



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2017 – 06:58 AM EST

PDB ID : 5TXV
Title : HslU P21 cell with 4 hexamers
Authors : Grant, R.A.; Chen, J.; Glynn, S.E.; Sauer, R.T.
Deposited on : 2016-11-17
Resolution : 7.09 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

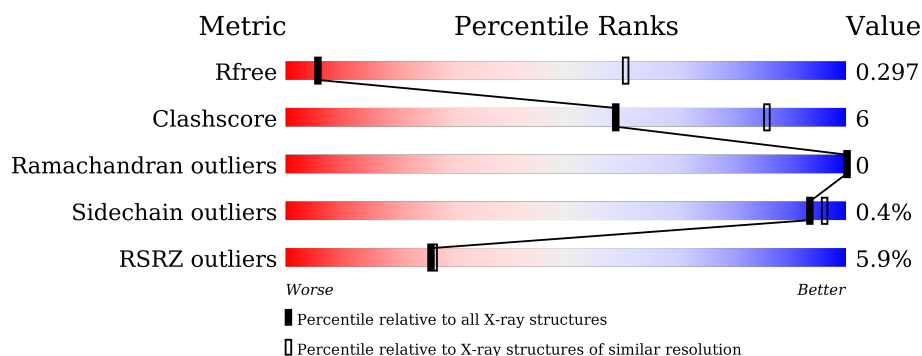
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	442	<div> <div>5%</div> <div>68% 7% 25%</div> </div>
1	B	442	<div> <div>5%</div> <div>65% 11% 24%</div> </div>
1	C	442	<div> <div>3%</div> <div>71% 12% 17%</div> </div>
1	D	442	<div> <div>5%</div> <div>65% 11% 25%</div> </div>
1	E	442	<div> <div>3%</div> <div>69% 12% 19%</div> </div>
1	F	442	<div> <div>4%</div> <div>68% 8% 24%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	442	
1	H	442	
1	I	442	
1	J	442	
1	K	442	
1	L	442	
1	M	442	
1	N	442	
1	O	442	
1	P	442	
1	Q	442	
1	R	442	
1	S	442	
1	T	442	
1	U	442	
1	V	442	
1	W	442	
1	X	442	

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
2	ADP	B	501	-	-	-	X
2	ADP	C	501	-	-	-	X
2	ADP	D	501	-	-	-	X
2	ADP	H	501	-	-	-	X
2	ADP	I	501	-	-	-	X
2	ADP	J	501	-	-	-	X
2	ADP	K	501	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	L	501	-	-	-	X
2	ADP	N	501	-	-	-	X
2	ADP	O	501	-	-	-	X
2	ADP	R	501	-	-	-	X
2	ADP	T	501	-	-	-	X
2	ADP	V	501	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 64889 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 ATP-dependent protease ATPase subunit HslU.

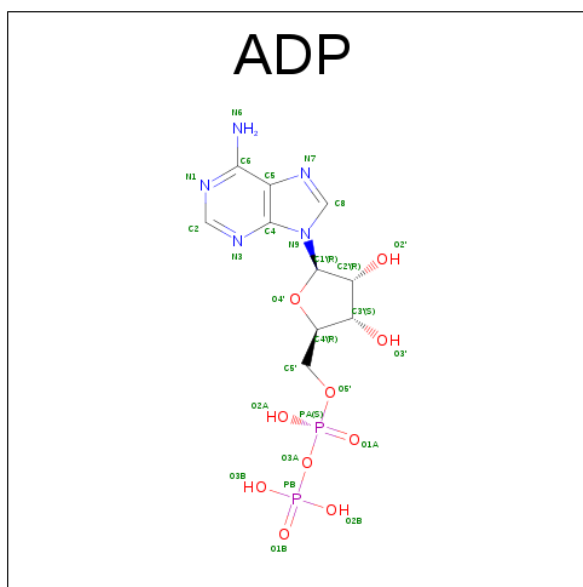
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2586	1615	456	506	9			
1	B	337	Total	C	N	O	S	0	0	0
			2638	1650	466	513	9			
1	C	366	Total	C	N	O	S	0	0	0
			2867	1792	509	556	10			
1	D	333	Total	C	N	O	S	0	0	0
			2609	1629	460	511	9			
1	E	359	Total	C	N	O	S	0	0	0
			2817	1764	501	542	10			
1	F	338	Total	C	N	O	S	0	0	0
			2654	1657	467	520	10			
1	G	327	Total	C	N	O	S	0	0	0
			2568	1606	454	498	10			
1	H	371	Total	C	N	O	S	0	0	0
			2915	1825	517	563	10			
1	I	348	Total	C	N	O	S	0	0	0
			2743	1712	490	531	10			
1	J	332	Total	C	N	O	S	0	0	0
			2608	1633	458	507	10			
1	K	337	Total	C	N	O	S	0	0	0
			2646	1651	467	519	9			
1	L	371	Total	C	N	O	S	0	0	0
			2915	1822	517	566	10			
1	M	342	Total	C	N	O	S	0	0	0
			2695	1687	481	519	8			
1	N	328	Total	C	N	O	S	0	0	0
			2581	1614	456	502	9			
1	O	348	Total	C	N	O	S	0	0	0
			2742	1715	489	529	9			
1	P	305	Total	C	N	O	S	0	0	0
			2387	1491	422	465	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	370	Total	C	N	O	S	0	0	0
			2906	1819	516	561	10			
1	R	338	Total	C	N	O	S	0	0	0
			2667	1664	479	515	9			
1	S	310	Total	C	N	O	S	0	0	0
			2436	1522	434	471	9			
1	T	318	Total	C	N	O	S	0	0	0
			2503	1564	444	487	8			
1	U	321	Total	C	N	O	S	0	0	0
			2511	1568	447	487	9			
1	V	352	Total	C	N	O	S	0	0	0
			2768	1730	493	535	10			
1	W	336	Total	C	N	O	S	0	0	0
			2637	1649	465	514	9			
1	X	360	Total	C	N	O	S	0	0	0
			2842	1779	504	549	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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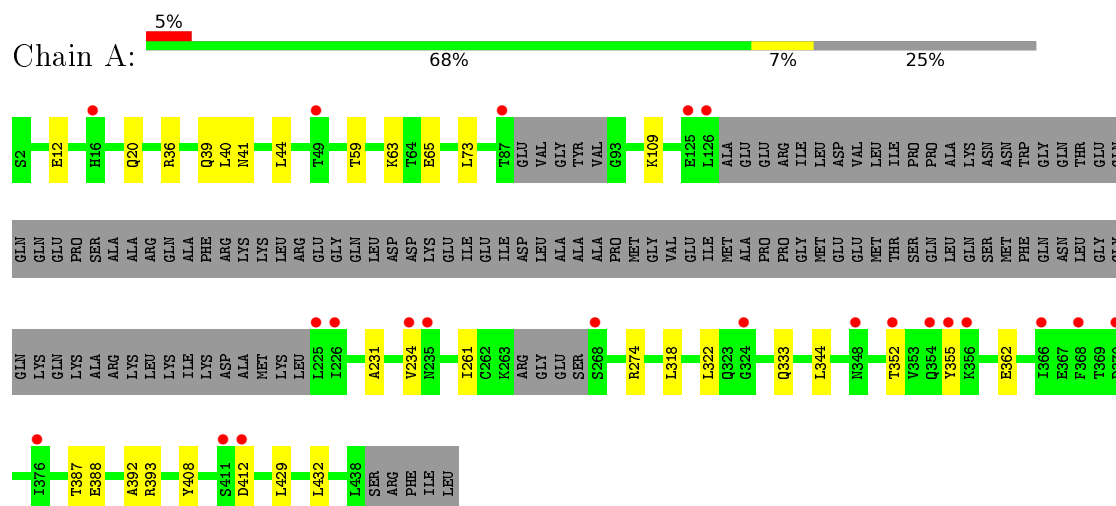
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	M	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	N	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	O	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	P	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	Q	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	R	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	S	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	T	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	U	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	V	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	W	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	X	1	Total 27	C 10	N 5	O 10	P 2	0	0

