	C3'-C4'	-9.44	1.28	1.53
3	C	401	ATP	C3'-C4'	-9.42	1.28	1.53
3	U	401	ATP	C3'-C4'	-9.42	1.28	1.53
3	E	401	ATP	C3'-C4'	-9.41	1.28	1.53
3	M	401	ATP	C3'-C4'	-9.38	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	K	401	ATP	PA-O5'	2.50	1.69	1.59
3	X	401	ATP	O3'-C3'	2.51	1.48	1.43
3	S	401	ATP	PA-O5'	2.52	1.69	1.59
3	E	401	ATP	O3'-C3'	2.54	1.48	1.43
3	S	401	ATP	O3'-C3'	2.54	1.48	1.43
3	O	401	ATP	O3'-C3'	2.54	1.48	1.43
3	A	401	ATP	O3'-C3'	2.55	1.48	1.43
3	G	401	ATP	O3'-C3'	2.56	1.48	1.43
3	U	401	ATP	O3'-C3'	2.56	1.48	1.43
3	K	401	ATP	O3'-C3'	2.56	1.48	1.43
3	I	401	ATP	O3'-C3'	2.56	1.48	1.43
3	Q	401	ATP	O3'-C3'	2.57	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	401	ATP	O3'-C3'	2.57	1.48	1.43
3	C	401	ATP	O3'-C3'	2.59	1.48	1.43
3	Q	401	ATP	C6-N6	3.80	1.49	1.34
3	I	401	ATP	C6-N6	3.81	1.49	1.34
3	G	401	ATP	C6-N6	3.82	1.49	1.34
3	X	401	ATP	C6-N6	3.82	1.49	1.34
3	C	401	ATP	C6-N6	3.82	1.49	1.34
3	K	401	ATP	C6-N6	3.82	1.49	1.34
3	S	401	ATP	C6-N6	3.82	1.49	1.34
3	E	401	ATP	C6-N6	3.82	1.49	1.34
3	A	401	ATP	C6-N6	3.83	1.49	1.34
3	M	401	ATP	C6-N6	3.83	1.49	1.34
3	O	401	ATP	C6-N6	3.83	1.49	1.34
3	U	401	ATP	C6-N6	3.84	1.49	1.34
3	A	401	ATP	C2'-C3'	4.37	1.65	1.53
3	I	401	ATP	C2'-C3'	4.39	1.65	1.53
3	S	401	ATP	C2'-C3'	4.39	1.65	1.53
3	Q	401	ATP	C2'-C3'	4.39	1.65	1.53
3	K	401	ATP	C2'-C3'	4.39	1.65	1.53
3	G	401	ATP	C2'-C3'	4.39	1.65	1.53
3	X	401	ATP	C2'-C3'	4.40	1.65	1.53
3	M	401	ATP	C2'-C3'	4.41	1.65	1.53
3	U	401	ATP	C2'-C3'	4.41	1.65	1.53
3	C	401	ATP	C2'-C3'	4.43	1.65	1.53
3	E	401	ATP	C2'-C3'	4.47	1.65	1.53
3	O	401	ATP	C2'-C3'	4.54	1.65	1.53
3	O	401	ATP	O4'-C4'	4.78	1.55	1.45
3	S	401	ATP	O4'-C4'	4.95	1.56	1.45
3	K	401	ATP	O4'-C4'	5.01	1.56	1.45
3	Q	401	ATP	O4'-C4'	5.07	1.56	1.45
3	U	401	ATP	O4'-C4'	5.07	1.56	1.45
3	X	401	ATP	O4'-C4'	5.07	1.56	1.45
3	G	401	ATP	O4'-C4'	5.08	1.56	1.45
3	I	401	ATP	O4'-C4'	5.09	1.56	1.45
3	A	401	ATP	O4'-C4'	5.10	1.56	1.45
3	C	401	ATP	O4'-C4'	5.11	1.56	1.45
3	E	401	ATP	O4'-C4'	5.16	1.56	1.45
3	M	401	ATP	O4'-C4'	5.16	1.56	1.45
3	K	401	ATP	PG-O3B	5.39	1.68	1.60
3	A	401	ATP	PG-O3B	5.43	1.68	1.60