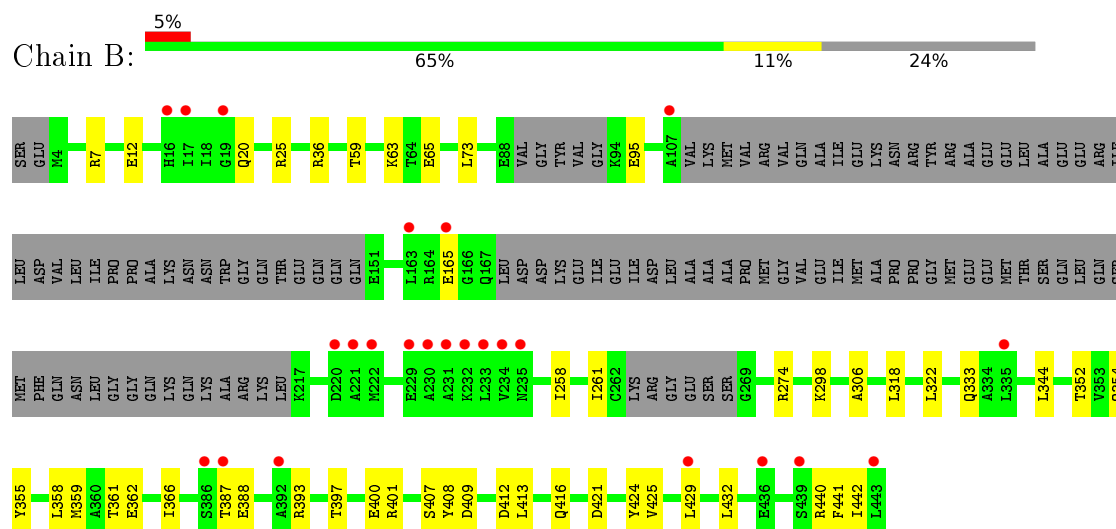
3 Residue-property plots

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

- Molecule 1: ATP-dependent protease ATPase subunit HslU

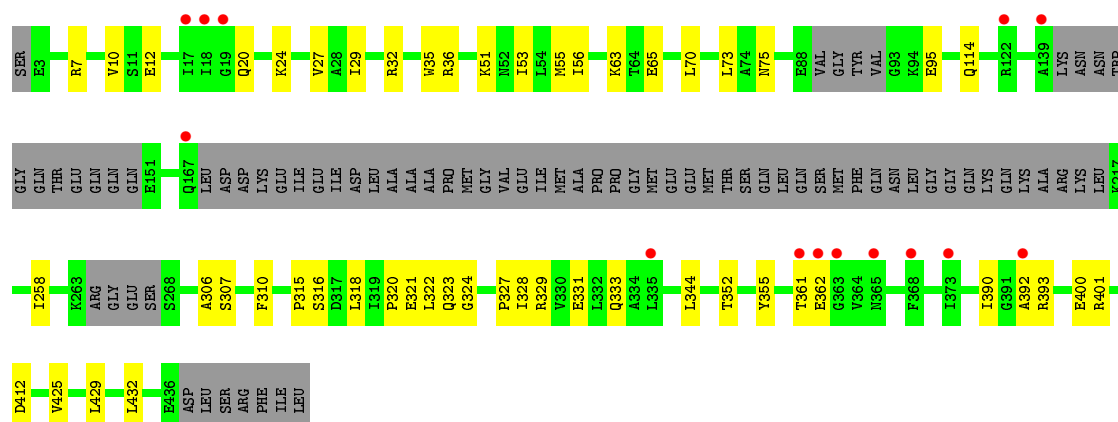


- Molecule 1: ATP-dependent protease ATPase subunit HslU

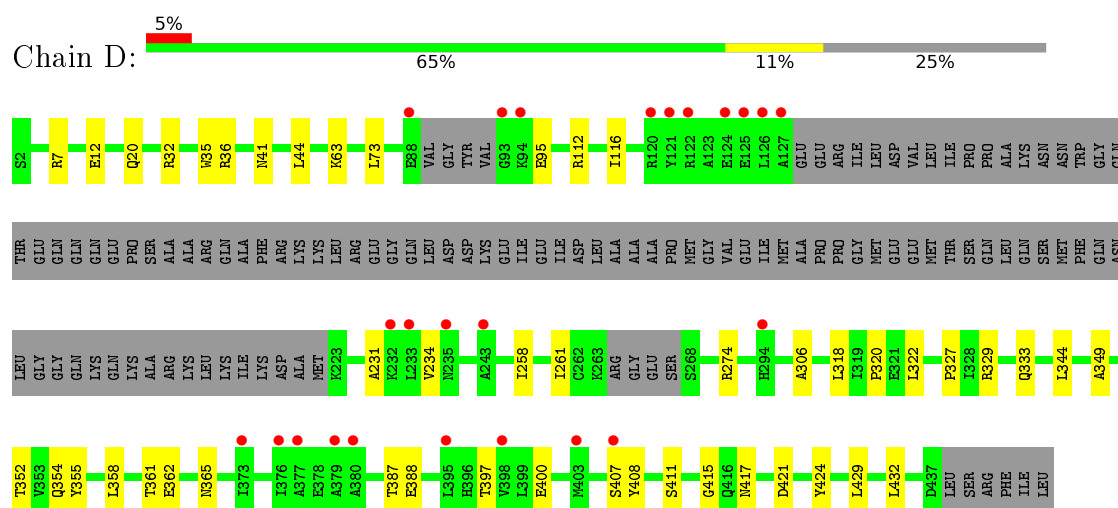


- Molecule 1: ATP-dependent protease ATPase subunit HslU

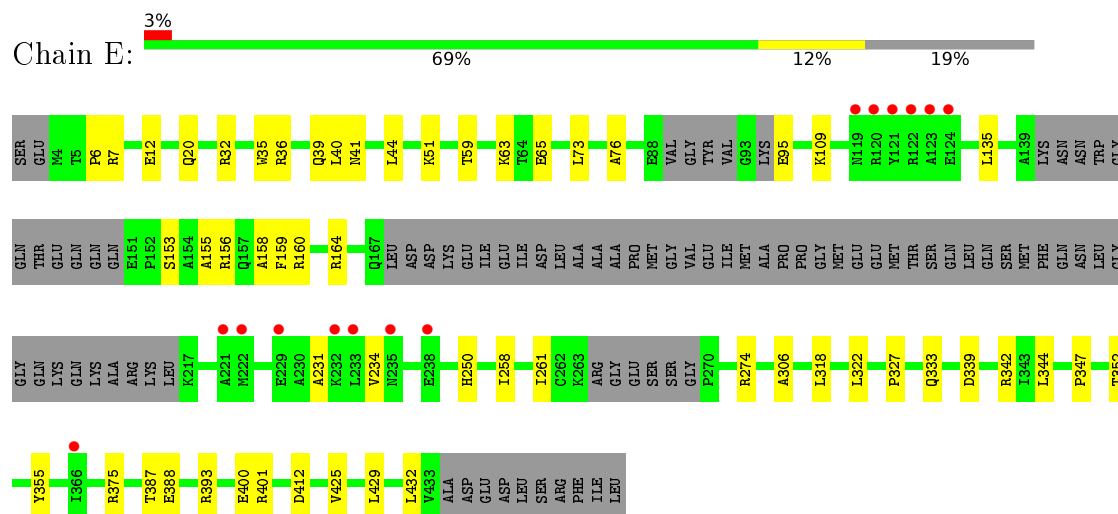




- Molecule 1: ATP-dependent protease ATPase subunit HslU

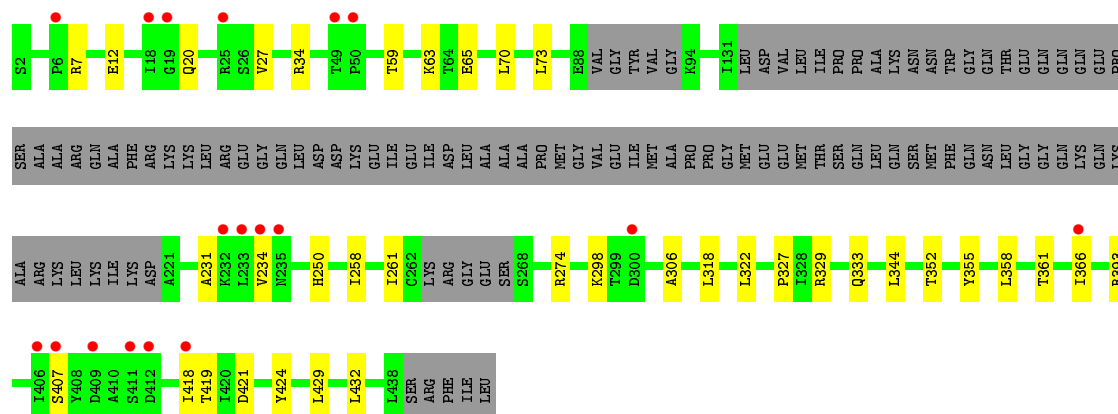


- Molecule 1: ATP-dependent protease ATPase subunit HslU

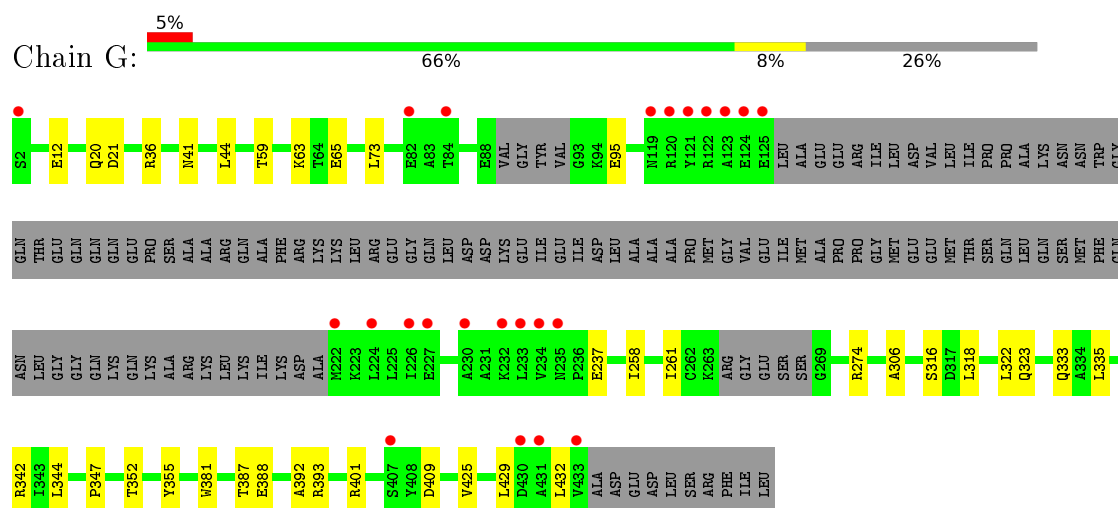


- Molecule 1: ATP-dependent protease ATPase subunit HslU

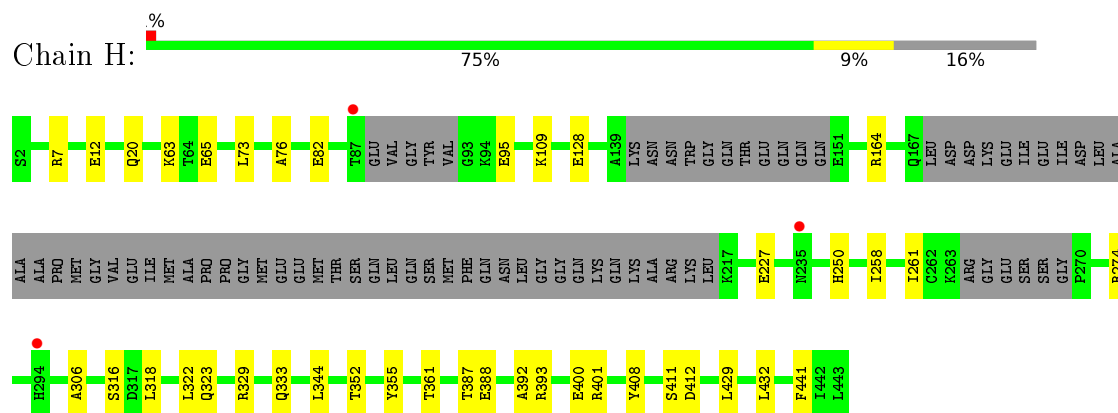




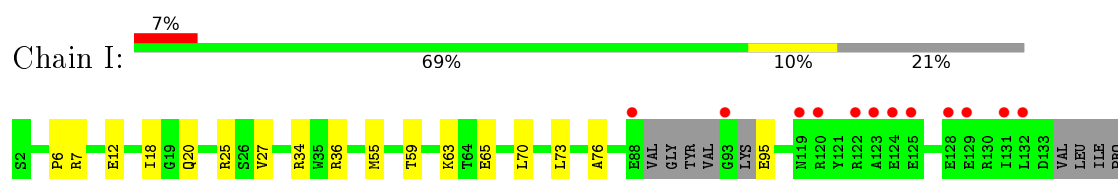
- Molecule 1: ATP-dependent protease ATPase subunit HslU

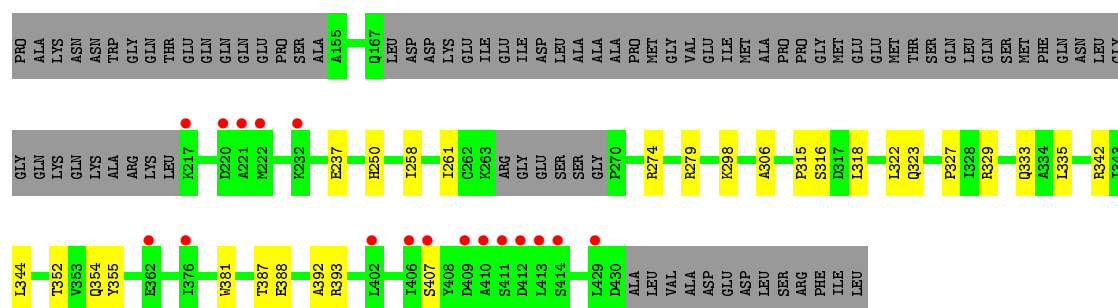


- Molecule 1: ATP-dependent protease ATPase subunit HslU

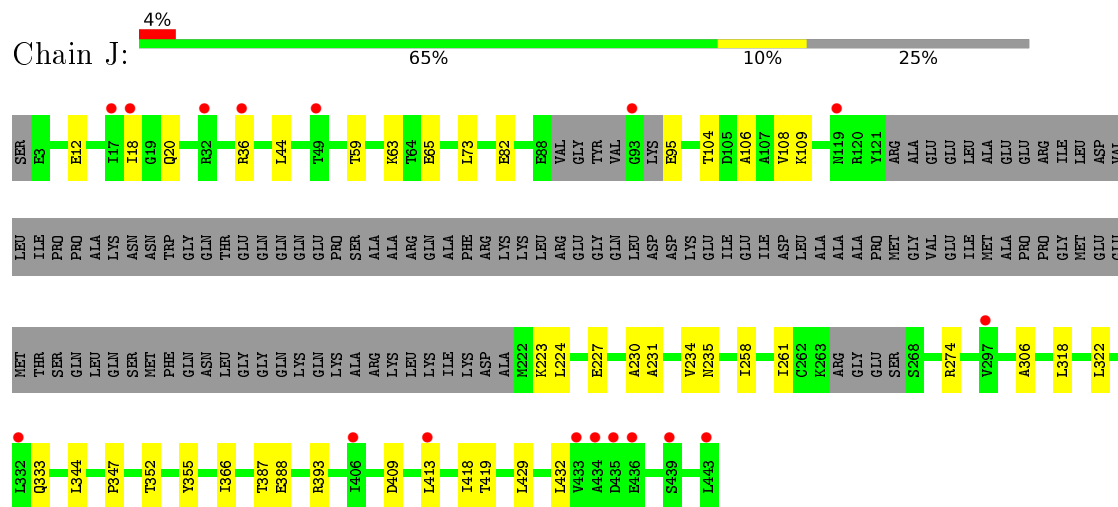


- Molecule 1: ATP-dependent protease ATPase subunit HslU

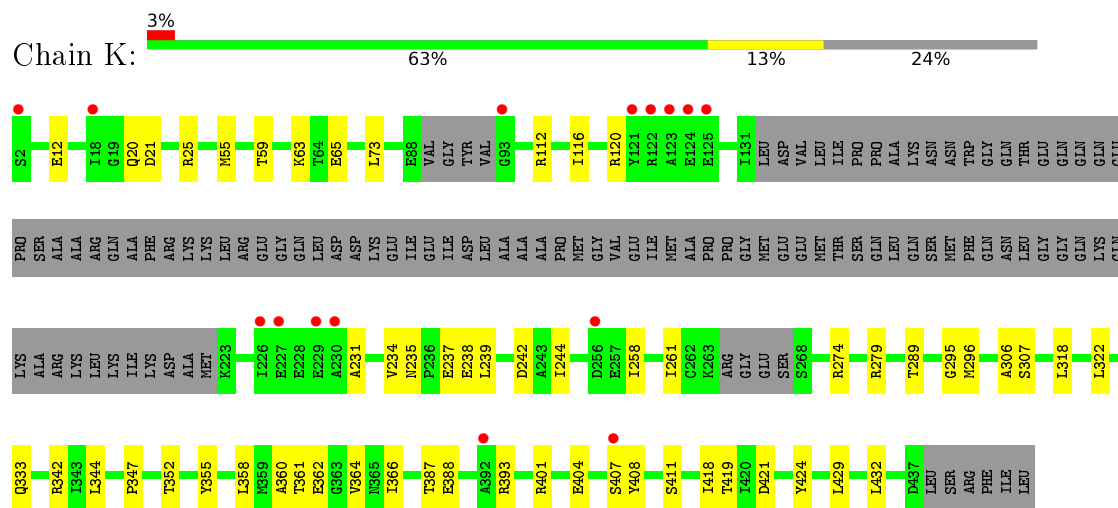




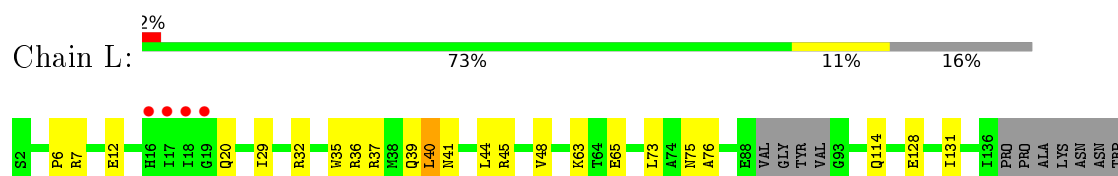
- Molecule 1: ATP-dependent protease ATPase subunit HslU

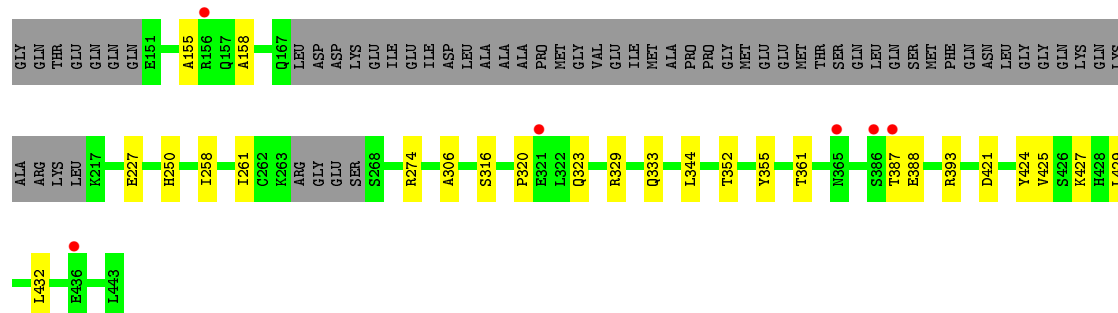


- Molecule 1: ATP-dependent protease ATPase subunit HslU

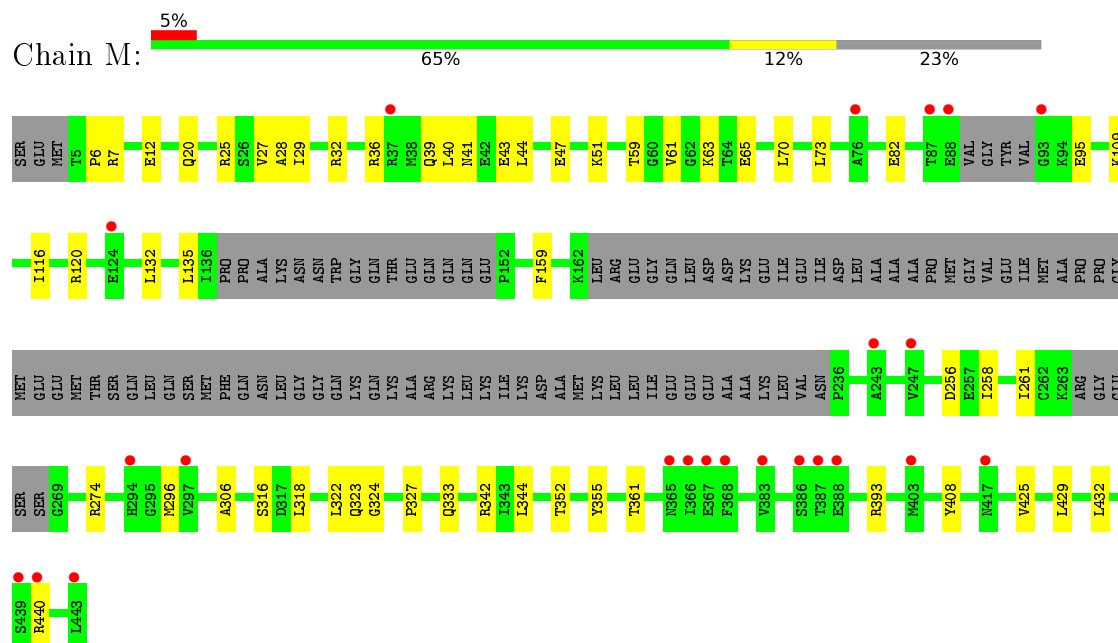


- Molecule 1: ATP-dependent protease ATPase subunit HslU

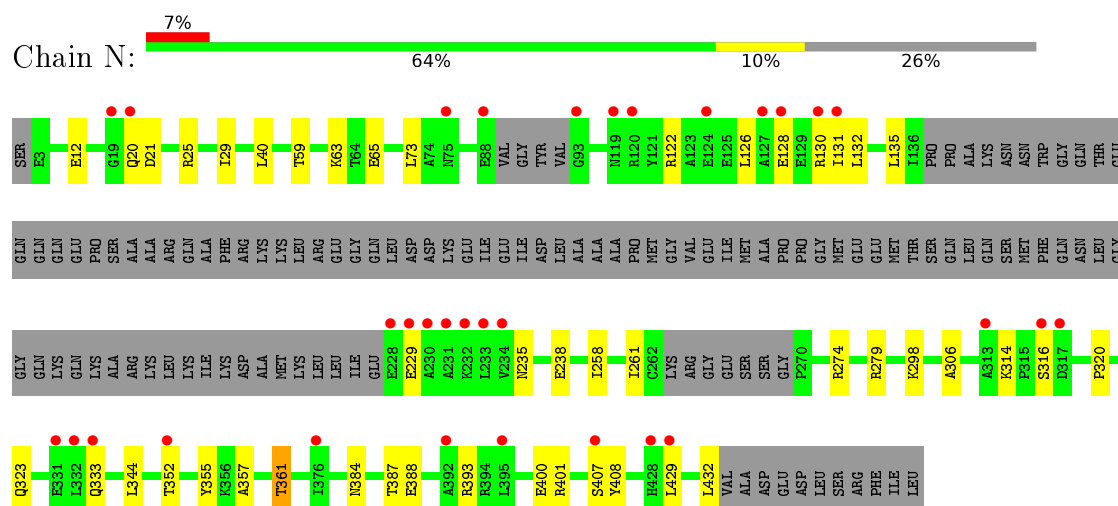




- Molecule 1: ATP-dependent protease ATPase subunit HslU

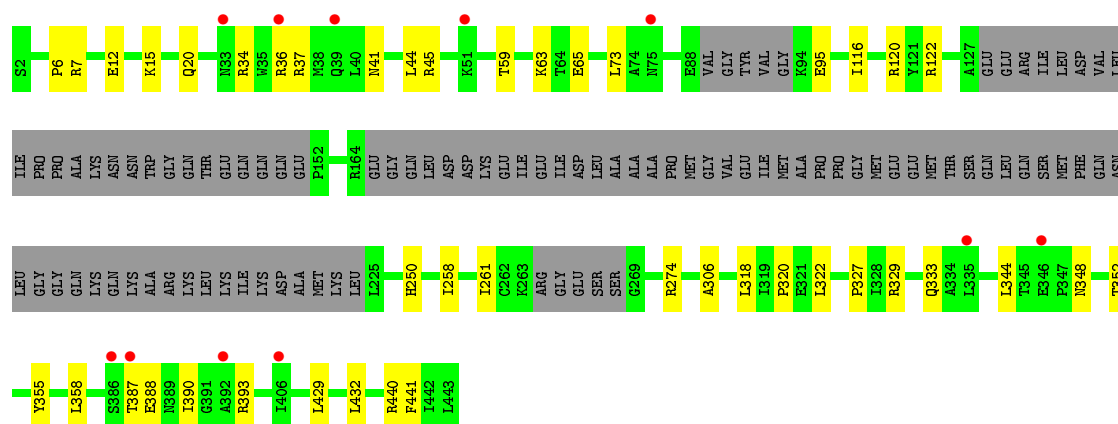


- Molecule 1: ATP-dependent protease ATPase subunit HslU

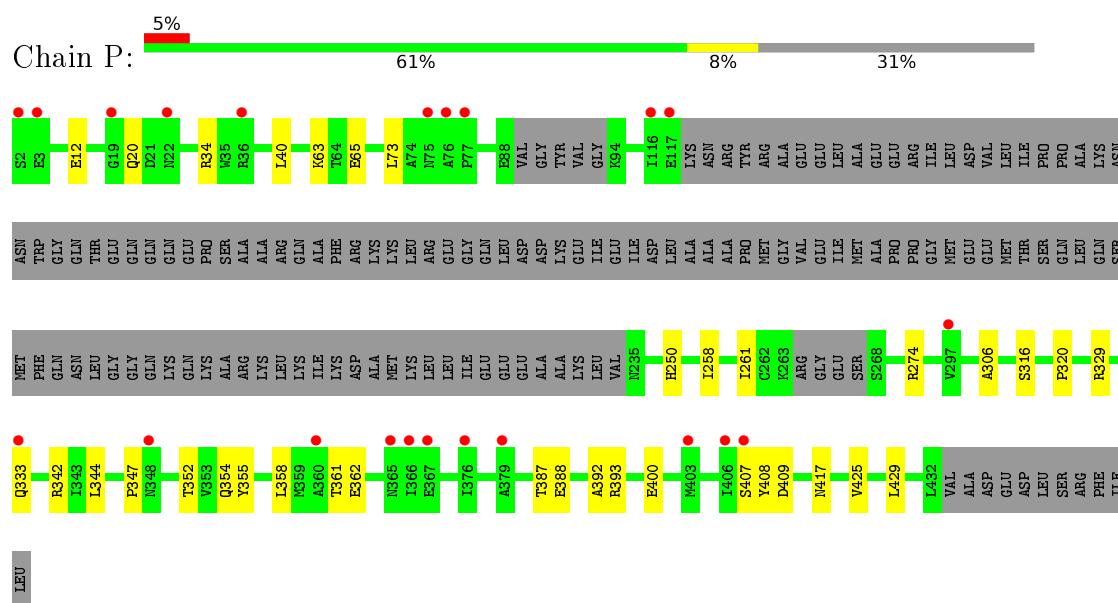


- Molecule 1: ATP-dependent protease ATPase subunit HslU

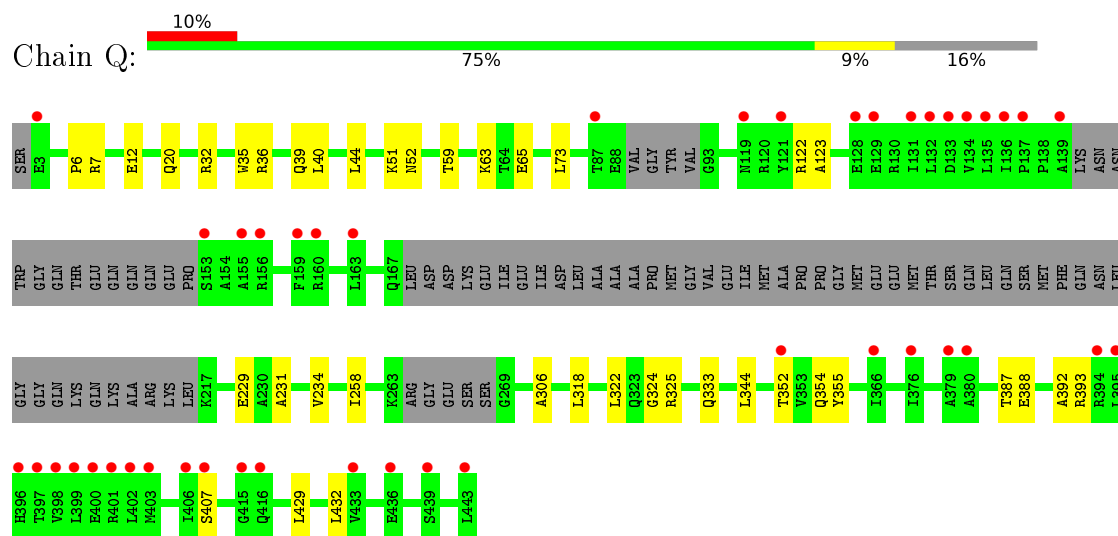




- Molecule 1: ATP-dependent protease ATPase subunit HslU



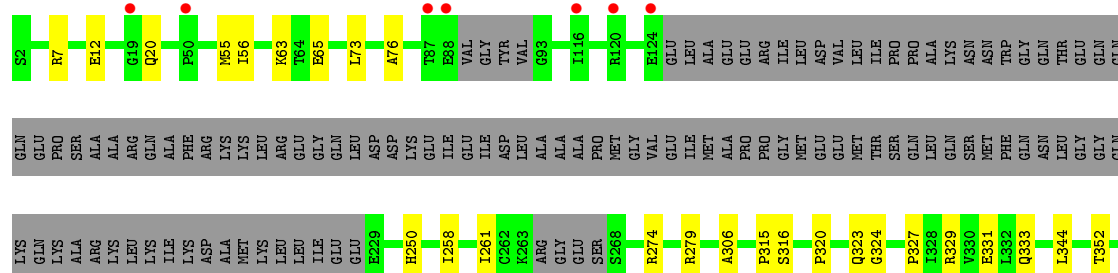
- Molecule 1: ATP-dependent protease ATPase subunit HslU