3	G	401	ATP	PG-O3B	5.49	1.68	1.60
3	O	401	ATP	PG-O3B	5.50	1.69	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	401	ATP	PG-O3B	5.50	1.69	1.60
3	U	401	ATP	PG-O3B	5.51	1.69	1.60
3	X	401	ATP	PG-O3B	5.52	1.69	1.60
3	C	401	ATP	PG-O3B	5.54	1.69	1.60
3	I	401	ATP	PG-O3B	5.54	1.69	1.60
3	S	401	ATP	PG-O3B	5.59	1.69	1.60
3	M	401	ATP	PG-O3B	5.59	1.69	1.60
3	E	401	ATP	PG-O3B	5.61	1.69	1.60
3	O	401	ATP	O4'-C1'	9.66	1.54	1.41
3	E	401	ATP	O4'-C1'	9.93	1.55	1.41
3	I	401	ATP	O4'-C1'	9.96	1.55	1.41
3	X	401	ATP	O4'-C1'	9.96	1.55	1.41
3	U	401	ATP	O4'-C1'	9.99	1.55	1.41
3	G	401	ATP	O4'-C1'	9.99	1.55	1.41
3	Q	401	ATP	O4'-C1'	10.02	1.55	1.41
3	S	401	ATP	O4'-C1'	10.02	1.55	1.41
3	A	401	ATP	O4'-C1'	10.02	1.55	1.41
3	C	401	ATP	O4'-C1'	10.03	1.55	1.41
3	K	401	ATP	O4'-C1'	10.03	1.55	1.41
3	M	401	ATP	O4'-C1'	10.05	1.55	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	401	ATP	N3-C2-N1	-10.24	119.94	128.86
3	A	401	ATP	N3-C2-N1	-10.20	119.98	128.86
3	Q	401	ATP	N3-C2-N1	-10.15	120.02	128.86
3	O	401	ATP	N3-C2-N1	-10.15	120.02	128.86
3	G	401	ATP	N3-C2-N1	-10.13	120.03	128.86
3	I	401	ATP	N3-C2-N1	-10.13	120.03	128.86
3	U	401	ATP	N3-C2-N1	-10.12	120.04	128.86
3	S	401	ATP	N3-C2-N1	-10.00	120.15	128.86
3	K	401	ATP	N3-C2-N1	-10.00	120.15	128.86
3	M	401	ATP	N3-C2-N1	-9.92	120.22	128.86
3	C	401	ATP	N3-C2-N1	-9.92	120.22	128.86
3	E	401	ATP	N3-C2-N1	-9.82	120.30	128.86
3	O	401	ATP	C1'-N9-C4	-8.04	112.75	126.64
3	K	401	ATP	C1'-N9-C4	-7.72	113.30	126.64
3	S	401	ATP	C1'-N9-C4	-7.60	113.51	126.64
3	C	401	ATP	C1'-N9-C4	-7.49	113.70	126.64
3	Q	401	ATP	C1'-N9-C4	-7.48	113.72	126.64
3	G	401	ATP	C1'-N9-C4	-7.45	113.76	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	401	ATP	C1'-N9-C4	-7.41	113.83	126.64
3	X	401	ATP	C1'-N9-C4	-7.41	113.83	126.64
3	U	401	ATP	C1'-N9-C4	-7.38	113.88	126.64
3	M	401	ATP	C1'-N9-C4	-7.36	113.92	126.64
3	E	401	ATP	C1'-N9-C4	-7.30	114.02	126.64
3	A	401	ATP	C1'-N9-C4	-7.29	114.03	126.64
3	O	401	ATP	C4'-O4'-C1'	-7.27	102.03	109.77
3	E	401	ATP	N6-C6-N1	-7.01	104.87	118.77
3	O	401	ATP	N6-C6-N1	-6.99	104.90	118.77
3	K	401	ATP	N6-C6-N1	-6.94	105.01	118.77
3	X	401	ATP	N6-C6-N1	-6.91	105.06	118.77
3	C	401	ATP	N6-C6-N1	-6.90	105.08	118.77
3	S	401	ATP	N6-C6-N1	-6.90	105.08	118.77
3	I	401	ATP	N6-C6-N1	-6.90	105.10	118.77
3	M	401	ATP	N6-C6-N1	-6.89	105.10	118.77
3	U	401	ATP	N6-C6-N1	-6.88	105.12	118.77
3	A	401	ATP	N6-C6-N1	-6.88	105.12	118.77
3	G	401	ATP	N6-C6-N1	-6.88	105.13	118.77
3	Q	401	ATP	N6-C6-N1	-6.88	105.13	118.77
3	S	401	ATP	C4'-O4'-C1'	-4.59	104.88	109.77
3	Q	401	ATP	C4'-O4'-C1'	-4.09	105.42	109.77
3	K	401	ATP	C4'-O4'-C1'	-4.01	105.50	109.77
3	G	401	ATP	C4'-O4'-C1'	-3.98	105.54	109.77
3	X	401	ATP	C4'-O4'-C1'	-3.95	105.56	109.77
3	I	401	ATP	C4'-O4'-C1'	-3.88	105.64	109.77
3	C	401	ATP	C4'-O4'-C1'	-3.84	105.68	109.77
3	M	401	ATP	C4'-O4'-C1'	-3.79	105.73	109.77
3	A	401	ATP	C4'-O4'-C1'	-3.79	105.74	109.77
3	U	401	ATP	C4'-O4'-C1'	-3.76	105.76	109.77
3	E	401	ATP	C4'-O4'-C1'	-3.63	105.91	109.77
3	E	401	ATP	C2'-C3'-C4'	2.01	106.54	102.62
3	M	401	ATP	C2'-C3'-C4'	2.02	106.55	102.62
3	C	401	ATP	C2'-C3'-C4'	2.07	106.65	102.62
3	A	401	ATP	C5-C6-N6	7.03	134.81	120.47
3	U	401	ATP	C5-C6-N6	7.04	134.82	120.47
3	G	401	ATP	C5-C6-N6	7.05	134.83	120.47
3	I	401	ATP	C5-C6-N6	7.06	134.87	120.47
3	S	401	ATP	C5-C6-N6	7.07	134.89	120.47
3	X	401	ATP	C5-C6-N6	7.08	134.89	120.47
3	M	401	ATP	C5-C6-N6	7.08	134.90	120.47
3	C	401	ATP	C5-C6-N6	7.08	134.91	120.47
3	Q	401	ATP	C5-C6-N6	7.09	134.91	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	K	401	ATP	C5-C6-N6	7.12	134.97	120.47
3	O	401	ATP	C5-C6-N6	7.16	135.07	120.47
3	E	401	ATP	C5-C6-N6	7.19	135.13	120.47

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	357/377 (94%)	0.46	28 (7%) 14 13	47, 76, 125, 154	0
1	C	358/377 (94%)	0.47	21 (5%) 23 19	50, 79, 125, 174	0
1	E	358/377 (94%)	0.53	25 (6%) 17 15	57, 89, 133, 161	0
1	G	356/377 (94%)	0.58	30 (8%) 12 12	57, 89, 130, 155	0
1	I	358/377 (94%)	0.44	23 (6%) 20 17	48, 76, 125, 168	0
1	K	357/377 (94%)	0.69	39 (10%) 6 7	62, 94, 144, 169	0
1	M	358/377 (94%)	0.49	25 (6%) 17 15	53, 79, 121, 171	0
1	O	355/377 (94%)	0.66	45 (12%) 4 5	61, 95, 144, 161	0