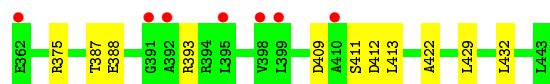
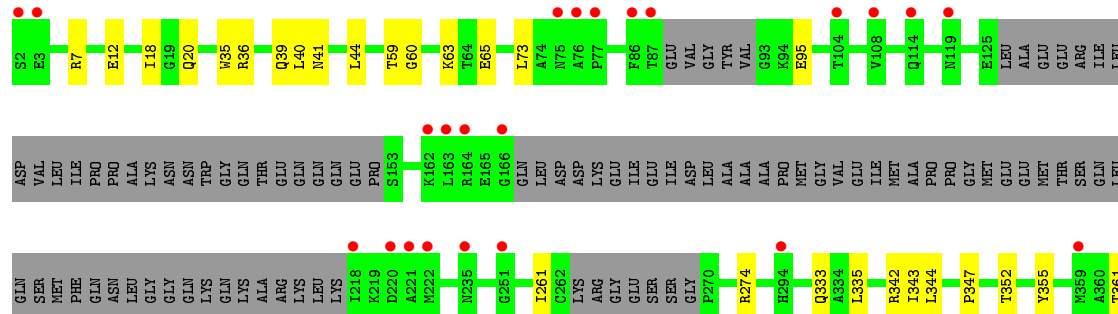
- Molecule 1: ATP-dependent protease ATPase subunit HslU



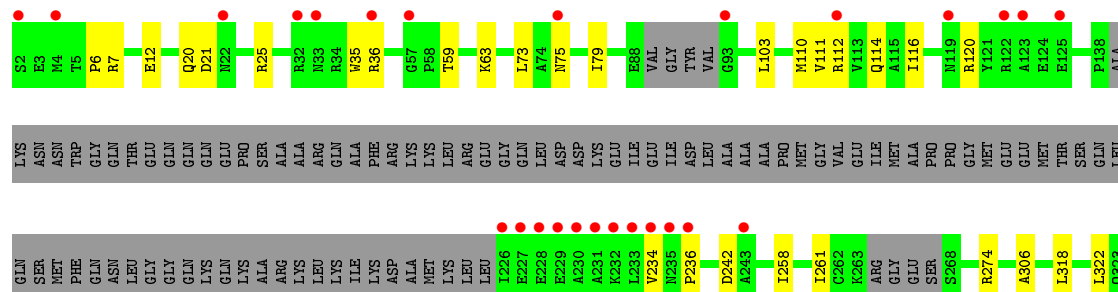
- Molecule 1: ATP-dependent protease ATPase subunit HslU

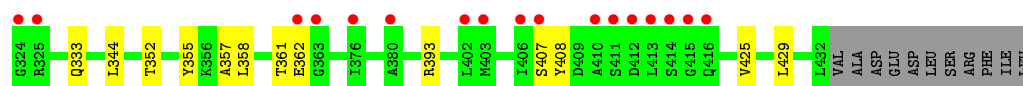


- Molecule 1: ATP-dependent protease ATPase subunit HslU

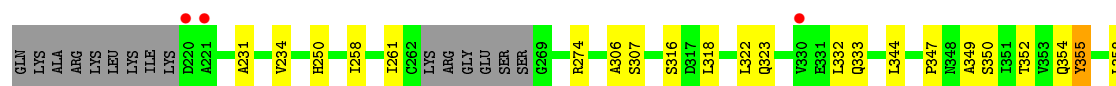
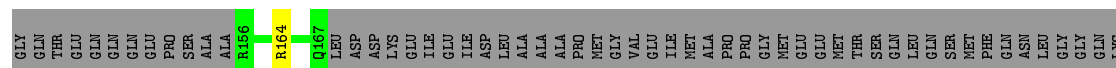
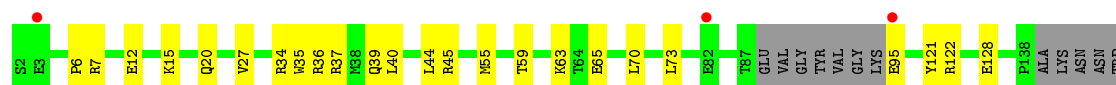


- Molecule 1: ATP-dependent protease ATPase subunit HslU





- Molecule 1: ATP-dependent protease ATPase subunit HslU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.50Å 420.86Å 176.42Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	49.19 – 7.09 49.19 – 7.09	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.19-7.09) 98.8 (49.19-7.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 7.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.274 , 0.298 0.270 , 0.297	Depositor DCC
R_{free} test set	1887 reflections (10.15%)	DCC
Wilson B-factor (Å ²)	397.2	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 357.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	64889	wwPDB-VP
Average B, all atoms (Å ²)	414.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: ADP

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	0.26	0/2615	0.42	0/3529
1	B	0.26	0/2668	0.42	0/3597
1	C	0.26	0/2899	0.43	0/3909
1	D	0.26	0/2638	0.43	0/3559
1	E	0.26	0/2848	0.44	0/3839
1	F	0.26	0/2683	0.42	0/3620
1	G	0.25	0/2597	0.42	0/3502
1	H	0.25	0/2948	0.42	0/3973
1	I	0.26	0/2771	0.42	0/3729
1	J	0.27	0/2637	0.42	0/3555
1	K	0.27	0/2675	0.44	0/3608
1	L	0.26	0/2946	0.45	1/3968 (0.0%)
1	M	0.27	0/2726	0.45	0/3672
1	N	0.25	0/2610	0.43	0/3522
1	O	0.26	0/2773	0.43	0/3735
1	P	0.26	0/2415	0.43	0/3260
1	Q	0.26	0/2938	0.43	0/3959
1	R	0.30	0/2697	0.44	0/3633
1	S	0.26	0/2465	0.44	0/3324
1	T	0.25	0/2533	0.42	0/3419
1	U	0.26	0/2540	0.42	0/3427
1	V	0.25	0/2798	0.43	0/3767
1	W	0.26	0/2668	0.43	0/3602
1	X	0.27	0/2874	0.44	0/3874
All	All	0.26	0/64962	0.43	1/87582 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	40	LEU	CA-CB-CG	5.62	128.24	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2586	0	2628	26	0
1	B	2638	0	2676	48	1
1	C	2867	0	2919	50	0
1	D	2609	0	2652	61	0
1	E	2817	0	2877	63	0
1	F	2654	0	2697	26	1
1	G	2568	0	2621	25	0
1	H	2915	0	2975	30	0
1	I	2743	0	2790	33	0
1	J	2608	0	2656	36	1
1	K	2646	0	2688	66	3
1	L	2915	0	2969	57	0
1	M	2695	0	2753	63	1
1	N	2581	0	2629	42	0
1	O	2742	0	2800	32	1
1	P	2387	0	2427	40	1
1	Q	2906	0	2965	39	1
1	R	2667	0	2718	47	0
1	S	2436	0	2483	57	0
1	T	2503	0	2538	36	1
1	U	2511	0	2558	37	0
1	V	2768	0	2822	38	0
1	W	2637	0	2685	39	0
1	X	2842	0	2900	65	3
2	A	27	0	12	4	0
2	B	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	12	4	0
2	D	27	0	12	1	0
2	E	27	0	12	4	0
2	F	27	0	12	2	0
2	G	27	0	12	5	0
2	H	27	0	12	5	0
2	I	27	0	12	4	0
2	J	27	0	12	3	0
2	K	27	0	12	4	0
2	L	27	0	12	3	0
2	M	27	0	12	5	0
2	N	27	0	12	2	0
2	O	27	0	12	3	0
2	P	27	0	12	5	0
2	Q	27	0	12	4	0
2	R	27	0	12	3	0
2	S	27	0	12	4	0
2	T	27	0	12	4	0
2	U	27	0	12	2	0
2	V	27	0	12	3	0
2	W	27	0	12	1	0
2	X	27	0	12	4	0
All	All	64889	0	65714	755	7

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 6.