1	Q	357/377 (94%)	0.61	31 (8%) 11 11	59, 87, 126, 171	0
1	S	358/377 (94%)	0.44	20 (5%) 25 21	53, 78, 123, 172	0
1	U	358/377 (94%)	0.61	35 (9%) 8 9	57, 87, 123, 167	0
1	X	358/377 (94%)	0.51	17 (4%) 32 26	52, 78, 125, 168	0
2	B	40/92 (43%)	-0.02	0 100 100	69, 85, 119, 129	0
2	D	38/92 (41%)	0.24	3 (7%) 13 13	71, 92, 129, 151	0
2	F	37/92 (40%)	0.30	0 100 100	95, 108, 133, 149	0
2	H	37/92 (40%)	0.18	0 100 100	24, 103, 125, 131	0
2	J	39/92 (42%)	-0.16	0 100 100	68, 83, 102, 113	0
2	L	37/92 (40%)	0.56	1 (2%) 55 46	95, 121, 165, 173	0
2	N	37/92 (40%)	0.27	0 100 100	78, 97, 111, 118	0
2	P	37/92 (40%)	1.11	9 (24%) 1 1	98, 115, 158, 172	0
2	R	37/92 (40%)	0.41	1 (2%) 55 46	87, 108, 127, 135	0
2	T	38/92 (41%)	0.16	0 100 100	73, 88, 116, 122	0
2	V	37/92 (40%)	0.44	2 (5%) 26 22	92, 113, 126, 130	0
2	Y	37/92 (40%)	0.02	0 100 100	79, 93, 107, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4739/5628 (84%)	0.52	355 (7%) 15 14	24, 86, 130, 174	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	236	LEU	5.9
1	M	236	LEU	5.8
1	G	198	TYR	5.8
1	S	247	VAL	5.4
1	C	250	ILE	5.4
1	E	250	ILE	5.3
1	G	236	LEU	5.2
1	E	240	TYR	5.2
1	S	250	ILE	5.2
1	E	216	LEU	5.0
1	K	236	LEU	5.0
1	O	236	LEU	4.9
1	A	238	LYS	4.9
1	A	247	VAL	4.8
1	O	246	GLN	4.7
1	C	247	VAL	4.7
1	G	250	ILE	4.7
1	M	250	ILE	4.4
1	O	250	ILE	4.3
2	P	726	ILE	4.3
1	I	200	PHE	4.3
1	C	199	SER	4.3
1	E	220	ALA	4.3
1	E	236	LEU	4.2
1	E	247	VAL	4.1
1	S	198	TYR	4.1
1	X	218	TYR	4.1
1	S	200	PHE	4.0
1	K	250	ILE	4.0
1	C	236	LEU	4.0
1	U	208	ILE	3.9
1	U	26	ALA	3.9
1	A	240	TYR	3.9
1	S	239	SER	3.9
1	G	240	TYR	3.9
1	A	250	ILE	3.9
1	K	231	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	356	TRP	3.7
1	X	199	SER	3.7
1	Q	40	HIS	3.6
1	A	249	THR	3.6
1	C	255	PHE	3.6
1	Q	198	TYR	3.6
1	X	200	PHE	3.6
1	E	200	PHE	3.5
1	G	218	TYR	3.5
1	K	6	THR	3.5
1	S	240	TYR	3.5
1	I	236	LEU	3.5
1	X	22	ALA	3.5
1	K	240	TYR	3.5
1	G	216	LEU	3.5
1	O	26	ALA	3.5
1	U	232	SER	3.5
1	I	250	ILE	3.5
1	K	100	GLU	3.4
1	M	218	TYR	3.4
1	K	212	ILE	3.4
1	K	5	THR	3.4
1	I	221	LEU	3.4
1	G	245	GLY	3.4
1	G	241	GLU	3.4
1	Q	236	LEU	3.4