All (755) 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:D:407:SER:O	1:E:36:ARG:NH2	1.65	1.30
1:P:407:SER:O	1:Q:36:ARG:NH2	1.79	1.14
1:D:407:SER:OG	1:E:36:ARG:NH1	1.80	1.14
1:K:407:SER:O	1:L:36:ARG:NH1	1.80	1.12
1:B:401:ARG:NH2	1:C:329:ARG:O	1.88	1.06
1:P:407:SER:OG	1:Q:36:ARG:NH1	1.88	1.06
1:M:39:GLN:HB3	1:R:361:THR:HG21	1.35	1.02
1:S:82:GLU:HG3	1:T:279:ARG:HD2	1.46	0.97
1:U:407:SER:O	1:V:36:ARG:NH2	1.98	0.96
1:D:415:GLY:O	1:S:333:GLN:NE2	1.99	0.95
1:W:407:SER:O	1:X:36:ARG:NH2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ASP:OD2	1:D:7:ARG:NE	2.02	0.92
1:W:358:LEU:CD2	1:X:40:LEU:HD11	2.02	0.90
1:M:327:PRO:HA	1:R:397:THR:HG22	1.51	0.90
1:A:412:ASP:OD2	1:B:7:ARG:NH2	2.07	0.87
1:W:358:LEU:HA	1:X:40:LEU:HD21	1.57	0.87
1:M:82:GLU:HG3	1:N:279:ARG:HB3	1.56	0.86
1:D:354:GLN:HG2	1:E:44:LEU:HD22	1.58	0.86
1:F:59:THR:OG1	1:F:393:ARG:NH2	2.08	0.86
1:M:36:ARG:NH2	1:R:407:SER:O	2.09	0.86
1:O:441:PHE:O	1:P:329:ARG:NH1	2.10	0.84
1:H:412:ASP:OD2	1:I:7:ARG:NE	2.10	0.84
1:O:59:THR:OG1	1:O:393:ARG:NH2	2.11	0.83
1:M:393:ARG:NH1	2:M:501:ADP:O5'	2.11	0.83
1:D:415:GLY:HA3	1:S:22:ASN:ND2	1.94	0.82
1:T:401:ARG:NH2	1:U:329:ARG:O	2.14	0.81
1:B:441:PHE:HA	1:C:315:PRO:HG2	1.63	0.81
1:P:408:TYR:CD1	1:Q:6:PRO:HB2	2.16	0.81
1:D:415:GLY:HA3	1:S:22:ASN:HD22	1.44	0.80
1:W:358:LEU:HD21	1:X:40:LEU:HD11	1.62	0.80
1:T:59:THR:OG1	1:T:393:ARG:NH2	2.15	0.79
1:J:109:LYS:HB2	1:K:296:MET:HG2	1.62	0.79
1:W:59:THR:OG1	1:W:393:ARG:NH2	2.16	0.79
1:R:152:PRO:HB2	1:R:157:GLN:HE21	1.47	0.79
1:D:417:ASN:ND2	1:S:333:GLN:OE1	2.16	0.78
1:K:407:SER:O	1:L:36:ARG:CZ	2.31	0.78
1:V:59:THR:OG1	1:V:393:ARG:NH2	2.16	0.77
1:B:442:ILE:HD11	1:C:331:GLU:HG3	1.66	0.77
1:S:29:ILE:HD13	1:X:404:GLU:HB2	1.66	0.77
1:T:400:GLU:HG3	1:U:327:PRO:HB2	1.67	0.77
1:S:59:THR:OG1	1:S:393:ARG:NH2	2.17	0.76
1:K:116:ILE:O	1:K:120:ARG:N	2.18	0.76
1:J:224:LEU:HD21	1:K:235:ASN:HB3	1.66	0.76
1:K:407:SER:C	1:L:36:ARG:HH12	1.90	0.76
1:B:441:PHE:HD2	1:C:56:ILE:HG21	1.51	0.75
1:P:361:THR:HG21	1:Q:39:GLN:HG3	1.67	0.75
1:P:407:SER:HG	1:Q:36:ARG:HH12	1.31	0.75
1:H:82:GLU:HG3	1:I:279:ARG:HB3	1.68	0.75
1:K:59:THR:OG1	1:K:393:ARG:NH2	2.20	0.75
1:K:404:GLU:HB2	1:L:29:ILE:HD13	1.69	0.75
1:P:354:GLN:HG2	1:Q:44:LEU:HD22	1.69	0.74
1:M:39:GLN:HB3	1:R:361:THR:CG2	2.14	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:7:ARG:HG2	1:X:408:TYR:HE2	1.52	0.74
1:B:393:ARG:HB3	1:C:324:GLY:HA3	1.69	0.73
1:R:393:ARG:NH1	2:R:501:ADP:O5'	2.20	0.73
1:B:412:ASP:OD2	1:C:7:ARG:NE	2.21	0.72
1:M:132:LEU:HD22	1:M:159:PHE:CG	2.25	0.72
1:W:110:MET:HG2	1:W:114:GLN:HE22	1.54	0.72
1:J:109:LYS:NZ	1:K:296:MET:O	2.18	0.72
1:E:59:THR:OG1	1:E:393:ARG:NH2	2.23	0.72
1:E:412:ASP:OD2	1:F:7:ARG:NE	2.23	0.71
1:M:44:LEU:HD22	1:R:354:GLN:HG2	1.71	0.71
1:M:32:ARG:NH2	1:R:411:SER:OG	2.24	0.71
1:J:231:ALA:HA	1:J:234:VAL:HG12	1.72	0.71
1:C:362:GLU:OE2	1:D:32:ARG:NE	2.22	0.71
1:M:393:ARG:HE	1:N:320:PRO:HB2	1.56	0.71
1:K:407:SER:O	1:L:36:ARG:NH2	2.23	0.71
1:N:401:ARG:NH2	1:O:329:ARG:O	2.23	0.71
1:M:51:LYS:HE2	1:R:400:GLU:OE2	1.91	0.71
1:M:324:GLY:HA3	1:R:393:ARG:HD2	1.72	0.70
1:N:126:LEU:HB2	1:N:229:GLU:HG2	1.72	0.70
1:V:412:ASP:OD2	1:W:7:ARG:NE	2.24	0.70
1:F:63:LYS:N	2:F:501:ADP:O1B	2.25	0.70
1:S:327:PRO:HA	1:X:397:THR:HG22	1.71	0.70
1:M:7:ARG:HG3	1:R:408:TYR:CZ	2.27	0.70
1:S:7:ARG:NH2	1:X:409:ASP:OD1	2.25	0.70
1:P:358:LEU:HD21	1:Q:40:LEU:HD11	1.74	0.70
1:S:362:GLU:OE2	1:T:36:ARG:NE	2.24	0.70
1:B:59:THR:OG1	1:B:393:ARG:NH2	2.26	0.69
1:A:63:LYS:N	2:A:501:ADP:O1B	2.26	0.69
1:Q:407:SER:O	1:R:36:ARG:NH2	2.26	0.69
1:C:361:THR:HG21	1:D:36:ARG:HA	1.75	0.69
1:K:408:TYR:CZ	1:L:6:PRO:HB2	2.28	0.69
1:K:362:GLU:OE2	1:L:35:TRP:HZ3	1.75	0.69
1:W:408:TYR:CE1	1:X:6:PRO:HB2	2.28	0.68
1:J:227:GLU:HB2	1:K:237:GLU:HG2	1.75	0.68
1:A:408:TYR:CE2	1:B:25:ARG:NH2	2.62	0.68
1:X:63:LYS:N	2:X:501:ADP:O1B	2.26	0.68
1:D:362:GLU:OE2	1:E:35:TRP:CZ3	2.47	0.67
1:U:361:THR:HG23	1:V:39:GLN:HB2	1.77	0.67
1:H:401:ARG:NH2	1:I:329:ARG:O	2.28	0.67
1:I:344:LEU:O	1:I:352:THR:OG1	2.11	0.67
1:I:63:LYS:N	2:I:501:ADP:O1B	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ASN:HD21	1:S:333:GLN:HA	1.59	0.67
1:H:63:LYS:N	2:H:501:ADP:O1B	2.28	0.67
1:S:63:LYS:N	2:S:501:ADP:O3B	2.27	0.67
1:B:441:PHE:CD2	1:C:56:ILE:HG21	2.29	0.66
1:J:223:LYS:HD2	1:K:238:GLU:CD	2.16	0.66
1:H:393:ARG:NH1	2:H:501:ADP:O5'	2.29	0.66
1:U:63:LYS:N	2:U:501:ADP:O3B	2.27	0.66
1:C:361:THR:HG22	1:D:35:TRP:CZ3	2.31	0.66
1:L:393:ARG:NH1	2:L:501:ADP:O5'	2.28	0.66
1:K:408:TYR:OH	1:L:7:ARG:HA	1.96	0.65
1:Q:63:LYS:N	2:Q:501:ADP:O3B	2.29	0.65
1:K:63:LYS:N	2:K:501:ADP:O3B	2.28	0.65
1:N:63:LYS:N	2:N:501:ADP:O3B	2.29	0.65
1:H:400:GLU:HG3	1:I:327:PRO:HB2	1.78	0.65
1:U:20:GLN:NE2	1:U:333:GLN:O	2.29	0.65
1:U:361:THR:CG2	1:V:39:GLN:HB2	2.27	0.65
1:T:63:LYS:N	2:T:501:ADP:O3B	2.29	0.65
1:J:230:ALA:O	1:J:234:VAL:HG12	1.97	0.65
1:J:223:LYS:NZ	1:K:238:GLU:OE2	2.22	0.65
1:T:366:ILE:HD13	1:T:418:ILE:HB	1.78	0.65
1:R:355:TYR:HA	1:R:358:LEU:HD12	1.79	0.65
1:B:440:ARG:O	1:C:315:PRO:HB2	1.97	0.64
1:K:358:LEU:HD23	1:L:40:LEU:HD11	1.78	0.64
1:F:20:GLN:NE2	1:F:333:GLN:O	2.30	0.64
1:D:415:GLY:CA	1:S:22:ASN:ND2	2.59	0.64
1:S:329:ARG:HB2	1:X:442:ILE:HA	1.79	0.64
1:I:392:ALA:HB3	2:I:501:ADP:C8	2.33	0.64
1:D:63:LYS:N	2:D:501:ADP:O3B	2.31	0.64
1:A:109:LYS:HE2	1:B:298:LYS:HB2	1.80	0.64
1:S:324:GLY:HA3	1:X:393:ARG:HB3	1.79	0.64
1:N:59:THR:OG1	1:N:393:ARG:NH2	2.31	0.64
1:D:361:THR:CG2	1:E:39:GLN:HG3	2.28	0.63
1:M:59:THR:OG1	1:M:393:ARG:NH2	2.31	0.63
1:W:407:SER:O	1:X:36:ARG:CZ	2.46	0.63
1:E:63:LYS:N	2:E:501:ADP:O1B	2.30	0.63
1:J:63:LYS:N	2:J:501:ADP:O1B	2.31	0.63
1:O:63:LYS:N	2:O:501:ADP:O3B	2.31	0.63
1:W:362:GLU:OE2	1:X:35:TRP:HZ3	1.82	0.63
1:S:393:ARG:NE	1:T:320:PRO:HB2	2.14	0.63
1:B:362:GLU:OE2	1:C:32:ARG:NE	2.27	0.62
1:C:63:LYS:N	2:C:501:ADP:O3B	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:407:SER:O	1:O:36:ARG:NH2	2.29	0.62
1:P:20:GLN:NE2	1:P:333:GLN:O	2.30	0.62
1:H:20:GLN:NE2	1:H:333:GLN:O	2.30	0.62
1:P:400:GLU:OE2	1:Q:51:LYS:HE2	1.99	0.62
1:L:63:LYS:N	2:L:501:ADP:O3B	2.33	0.62
1:W:361:THR:HG21	1:X:39:GLN:HB2	1.80	0.62
1:M:109:LYS:HE2	1:N:298:LYS:HB2	1.81	0.62
1:P:358:LEU:CD2	1:Q:40:LEU:HD11	2.30	0.62
1:F:366:ILE:HD13	1:F:418:ILE:HB	1.82	0.62
1:M:63:LYS:N	2:M:501:ADP:O1B	2.31	0.62
1:O:440:ARG:HB3	1:P:316:SER:HB3	1.82	0.61
1:K:408:TYR:CE1	1:L:6:PRO:HB2	2.35	0.61
1:V:63:LYS:N	2:V:501:ADP:O3B	2.33	0.61
1:H:227:GLU:CD	1:I:237:GLU:HG2	2.20	0.61
1:H:109:LYS:HE2	1:I:298:LYS:HB2	1.82	0.61
1:P:63:LYS:N	2:P:501:ADP:O3B	2.34	0.61
1:D:361:THR:HG21	1:E:39:GLN:HG3	1.83	0.61
1:M:361:THR:OG1	1:N:40:LEU:HD21	1.99	0.61
1:P:409:ASP:OD1	1:Q:7:ARG:NH2	2.34	0.61
1:K:344:LEU:O	1:K:352:THR:OG1	2.13	0.61
1:P:393:ARG:NH1	2:P:501:ADP:O5'	2.33	0.61
1:L:20:GLN:NE2	1:L:333:GLN:O	2.33	0.60
1:P:408:TYR:CE2	1:Q:7:ARG:HG2	2.36	0.60
1:G:63:LYS:N	2:G:501:ADP:O3B	2.34	0.60
1:J:223:LYS:HD2	1:K:238:GLU:OE2	2.00	0.60
1:J:393:ARG:NH1	2:J:501:ADP:O5'	2.35	0.60
1:W:63:LYS:N	2:W:501:ADP:O1B	2.33	0.60
1:C:344:LEU:O	1:C:352:THR:OG1	2.12	0.60
1:K:408:TYR:HE2	1:L:7:ARG:CG	2.14	0.60
1:C:400:GLU:HG3	1:D:327:PRO:HB2	1.83	0.60
1:W:408:TYR:CZ	1:X:6:PRO:HB2	2.36	0.60