1	Q	247	VAL	3.4
1	C	200	PHE	3.4
2	P	701	PHE	3.4
1	E	249	THR	3.4
1	X	239	SER	3.3
1	U	236	LEU	3.3
2	P	735	MET	3.3
1	C	240	TYR	3.3
1	X	247	VAL	3.3
1	G	251	GLY	3.3
1	Q	223	PHE	3.3
1	S	199	SER	3.3
1	Q	243	PRO	3.3
1	I	40	HIS	3.3
1	O	131	ALA	3.2
1	O	198	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	240	TYR	3.2
1	A	246	GLN	3.2
1	E	246	GLN	3.2
1	I	231	ALA	3.2
1	O	360	GLN	3.1
1	K	237	GLU	3.1
1	X	250	ILE	3.1
1	Q	208	ILE	3.1
2	L	726	ILE	3.1
1	O	356	TRP	3.1
1	E	241	GLU	3.1
1	E	239	SER	3.1
1	M	216	LEU	3.1
1	A	232	SER	3.0
1	U	286	ASP	3.0
1	I	220	ALA	3.0
1	A	236	LEU	3.0
1	S	251	GLY	3.0
1	X	240	TYR	3.0
1	U	200	PHE	2.9
1	C	246	GLN	2.9
1	O	8	LEU	2.9
1	M	239	SER	2.9
1	C	238	LYS	2.9
1	K	232	SER	2.9
1	G	239	SER	2.9
1	A	241	GLU	2.9
1	S	255	PHE	2.9
1	K	129	VAL	2.9
1	E	251	GLY	2.9
1	K	103	THR	2.9
1	O	218	TYR	2.9
1	A	200	PHE	2.9
1	G	257	CYS	2.9
1	Q	242	LEU	2.9
1	U	242	LEU	2.9
1	O	130	PRO	2.8
1	O	225	ASN	2.8
1	G	220	ALA	2.8
1	U	100	GLU	2.8
1	M	200	PHE	2.8
1	G	101	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	240	TYR	2.8
1	M	246	GLN	2.8
1	O	240	TYR	2.8
1	S	238	LYS	2.8
1	U	197	GLY	2.8
1	S	236	LEU	2.8
1	G	247	VAL	2.8
1	O	21	PHE	2.8
1	M	100	GLU	2.8
1	Q	225	ASN	2.8
1	G	200	PHE	2.8
1	S	249	THR	2.7
1	C	251	GLY	2.7
1	U	27	PRO	2.7
1	E	245	GLY	2.7
1	M	220	ALA	2.7
1	U	218	TYR	2.7
1	X	232	SER	2.7
1	U	257	CYS	2.7
1	G	25	ASP	2.7
2	V	726	ILE	2.7
1	I	185	LEU	2.7
1	A	220	ALA	2.7
1	K	363	ASP	2.7
1	K	192	ILE	2.7
1	Q	246	GLN	2.7
1	K	227	MET	2.7
1	U	358	THR	2.7
1	M	247	VAL	2.7
1	O	27	PRO	2.7
1	X	245	GLY	2.7
1	U	225	ASN	2.7
1	O	197	GLY	2.7
1	U	250	ILE	2.7
1	X	198	TYR	2.6
1	M	196	ARG	2.6
1	Q	25	ASP	2.6
1	E	196	ARG	2.6
1	O	255	PHE	2.6
1	G	217	CYS	2.6
1	O	103	THR	2.6
1	E	101	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	198	TYR	2.6
1	E	21	PHE	2.6
1	A	221	LEU	2.6
1	K	218	TYR	2.6
1	K	245	GLY	2.6
1	I	222	ASP	2.6
1	G	128	ASN	2.6
1	O	248	ILE	2.6
1	E	188	TYR	2.6
1	Q	257	CYS	2.6
1	Q	232	SER	2.6
1	E	217	CYS	2.6
1	O	192	ILE	2.6
1	O	208	ILE	2.5
1	A	196	ARG	2.5
1	A	231	ALA	2.5
1	G	100	GLU	2.5
1	Q	100	GLU	2.5
1	K	247	VAL	2.5
1	K	8	LEU	2.5