1:A:36:ARG:NH1	1:F:407:SER:O	2.34	0.60
1:W:75:ASN:HD21	1:W:114:GLN:CD	2.04	0.60
1:W:20:GLN:NE2	1:W:333:GLN:O	2.32	0.60
1:V:18:ILE:CG1	1:V:347:PRO:HG3	2.32	0.60
1:A:362:GLU:OE2	1:B:36:ARG:NE	2.33	0.59
1:J:409:ASP:O	1:J:413:LEU:HG	2.02	0.59
1:M:393:ARG:HH12	2:M:501:ADP:PA	2.25	0.59
1:O:344:LEU:O	1:O:352:THR:OG1	2.14	0.59
1:B:400:GLU:HG3	1:C:327:PRO:HB2	1.83	0.59
1:S:7:ARG:CG	1:X:408:TYR:HE2	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:ARG:NH2	1:D:329:ARG:O	2.35	0.59
1:S:53:ILE:HA	1:S:328:ILE:O	2.02	0.59
1:S:408:TYR:HD1	1:T:29:ILE:HD11	1.67	0.59
1:U:361:THR:HG23	1:V:39:GLN:CB	2.32	0.59
1:A:20:GLN:NE2	1:A:333:GLN:O	2.31	0.59
1:K:393:ARG:NH1	2:K:501:ADP:O5'	2.35	0.59
1:J:109:LYS:HB2	1:K:296:MET:CG	2.30	0.58
1:N:361:THR:HG21	1:O:36:ARG:HA	1.84	0.58
1:D:407:SER:HG	1:E:36:ARG:NH1	2.00	0.58
1:W:358:LEU:HD23	1:X:40:LEU:HD11	1.84	0.58
1:C:20:GLN:NE2	1:C:333:GLN:O	2.34	0.58
1:D:365:ASN:OD1	1:S:336:THR:HG21	2.03	0.58
1:H:441:PHE:HA	1:I:315:PRO:HD2	1.84	0.58
1:D:400:GLU:OE2	1:E:51:LYS:HE2	2.03	0.58
1:R:63:LYS:N	2:R:501:ADP:O1B	2.37	0.58
1:K:358:LEU:CD2	1:L:40:LEU:HD11	2.33	0.58
1:S:36:ARG:NH1	1:X:407:SER:OG	2.37	0.58
1:T:344:LEU:O	1:T:352:THR:OG1	2.14	0.58
1:E:155:ALA:HA	1:E:158:ALA:HB3	1.85	0.58
1:N:408:TYR:HE2	1:O:7:ARG:HG2	1.67	0.58
1:B:20:GLN:NE2	1:B:333:GLN:O	2.34	0.57
1:D:408:TYR:CE2	1:E:7:ARG:HG2	2.38	0.57
1:Q:344:LEU:O	1:Q:352:THR:OG1	2.14	0.57
1:S:82:GLU:CG	1:T:279:ARG:HD2	2.29	0.57
1:B:63:LYS:N	2:B:501:ADP:O3B	2.37	0.57
1:A:36:ARG:NH2	1:F:407:SER:O	2.37	0.57
1:L:12:GLU:HG2	1:L:73:LEU:HD13	1.86	0.57
1:B:441:PHE:HD2	1:C:56:ILE:HD13	1.69	0.57
1:H:344:LEU:O	1:H:352:THR:OG1	2.18	0.57
1:O:116:ILE:O	1:O:120:ARG:N	2.35	0.57
1:R:20:GLN:NE2	1:R:333:GLN:O	2.36	0.57
1:M:7:ARG:H	1:R:408:TYR:HE1	1.51	0.57
1:F:344:LEU:O	1:F:352:THR:OG1	2.15	0.57
1:M:135:LEU:HB2	1:M:159:PHE:CE1	2.40	0.57
1:P:344:LEU:O	1:P:352:THR:OG1	2.18	0.57
1:V:344:LEU:O	1:V:352:THR:OG1	2.12	0.56
1:I:59:THR:OG1	1:I:393:ARG:NH2	2.37	0.56
1:L:344:LEU:O	1:L:352:THR:OG1	2.14	0.56
1:D:408:TYR:CE1	1:E:6:PRO:HB2	2.40	0.56
1:K:20:GLN:NE2	1:K:333:GLN:O	2.38	0.56
1:U:407:SER:OG	1:V:36:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:GLN:NE2	1:G:333:GLN:O	2.34	0.56
1:C:393:ARG:NH1	2:C:501:ADP:O5'	2.38	0.56
1:D:362:GLU:OE2	1:E:32:ARG:NH2	2.39	0.56
1:G:393:ARG:NH1	2:G:501:ADP:O5'	2.39	0.56
1:M:256:ASP:OD2	1:N:279:ARG:NH1	2.39	0.56
1:G:344:LEU:O	1:G:352:THR:OG1	2.17	0.55
1:S:344:LEU:O	1:S:352:THR:OG1	2.13	0.55
1:D:358:LEU:HD22	1:E:36:ARG:HB3	1.88	0.55
1:M:135:LEU:HB2	1:M:159:PHE:HE1	1.71	0.55
1:J:366:ILE:HD13	1:J:418:ILE:HB	1.87	0.55
1:W:358:LEU:HD23	1:X:40:LEU:HD21	1.89	0.55
1:D:344:LEU:O	1:D:352:THR:OG1	2.15	0.55
1:H:109:LYS:CE	1:I:298:LYS:HB2	2.36	0.55
1:M:63:LYS:NZ	2:M:501:ADP:O3B	2.32	0.55
1:J:429:LEU:O	1:J:432:LEU:N	2.38	0.55
1:M:36:ARG:CZ	1:R:407:SER:HB3	2.36	0.55
1:J:344:LEU:O	1:J:352:THR:OG1	2.16	0.55
1:M:82:GLU:CG	1:N:279:ARG:HB3	2.33	0.55
1:D:361:THR:OG1	1:E:39:GLN:HB2	2.07	0.55
1:S:36:ARG:HA	1:X:361:THR:HG21	1.88	0.55
1:B:441:PHE:HE2	1:C:310:PHE:HB2	1.72	0.54
1:M:59:THR:HG21	1:N:320:PRO:HG3	1.88	0.54
1:U:407:SER:O	1:V:36:ARG:CZ	2.54	0.54
1:C:392:ALA:HB3	2:C:501:ADP:C8	2.42	0.54
1:S:29:ILE:CD1	1:X:404:GLU:HB2	2.37	0.54
1:J:234:VAL:HG22	1:J:235:ASN:N	2.23	0.54
1:B:359:MET:HG3	1:B:366:ILE:HG13	1.89	0.54
1:Q:407:SER:OG	1:R:36:ARG:NH1	2.41	0.54
1:E:344:LEU:O	1:E:352:THR:OG1	2.15	0.54
1:E:375:ARG:HH21	1:G:21:ASP:HB2	1.73	0.54
1:V:41:ASN:HD21	1:V:44:LEU:HD12	1.73	0.54
1:D:20:GLN:NE2	1:D:333:GLN:O	2.36	0.54
1:Q:20:GLN:NE2	1:Q:333:GLN:O	2.37	0.54
1:S:412:ASP:OD2	1:T:7:ARG:NH2	2.33	0.54
1:D:358:LEU:HA	1:E:40:LEU:HD21	1.90	0.53
1:B:400:GLU:OE2	1:C:51:LYS:HE2	2.08	0.53
1:P:354:GLN:HG2	1:Q:44:LEU:CD2	2.36	0.53
1:T:412:ASP:OD2	1:U:7:ARG:NE	2.39	0.53
1:S:56:ILE:HG21	1:X:441:PHE:CE2	2.44	0.53
1:B:441:PHE:CD2	1:C:56:ILE:HD13	2.43	0.53
1:E:401:ARG:NH2	1:F:329:ARG:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:GLU:HG3	2:J:501:ADP:H2'	1.90	0.53
1:P:358:LEU:HD22	1:Q:36:ARG:HB3	1.90	0.53
1:M:6:PRO:HB3	1:M:28:ALA:HB1	1.90	0.53
1:U:429:LEU:O	1:U:432:LEU:N	2.41	0.53
1:V:411:SER:OG	1:W:6:PRO:HD2	2.08	0.53
1:J:82:GLU:HG3	1:K:279:ARG:HB3	1.89	0.53
1:Q:59:THR:OG1	1:Q:393:ARG:NH2	2.42	0.53
1:T:442:ILE:HD11	1:U:331:GLU:HG3	1.90	0.53
1:K:408:TYR:CE2	1:L:6:PRO:HB2	2.44	0.53
1:K:408:TYR:HE2	1:L:7:ARG:HG2	1.74	0.53
1:T:429:LEU:O	1:T:432:LEU:N	2.41	0.53
1:J:231:ALA:HA	1:J:234:VAL:CG1	2.39	0.53
1:B:397:THR:HG22	1:C:327:PRO:HA	1.92	0.53
1:X:344:LEU:O	1:X:352:THR:OG1	2.15	0.53
1:O:20:GLN:NE2	1:O:333:GLN:O	2.39	0.52
1:S:56:ILE:HD13	1:X:441:PHE:CD2	2.44	0.52
1:E:109:LYS:HE2	1:F:298:LYS:HB2	1.91	0.52
1:U:344:LEU:O	1:U:352:THR:OG1	2.16	0.52
1:A:344:LEU:O	1:A:352:THR:OG1	2.16	0.52
1:T:393:ARG:NH1	2:T:501:ADP:O5'	2.43	0.52
1:M:116:ILE:O	1:M:120:ARG:N	2.41	0.52
1:S:20:GLN:NE2	1:S:333:GLN:O	2.38	0.52
1:S:44:LEU:HD23	1:X:349:ALA:HB1	1.90	0.52
1:K:388:GLU:HB2	1:L:316:SER:HB2	1.91	0.52
1:M:20:GLN:NE2	1:M:333:GLN:O	2.42	0.52
1:W:75:ASN:OD1	1:W:114:GLN:NE2	2.43	0.52
1:X:318:LEU:HD22	1:X:322:LEU:HD23	1.92	0.52
1:I:393:ARG:NH1	2:I:501:ADP:O5'	2.43	0.51
1:M:344:LEU:O	1:M:352:THR:OG1	2.14	0.51
1:C:53:ILE:HA	1:C:328:ILE:O	2.09	0.51
1:D:408:TYR:CE2	1:E:7:ARG:CG	2.94	0.51
1:F:429:LEU:O	1:F:432:LEU:N	2.42	0.51
1:P:362:GLU:OE2	1:Q:32:ARG:NH2	2.40	0.51
1:K:366:ILE:HD13	1:K:418:ILE:HB	1.92	0.51
1:N:20:GLN:NE2	1:N:333:GLN:O	2.40	0.51
1:W:12:GLU:HG2	1:W:73:LEU:HD13	1.90	0.51
1:P:361:THR:HG21	1:Q:39:GLN:CG	2.39	0.51
1:W:116:ILE:O	1:W:120:ARG:N	2.38	0.51
1:D:408:TYR:CD1	1:E:6:PRO:HB2	2.45	0.51
1:K:65:GLU:HG3	2:K:501:ADP:H2'	1.93	0.51
1:Q:354:GLN:HG2	1:R:44:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:20:GLN:NE2	1:T:333:GLN:O	2.39	0.51
1:C:390:ILE:HG22	1:D:320:PRO:HB3	1.92	0.51
1:L:261:ILE:O	1:L:274:ARG:HB3	2.11	0.51
1:O:41:ASN:HD21	1:O:44:LEU:HD12	1.76	0.51
1:J:59:THR:OG1	1:J:393:ARG:NH2	2.44	0.51
1:K:361:THR:CG2	1:L:39:GLN:HB2	2.41	0.51
1:D:417:ASN:OD1	1:S:333:GLN:HB3	2.10	0.51
1:E:12:GLU:HG2	1:E:73:LEU:HD13	1.93	0.51
1:K:408:TYR:HE2	1:L:7:ARG:HG3	1.76	0.51
1:N:407:SER:O	1:O:36:ARG:NH1	2.41	0.51
1:A:393:ARG:NH1	2:A:501:ADP:O5'	2.44	0.51
1:Q:392:ALA:HB3	2:Q:501:ADP:C8	2.46	0.51
1:T:21:ASP:O	1:T:25:ARG:HG3	2.11	0.50
1:W:407:SER:OG	1:X:36:ARG:NH1	2.44	0.50
1:R:355:TYR:HE1	1:R:407:SER:OG	1.94	0.50
1:I:407:SER:O	1:J:36:ARG:NH2	2.40	0.50
1:U:358:LEU:HA	1:V:40:LEU:HD21	1.93	0.50
1:E:20:GLN:NE2	1:E:333:GLN:O	2.42	0.50
1:F:65:GLU:HG3	2:F:501:ADP:H2'	1.93	0.50
1:N:131:ILE:O	1:N:135:LEU:HG	2.12	0.50
1:U:407:SER:O	1:V:36:ARG:NH1	2.45	0.50
1:H:12:GLU:HG2	1:H:73:LEU:HD13	1.93	0.50
1:M:40:LEU:HD21	1:R:358:LEU:HA	1.94	0.50
1:R:95:GLU:OE1	1:R:95:GLU:N	2.45	0.50
1:S:56:ILE:HG21	1:X:441:PHE:CD2	2.47	0.50
1:A:392:ALA:HB3	2:A:501:ADP:C8	2.46	0.50
1:F:318:LEU:HD22	1:F:322:LEU:HD23	1.92	0.50
1:O:429:LEU:O	1:O:432:LEU:N	2.44	0.50
1:P:408:TYR:CE1	1:Q:6:PRO:HB2	2.46	0.50
1:B:407:SER:OG	1:C:36:ARG:NH1	2.35	0.50
1:D:12:GLU:HG2	1:D:73:LEU:HD13	1.94	0.50
1:E:342:ARG:HH11	1:L:427:LYS:HG3	1.75	0.50
1:D:408:TYR:OH	1:E:7:ARG:HG2	2.11	0.50
1:M:6:PRO:HB2	1:R:408:TYR:CD1	2.47	0.50
1:K:358:LEU:HD21	1:L:48:VAL:HG21	1.94	0.49
1:M:393:ARG:NE	1:N:320:PRO:HB2	2.25	0.49
1:P:392:ALA:HB3	2:P:501:ADP:C8	2.47	0.49
1:X:392:ALA:HB3	2:X:501:ADP:C8	2.47	0.49
1:D:408:TYR:HE2	1:E:7:ARG:CG	2.25	0.49
1:M:40:LEU:HD21	1:R:358:LEU:CA	2.41	0.49
1:E:393:ARG:NH1	2:E:501:ADP:O5'	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:GLU:HG3	2:H:501:ADP:H2'	1.94	0.49
1:J:224:LEU:HD21	1:K:235:ASN:CB	2.37	0.49
1:U:12:GLU:HG2	1:U:73:LEU:HD13	1.94	0.49
1:V:12:GLU:HG2	1:V:73:LEU:HD13	1.94	0.49
1:H:361:THR:HG21	1:I:36:ARG:HA	1.94	0.49
1:A:65:GLU:HG3	2:A:501:ADP:H2'	1.93	0.49
1:E:63:LYS:NZ	2:E:501:ADP:O3B	2.33	0.49
1:W:408:TYR:OH	1:X:7:ARG:HG2	2.12	0.49
1:O:318:LEU:HD22	1:O:322:LEU:HD23	1.93	0.49
1:S:48:VAL:HG22	1:X:354:GLN:HB3	1.95	0.49
1:B:441:PHE:CE2	1:C:310:PHE:HB2	2.48	0.49
1:G:12:GLU:HG2	1:G:73:LEU:HD13	1.94	0.49
1:L:41:ASN:HD21	1:L:44:LEU:HD12	1.77	0.49
1:V:375:ARG:HD2	1:V:422:ALA:HB1	1.95	0.49
1:D:354:GLN:HG2	1:E:44:LEU:CD2	2.37	0.49
1:M:82:GLU:OE1	1:N:279:ARG:HD2	2.13	0.49
1:P:258:ILE:HG21	1:P:306:ALA:HB1	1.95	0.49
1:T:441:PHE:HA	1:U:315:PRO:HG2	1.94	0.49
1:I:354:GLN:HG2	1:J:44:LEU:HD22	1.95	0.48
1:D:41:ASN:HD21	1:D:44:LEU:HD12	1.79	0.48
1:V:429:LEU:O	1:V:432:LEU:N	2.45	0.48
1:J:20:GLN:NE2	1:J:333:GLN:O	2.41	0.48
1:K:112:ARG:HA	1:K:239:LEU:HD11	1.95	0.48
1:T:65:GLU:HG3	2:T:501:ADP:H2'	1.94	0.48
1:C:55:MET:O	1:C:307:SER:HA	2.13	0.48
1:G:387:THR:OG1	1:G:388:GLU:N	2.47	0.48
1:G:59:THR:OG1	1:G:393:ARG:NH2	2.47	0.48
1:N:235:ASN:HB2	1:N:238:GLU:HB3	1.96	0.48
1:W:21:ASP:O	1:W:25:ARG:HG3	2.12	0.48
1:K:429:LEU:O	1:K:432:LEU:N	2.45	0.48
1:P:261:ILE:O	1:P:274:ARG:HB3	2.13	0.48
1:I:65:GLU:HG3	2:I:501:ADP:H2'	1.96	0.48
1:K:318:LEU:HD22	1:K:322:LEU:HD23	1.96	0.48
1:S:316:SER:HB2	1:X:388:GLU:OE1	2.14	0.48
1:B:429:LEU:O	1:B:432:LEU:N	2.45	0.48
1:H:392:ALA:HB3	2:H:501:ADP:C8	2.49	0.48
1:P:393:ARG:HD2	1:Q:324:GLY:HA3	1.96	0.48
1:W:75:ASN:ND2	1:W:114:GLN:OE1	2.44	0.48
1:G:36:ARG:HA	1:L:361:THR:HG21	1.95	0.48
1:H:318:LEU:HD22	1:H:322:LEU:HD23	1.96	0.48
1:P:12:GLU:HG2	1:P:73:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:261:ILE:O	1:W:274:ARG:HB3	2.14	0.48
1:E:261:ILE:O	1:E:274:ARG:HB3	2.14	0.47
1:K:408:TYR:O	1:L:6:PRO:HG2	2.14	0.47
1:M:316:SER:O	1:M:323:GLN:NE2	2.47	0.47
1:S:7:ARG:HG2	1:X:408:TYR:CE2	2.42	0.47
1:D:400:GLU:CD	1:E:51:LYS:HE2	2.33	0.47
1:E:400:GLU:HG3	1:F:327:PRO:HB2	1.95	0.47
1:G:258:ILE:HG21	1:G:306:ALA:HB1	1.96	0.47
1:K:361:THR:OG1	1:L:40:LEU:HD23	2.14	0.47
1:S:37:ARG:O	1:S:45:ARG:HG2	2.13	0.47
1:W:318:LEU:HD22	1:W:322:LEU:HD23	1.96	0.47
1:D:358:LEU:CA	1:E:40:LEU:HD21	2.44	0.47
1:S:12:GLU:HG2	1:S:73:LEU:HD13	1.96	0.47
1:B:393:ARG:NH2	1:C:321:GLU:HG3	2.29	0.47
1:C:318:LEU:HD22	1:C:322:LEU:HD23	1.96	0.47
1:D:361:THR:OG1	1:E:39:GLN:CB	2.63	0.47
1:A:40:LEU:HD11	1:F:358:LEU:HD23	1.95	0.47
1:R:12:GLU:HG2	1:R:73:LEU:HD13	1.96	0.47
1:O:387:THR:OG1	1:O:388:GLU:N	2.48	0.47
1:N:344:LEU:O	1:N:352:THR:OG1	2.16	0.47
1:A:40:LEU:CD2	1:F:361:THR:OG1	2.62	0.47
1:R:344:LEU:O	1:R:352:THR:OG1	2.17	0.47
1:U:357:ALA:HB3	1:V:44:LEU:HD13	1.95	0.47
1:E:65:GLU:HG3	2:E:501:ADP:H2'	1.96	0.47
1:K:408:TYR:CE2	1:L:7:ARG:HG2	2.50	0.47
1:O:390:ILE:HG22	1:P:320:PRO:HB3	1.95	0.47
1:J:104:THR:O	1:J:108:VAL:HG23	2.15	0.47
1:J:106:ALA:HA	1:K:289:THR:HB	1.96	0.47
1:N:316:SER:O	1:N:323:GLN:NE2	2.47	0.47
1:A:39:GLN:HB2	1:F:361:THR:CG2	2.45	0.46
1:M:261:ILE:O	1:M:274:ARG:HB3	2.15	0.46
1:J:12:GLU:HG2	1:J:73:LEU:HD13	1.97	0.46
1:N:128:GLU:O	1:N:131:ILE:HG22	2.15	0.46
1:Q:429:LEU:O	1:Q:432:LEU:N	2.48	0.46
1:D:318:LEU:HD22	1:D:322:LEU:HD23	1.98	0.46
1:G:261:ILE:O	1:G:274:ARG:HB3	2.15	0.46
1:N:126:LEU:O	1:N:130:ARG:HG2	2.15	0.46
1:Q:318:LEU:HD22	1:Q:322:LEU:HD23	1.98	0.46
1:M:6:PRO:N	1:R:408:TYR:HE1	2.13	0.46
1:S:318:LEU:HD22	1:S:322:LEU:HD23	1.97	0.46
1:B:258:ILE:HG21	1:B:306:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:425:VAL:HG13	1:G:429:LEU:HD12	1.98	0.46
1:R:161:LYS:HE3	1:R:165:GLU:OE2	2.16	0.46
1:W:344:LEU:O	1:W:352:THR:OG1	2.19	0.46
1:C:12:GLU:HG2	1:C:73:LEU:HD13	1.97	0.46
1:E:41:ASN:HD21	1:E:44:LEU:HD12	1.81	0.46
1:K:408:TYR:CE1	1:L:6:PRO:CB	2.99	0.46
1:S:56:ILE:HD13	1:X:441:PHE:HD2	1.81	0.46
1:A:429:LEU:O	1:A:432:LEU:N	2.44	0.46
1:E:425:VAL:HG13	1:E:429:LEU:HD12	1.97	0.46
1:H:258:ILE:HG21	1:H:306:ALA:HB1	1.97	0.46
1:M:408:TYR:HB2	1:N:29:ILE:HD11	1.98	0.46
1:Q:63:LYS:NZ	2:Q:501:ADP:O1B	2.33	0.46
1:R:65:GLU:HG3	2:R:501:ADP:H2'	1.98	0.46
1:X:65:GLU:HG3	2:X:501:ADP:H2'	1.98	0.46
1:E:95:GLU:N	1:E:95:GLU:OE1	2.48	0.46
1:K:21:ASP:O	1:K:25:ARG:HG3	2.16	0.46
1:X:55:MET:N	1:X:306:ALA:O	2.46	0.46
1:J:231:ALA:CA	1:J:234:VAL:HG12	2.44	0.46
1:P:408:TYR:OH	1:Q:7:ARG:HA	2.16	0.46
1:N:126:LEU:CB	1:N:229:GLU:HG2	2.44	0.46
1:S:63:LYS:NZ	2:S:501:ADP:O2B	2.32	0.46
1:A:261:ILE:O	1:A:274:ARG:HB3	2.15	0.45
1:D:349:ALA:HB1	1:E:44:LEU:HD23	1.98	0.45
1:E:231:ALA:HA	1:E:234:VAL:HG12	1.98	0.45
1:D:361:THR:HG23	1:E:39:GLN:HG3	1.97	0.45
1:M:40:LEU:HD21	1:R:358:LEU:N	2.31	0.45
1:W:425:VAL:HG13	1:W:429:LEU:HD12	1.99	0.45
1:C:258:ILE:HG21	1:C:306:ALA:HB1	1.97	0.45
1:C:27:VAL:HB	1:C:70:LEU:HD22	1.98	0.45
1:G:318:LEU:HD22	1:G:322:LEU:HD23	1.97	0.45
1:K:63:LYS:NZ	2:K:501:ADP:O2B	2.38	0.45
1:O:37:ARG:O	1:O:45:ARG:HG2	2.15	0.45
1:S:65:GLU:HG3	2:S:501:ADP:H2'	1.97	0.45
1:U:362:GLU:OE2	1:V:35:TRP:HZ3	1.98	0.45
1:W:234:VAL:HG13	1:W:236:PRO:HD3	1.98	0.45
1:B:261:ILE:O	1:B:274:ARG:HB3	2.16	0.45
1:B:12:GLU:HG2	1:B:73:LEU:HD13	1.98	0.45
1:D:258:ILE:HG21	1:D:306:ALA:HB1	1.99	0.45
1:K:401:ARG:NH2	1:L:329:ARG:O	2.49	0.45
1:K:411:SER:OG	1:L:32:ARG:NH2	2.36	0.45
1:O:358:LEU:CD2	1:P:40:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:258:ILE:HG21	1:T:306:ALA:HB1	1.97	0.45
1:V:261:ILE:O	1:V:274:ARG:HB3	2.16	0.45
1:V:335:LEU:HD13	1:V:343:ILE:CD1	2.47	0.45
1:S:36:ARG:NH2	1:X:407:SER:O	2.41	0.45
1:T:12:GLU:HG2	1:T:73:LEU:HD13	1.97	0.45
1:W:258:ILE:HG21	1:W:306:ALA:HB1	1.99	0.45
1:G:95:GLU:OE1	1:G:95:GLU:N	2.49	0.45
1:O:65:GLU:HG3	2:O:501:ADP:H2'	1.98	0.45
1:K:387:THR:OG1	1:K:388:GLU:N	2.50	0.45
1:A:12:GLU:HG2	1:A:73:LEU:HD13	1.99	0.45
1:D:362:GLU:OE2	1:E:35:TRP:HZ3	1.98	0.45
1:D:429:LEU:O	1:D:432:LEU:N	2.48	0.45
1:F:12:GLU:HG2	1:F:73:LEU:HD13	1.99	0.45
1:G:65:GLU:HG3	2:G:501:ADP:H2'	1.97	0.45
1:L:421:ASP:OD1	1:L:424:TYR:N	2.43	0.45
1:S:109:LYS:HD3	1:T:289:THR:OG1	2.16	0.45
1:A:59:THR:OG1	1:A:393:ARG:NH2	2.49	0.45
1:M:39:GLN:HB3	1:R:361:THR:CB	2.46	0.45
1:N:12:GLU:HG2	1:N:73:LEU:HD13	1.99	0.45
1:V:65:GLU:HG3	2:V:501:ADP:H2'	1.98	0.45
1:K:361:THR:HG21	1:L:39:GLN:HB2	1.99	0.45
1:N:261:ILE:O	1:N:274:ARG:HB3	2.16	0.45
1:T:95:GLU:OE1	1:T:95:GLU:N	2.50	0.45
1:N:429:LEU:O	1:N:432:LEU:N	2.44	0.45
1:N:59:THR:HG21	1:O:320:PRO:CG	2.46	0.45
1:O:63:LYS:NZ	2:O:501:ADP:O2B	2.37	0.45
1:D:354:GLN:CG	1:E:44:LEU:HD22	2.38	0.44
1:G:401:ARG:NH2	1:H:329:ARG:O	2.50	0.44
1:M:44:LEU:HD22	1:R:354:GLN:CG	2.44	0.44
1:S:18:ILE:HG12	1:S:347:PRO:HG3	1.99	0.44
1:X:55:MET:O	1:X:307:SER:HA	2.17	0.44
1:B:318:LEU:HD22	1:B:322:LEU:HD23	1.98	0.44
1:J:387:THR:OG1	1:J:388:GLU:N	2.51	0.44
1:K:360:ALA:HA	1:K:364:VAL:O	2.17	0.44
1:K:408:TYR:OH	1:L:7:ARG:CA	2.66	0.44
1:M:27:VAL:HB	1:M:70:LEU:HD22	1.99	0.44