1	I	248	ILE	2.5
1	K	230	ALA	2.5
1	U	240	TYR	2.5
1	U	256	ARG	2.5
1	I	216	LEU	2.5
1	O	227	MET	2.5
1	A	239	SER	2.5
1	C	130	PRO	2.5
1	K	220	ALA	2.5
1	C	40	HIS	2.5
1	G	102	PRO	2.5
1	O	241	GLU	2.5
1	O	78	ASN	2.5
1	U	245	GLY	2.5
1	Q	231	ALA	2.5
1	I	239	SER	2.5
1	O	233	SER	2.5
1	K	94	LEU	2.4
1	M	240	TYR	2.4
1	U	243	PRO	2.4
1	O	101	HIS	2.4
1	C	239	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	196	ARG	2.4
1	S	100	GLU	2.4
1	S	201	VAL	2.4
1	S	216	LEU	2.4
1	O	223	PHE	2.4
1	A	243	PRO	2.4
1	X	220	ALA	2.4
1	A	242	LEU	2.4
1	A	257	CYS	2.4
1	C	241	GLU	2.4
1	I	306	TYR	2.4
1	S	212	ILE	2.4
1	Q	229	THR	2.4
1	G	248	ILE	2.4
1	Q	212	ILE	2.4
1	X	242	LEU	2.4
1	X	192	ILE	2.4
1	K	216	LEU	2.4
1	G	235	SER	2.4
2	V	732	MET	2.4
1	M	98	PRO	2.4
1	Q	27	PRO	2.4
1	U	246	GLN	2.3
1	I	230	ALA	2.3
1	M	192	ILE	2.3
1	Q	220	ALA	2.3
1	U	103	THR	2.3
1	K	270	GLU	2.3
1	E	25	ASP	2.3
1	Q	253	GLU	2.3
1	O	231	ALA	2.3
1	U	220	ALA	2.3
1	A	223	PHE	2.3
1	U	194	THR	2.3
1	Q	129	VAL	2.3
1	U	223	PHE	2.3
1	O	64	ILE	2.3
1	O	94	LEU	2.3
1	A	216	LEU	2.3
1	A	306	TYR	2.3
1	M	242	LEU	2.3
1	K	26	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	337	TYR	2.3
1	A	195	GLU	2.3
1	I	238	LYS	2.3
2	P	719	HIS	2.3
1	Q	26	ALA	2.3
1	Q	250	ILE	2.3
1	I	223	PHE	2.3
1	A	205	GLU	2.3
1	K	78	ASN	2.3
1	O	229	THR	2.3
1	Q	358	THR	2.3
2	D	731	LYS	2.3
1	M	243	PRO	2.3
1	I	247	VAL	2.3
1	M	198	TYR	2.3
1	M	245	GLY	2.3
1	K	249	THR	2.3
1	C	198	TYR	2.3
1	K	101	HIS	2.3
1	O	195	GLU	2.2
1	G	196	ARG	2.2
1	Q	21	PHE	2.2
1	O	355	MET	2.2
1	C	218	TYR	2.2
1	I	212	ILE	2.2
1	S	266	PHE	2.2
1	E	198	TYR	2.2
1	K	27	PRO	2.2
1	Q	227	MET	2.2
1	C	39	ARG	2.2
2	P	730	GLU	2.2
1	O	257	CYS	2.2
1	I	188	TYR	2.2
1	Q	221	LEU	2.2
1	U	21	PHE	2.2
1	O	247	VAL	2.2
2	D	737	ARG	2.2
1	U	227	MET	2.2
1	U	188	TYR	2.2
1	X	253	GLU	2.2
2	D	735	MET	2.2
1	Q	256	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	232	SER	2.2
1	K	234	SER	2.2
1	E	286	ASP	2.2
1	K	98	PRO	2.2
1	C	249	THR	2.2
1	K	22	ALA	2.1
1	K	21	PHE	2.1
1	C	193	LEU	2.1
1	U	22	ALA	2.1
1	K	96	VAL	2.1
1	S	237	GLU	2.1
2	P	734	GLU	2.1
1	U	216	LEU	2.1
1	C	208	ILE	2.1
1	A	255	PHE	2.1
1	S	195	GLU	2.1
1	Q	94	LEU	2.1
1	E	255	PHE	2.1
1	G	356	TRP	2.1
1	I	201	VAL	2.1
1	U	247	VAL	2.1
1	M	249	THR	2.1
1	M	251	GLY	2.1
1	K	255	PHE	2.1
1	O	200	PHE	2.1
1	M	253	GLU	2.1
1	M	252	ASN	2.1
1	O	230	ALA	2.1
1	O	347	ALA	2.1
1	E	248	ILE	2.1
1	G	212	ILE	2.1
1	G	219	VAL	2.1
1	U	354	GLN	2.1
1	O	7	ALA	2.1
2	P	721	SER	2.1
1	U	355	MET	2.1
1	X	77	THR	2.1
1	A	230	ALA	2.1
1	C	243	PRO	2.1
1	M	64	ILE	2.1
1	Q	216	LEU	2.1
1	A	217	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	257	CYS	2.0
1	O	249	THR	2.0
2	P	723	VAL	2.0
1	E	221	LEU	2.0
1	S	197	GLY	2.0
1	O	363	ASP	2.0
2	P	722	ARG	2.0
1	G	193	LEU	2.0
1	A	237	GLU	2.0
1	G	246	GLN	2.0
1	K	195	GLU	2.0
2	R	720	ASP	2.0
1	K	208	ILE	2.0
1	U	212	ILE	2.0
1	O	254	ARG	2.0
1	I	235	SER	2.0
1	M	221	LEU	2.0
1	G	223	PHE	2.0
1	G	333	PRO	2.0
1	U	98	PRO	2.0
1	K	355	MET	2.0
1	A	198	TYR	2.0
1	O	100	GLU	2.0
1	M	8	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	S	402	1/1	0.98	0.39	9.02	66,66,66,66	0
4	CA	M	402	1/1	0.98	0.38	8.50	67,67,67,67	0
4	CA	X	402	1/1	0.97	0.33	4.67	70,70,70,70	0
4	CA	I	402	1/1	0.93	0.41	4.27	72,72,72,72	0
4	CA	Q	402	1/1	0.95	0.31	3.18	68,68,68,68	0
4	CA	U	402	1/1	0.95	0.28	1.93	67,67,67,67	0
4	CA	A	402	1/1	0.95	0.31	1.46	62,62,62,62	0
4	CA	E	402	1/1	0.92	0.28	1.38	73,73,73,73	0
3	ATP	Q	401	31/31	0.91	0.25	0.12	69,88,94,95	0
3	ATP	O	401	31/31	0.89	0.23	0.01	81,94,104,111	0
3	ATP	A	401	31/31	0.92	0.25	0.01	66,77,85,89	0
3	ATP	I	401	31/31	0.92	0.25	-0.04	62,81,88,92	0
3	ATP	U	401	31/31	0.90	0.24	-0.06	69,90,98,108	0
3	ATP	K	401	31/31	0.90	0.23	-0.15	83,97,101,105	0
3	ATP	E	401	31/31	0.90	0.25	-0.30	76,91,107,118	0
3	ATP	C	401	31/31	0.92	0.21	-0.41	72,82,91,95	0
3	ATP	G	401	31/31	0.92	0.22	-0.54	75,91,100,102	0
3	ATP	S	401	31/31	0.93	0.20	-0.59	72,78,88,90	0
3	ATP	X	401	31/31	0.96	0.19	-1.21	73,81,87,89	0
3	ATP	M	401	31/31	0.95	0.17	-1.26	75,83,94,99	0
4	CA	G	402	1/1	0.93	0.31	-	80,80,80,80	0
4	CA	O	402	1/1	0.96	0.31	-	73,73,73,73	0
4	CA	C	402	1/1	0.97	0.38	-	65,65,65,65	0
4	CA	K	402	1/1	0.93	0.32	-	83,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.