1:B:413:LEU:HA	1:B:416:GLN:NE2	2.32	0.44
1:B:441:PHE:CE2	1:C:310:PHE:CB	3.01	0.44
1:I:316:SER:O	1:I:323:GLN:NE2	2.51	0.44
1:M:12:GLU:HG2	1:M:73:LEU:HD13	1.99	0.44
1:T:387:THR:OG1	1:T:388:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:258:ILE:HG21	1:U:306:ALA:HB1	1.99	0.44
1:V:361:THR:HG21	1:W:36:ARG:HA	1.98	0.44
1:I:95:GLU:OE1	1:I:95:GLU:N	2.51	0.44
1:K:408:TYR:OH	1:L:6:PRO:C	2.56	0.44
1:M:32:ARG:NH2	1:R:362:GLU:OE2	2.50	0.44
1:U:261:ILE:O	1:U:274:ARG:HB3	2.18	0.44
1:X:95:GLU:OE1	1:X:95:GLU:N	2.51	0.44
1:I:387:THR:OG1	1:I:388:GLU:N	2.50	0.44
1:M:425:VAL:HG13	1:M:429:LEU:HD12	2.00	0.44
1:X:261:ILE:O	1:X:274:ARG:HB3	2.18	0.44
1:L:258:ILE:HG21	1:L:306:ALA:HB1	2.00	0.44
1:L:75:ASN:OD1	1:L:114:GLN:NE2	2.49	0.44
1:P:342:ARG:O	1:P:347:PRO:HD3	2.18	0.44
1:J:261:ILE:O	1:J:274:ARG:HB3	2.17	0.44
1:O:258:ILE:HG21	1:O:306:ALA:HB1	2.00	0.44
1:P:34:ARG:NH1	1:P:250:HIS:HA	2.33	0.44
1:P:387:THR:OG1	1:P:388:GLU:N	2.50	0.44
1:P:361:THR:CG2	1:Q:39:GLN:HG3	2.43	0.44
1:X:20:GLN:NE2	1:X:333:GLN:O	2.42	0.44
1:B:361:THR:HG22	1:C:35:TRP:CH2	2.52	0.43
1:B:442:ILE:HA	1:C:329:ARG:HB2	2.00	0.43
1:B:407:SER:OG	1:C:29:ILE:HG23	2.18	0.43
1:G:429:LEU:O	1:G:432:LEU:N	2.50	0.43
1:L:387:THR:OG1	1:L:388:GLU:N	2.50	0.43
1:P:425:VAL:HG13	1:P:429:LEU:HD12	1.99	0.43
1:P:63:LYS:NZ	2:P:501:ADP:O2B	2.40	0.43
1:U:358:LEU:CD2	1:V:40:LEU:HD11	2.48	0.43
1:X:425:VAL:HG13	1:X:429:LEU:HD12	2.00	0.43
1:S:320:PRO:CB	1:X:59:THR:HG21	2.47	0.43
1:A:40:LEU:HD23	1:F:361:THR:OG1	2.18	0.43
1:B:65:GLU:HG3	2:B:501:ADP:H2'	2.00	0.43
1:D:407:SER:O	1:E:36:ARG:CZ	2.54	0.43
1:I:20:GLN:NE2	1:I:333:GLN:O	2.42	0.43
1:M:429:LEU:O	1:M:432:LEU:N	2.48	0.43
1:V:18:ILE:HG13	1:V:347:PRO:HG3	1.99	0.43
1:X:316:SER:O	1:X:323:GLN:NE2	2.51	0.43
1:E:339:ASP:OD1	1:L:427:LYS:NZ	2.51	0.43
1:I:12:GLU:HG2	1:I:73:LEU:HD13	2.00	0.43
1:P:65:GLU:HG3	2:P:501:ADP:H2'	2.00	0.43
1:T:393:ARG:HB3	1:U:324:GLY:HA3	1.99	0.43
1:V:342:ARG:O	1:V:347:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:258:ILE:HG21	1:M:306:ALA:HB1	2.00	0.43
1:S:15:LYS:HB3	1:S:348:ASN:ND2	2.33	0.43
1:X:355:TYR:HA	1:X:358:LEU:HD12	1.99	0.43
1:G:342:ARG:O	1:G:347:PRO:HD3	2.18	0.43
1:G:392:ALA:HB3	2:G:501:ADP:C8	2.53	0.43
1:H:76:ALA:HB1	1:H:250:HIS:O	2.18	0.43
1:J:95:GLU:N	1:J:95:GLU:OE1	2.52	0.43
1:O:12:GLU:HG2	1:O:73:LEU:HD13	2.01	0.43
1:M:324:GLY:HA3	1:R:393:ARG:HB3	2.00	0.43
1:D:387:THR:OG1	1:D:388:GLU:N	2.51	0.43
1:D:408:TYR:HE2	1:E:7:ARG:HG2	1.76	0.43
1:H:393:ARG:HH12	2:H:501:ADP:PA	2.42	0.43
1:N:258:ILE:HG21	1:N:306:ALA:HB1	2.01	0.43
1:O:358:LEU:HD23	1:P:40:LEU:HD11	2.00	0.43
1:I:18:ILE:HG21	1:I:342:ARG:HB2	2.00	0.43
1:G:335:LEU:O	1:G:381:TRP:HZ3	2.02	0.43
1:K:261:ILE:O	1:K:274:ARG:HB3	2.19	0.43
1:K:55:MET:N	1:K:306:ALA:O	2.46	0.43
1:N:21:ASP:O	1:N:25:ARG:HG3	2.19	0.43
1:R:316:SER:O	1:R:323:GLN:NE2	2.52	0.43
1:R:350:SER:O	1:R:354:GLN:HG3	2.19	0.43
1:J:18:ILE:HD11	1:J:347:PRO:HG3	2.00	0.43
1:K:12:GLU:HG2	1:K:73:LEU:HD13	2.01	0.43
1:M:41:ASN:HD21	1:M:44:LEU:HD12	1.83	0.43
1:N:122:ARG:O	1:N:126:LEU:HD23	2.19	0.43
1:B:95:GLU:N	1:B:95:GLU:OE1	2.51	0.43
1:E:135:LEU:HD13	1:E:159:PHE:CD1	2.54	0.43
1:E:318:LEU:HD22	1:E:322:LEU:HD23	2.00	0.43
1:E:342:ARG:NH1	1:L:427:LYS:HG3	2.34	0.43
1:L:429:LEU:O	1:L:432:LEU:N	2.52	0.43
1:H:261:ILE:O	1:H:274:ARG:HB3	2.19	0.42
1:L:41:ASN:ND2	1:L:44:LEU:HD12	2.33	0.42
1:P:362:GLU:OE2	1:Q:35:TRP:CZ3	2.72	0.42
1:V:361:THR:HG22	1:W:35:TRP:CZ3	2.54	0.42
1:X:128:GLU:OE1	1:X:164:ARG:NH2	2.52	0.42
1:X:27:VAL:HB	1:X:70:LEU:HD22	2.01	0.42
1:B:440:ARG:HG2	1:C:316:SER:HB3	2.00	0.42
1:C:429:LEU:O	1:C:432:LEU:N	2.51	0.42
1:J:258:ILE:HG21	1:J:306:ALA:HB1	2.00	0.42
1:L:37:ARG:O	1:L:45:ARG:HG2	2.19	0.42
1:T:15:LYS:HB3	1:T:348:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ARG:O	1:E:347:PRO:HD3	2.20	0.42
1:N:128:GLU:O	1:N:132:LEU:HG	2.19	0.42
1:R:318:LEU:HD22	1:R:322:LEU:HD23	2.01	0.42
1:V:95:GLU:OE1	1:V:95:GLU:N	2.50	0.42
1:W:111:VAL:HB	1:W:242:ASP:OD2	2.20	0.42
1:E:160:ARG:O	1:E:164:ARG:HG3	2.19	0.42
1:E:429:LEU:O	1:E:432:LEU:N	2.50	0.42
1:Q:258:ILE:HG21	1:Q:306:ALA:HB1	2.00	0.42
1:M:43:GLU:OE2	1:R:349:ALA:HB2	2.20	0.42
1:A:318:LEU:HD22	1:A:322:LEU:HD23	2.00	0.42
1:B:425:VAL:HG13	1:B:429:LEU:HD12	2.01	0.42
1:D:261:ILE:O	1:D:274:ARG:HB3	2.19	0.42
1:E:258:ILE:HG21	1:E:306:ALA:HB1	2.01	0.42
1:T:342:ARG:O	1:T:347:PRO:HD3	2.19	0.42
1:X:231:ALA:HA	1:X:234:VAL:HG12	2.01	0.42
1:X:63:LYS:NZ	2:X:501:ADP:O3B	2.35	0.42
1:C:425:VAL:HG13	1:C:429:LEU:HD12	2.02	0.42
1:C:75:ASN:OD1	1:C:114:GLN:NE2	2.51	0.42
1:C:95:GLU:OE1	1:C:95:GLU:N	2.50	0.42
1:H:95:GLU:OE1	1:H:95:GLU:N	2.52	0.42
1:I:27:VAL:HB	1:I:70:LEU:HD22	2.01	0.42
1:K:231:ALA:HA	1:K:234:VAL:HG12	2.00	0.42
1:L:76:ALA:HB1	1:L:250:HIS:O	2.19	0.42
1:O:261:ILE:O	1:O:274:ARG:HB3	2.20	0.42
1:R:27:VAL:HB	1:R:70:LEU:HD22	2.01	0.42
1:S:6:PRO:HG2	1:X:408:TYR:HA	2.00	0.42
1:T:15:LYS:O	1:T:348:ASN:N	2.35	0.42
1:U:55:MET:N	1:U:306:ALA:O	2.45	0.42
1:U:357:ALA:CB	1:V:44:LEU:HD13	2.49	0.42
1:W:79:ILE:HG22	1:W:103:LEU:HD13	2.01	0.42
1:W:112:ARG:O	1:W:116:ILE:HG13	2.20	0.42
1:B:344:LEU:O	1:B:352:THR:OG1	2.20	0.42
1:D:397:THR:HG22	1:E:327:PRO:HA	2.00	0.42
1:G:316:SER:O	1:G:323:GLN:NE2	2.52	0.42
1:H:387:THR:OG1	1:H:388:GLU:N	2.52	0.42
1:K:244:ILE:HD11	1:K:295:GLY:HA3	2.02	0.42
1:M:132:LEU:HD22	1:M:159:PHE:CD1	2.54	0.42
1:V:409:ASP:O	1:V:413:LEU:HG	2.20	0.42
1:D:112:ARG:O	1:D:116:ILE:HG13	2.19	0.42
1:I:261:ILE:O	1:I:274:ARG:HB3	2.20	0.42
1:M:318:LEU:HD22	1:M:322:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:258:ILE:HG21	1:S:306:ALA:HB1	2.01	0.42
1:V:40:LEU:HD13	1:V:44:LEU:HB3	2.01	0.42
1:D:358:LEU:N	1:E:40:LEU:HD21	2.35	0.42
1:F:231:ALA:HA	1:F:234:VAL:HG12	2.01	0.42
1:L:316:SER:O	1:L:323:GLN:NE2	2.52	0.42
1:L:425:VAL:HG13	1:L:429:LEU:HD12	2.00	0.42
1:M:20:GLN:NE2	1:M:61:VAL:HB	2.34	0.42
1:S:60:GLY:N	2:S:501:ADP:O2B	2.49	0.42
1:U:76:ALA:HB1	1:U:250:HIS:O	2.20	0.42
1:X:63:LYS:HG2	1:X:332:LEU:HD13	2.02	0.42
1:W:357:ALA:HB3	1:X:44:LEU:CD1	2.50	0.42
1:A:387:THR:OG1	1:A:388:GLU:N	2.51	0.42
1:C:65:GLU:HG3	2:C:501:ADP:H2'	2.02	0.42
1:D:421:ASP:OD1	1:D:424:TYR:N	2.46	0.42
1:L:65:GLU:HG3	2:L:501:ADP:H2'	2.02	0.42
1:R:342:ARG:O	1:R:347:PRO:HD3	2.20	0.42
1:T:441:PHE:HD2	1:U:56:ILE:HD13	1.85	0.42
1:X:387:THR:OG1	1:X:388:GLU:N	2.53	0.42
1:A:231:ALA:HA	1:A:234:VAL:HG12	2.01	0.41
1:C:10:VAL:HG13	1:C:24:LYS:HD3	2.01	0.41
1:F:258:ILE:HG21	1:F:306:ALA:HB1	2.02	0.41
1:M:296:MET:HG2	1:R:109:LYS:HD2	2.01	0.41
1:M:393:ARG:HD2	1:N:320:PRO:O	2.20	0.41
1:T:441:PHE:HD2	1:U:56:ILE:HG21	1.84	0.41
1:X:15:LYS:O	1:X:347:PRO:HA	2.19	0.41
1:B:387:THR:OG1	1:B:388:GLU:N	2.52	0.41
1:D:95:GLU:OE1	1:D:95:GLU:N	2.52	0.41
1:J:318:LEU:HD22	1:J:322:LEU:HD23	2.01	0.41
1:L:40:LEU:HD13	1:L:44:LEU:HB3	2.01	0.41
1:P:408:TYR:CD1	1:Q:6:PRO:CB	2.98	0.41
1:U:362:GLU:CD	1:V:35:TRP:HZ3	2.24	0.41
1:U:362:GLU:OE2	1:V:35:TRP:CZ3	2.73	0.41
1:W:408:TYR:CE1	1:X:6:PRO:CB	3.01	0.41
1:X:350:SER:O	1:X:354:GLN:HG3	2.20	0.41
1:I:55:MET:N	1:I:306:ALA:O	2.45	0.41
1:K:238:GLU:O	1:K:242:ASP:HB2	2.20	0.41
1:N:387:THR:OG1	1:N:388:GLU:N	2.52	0.41
1:S:316:SER:O	1:S:323:GLN:NE2	2.54	0.41
1:A:36:ARG:CZ	1:F:407:SER:O	2.69	0.41
1:A:41:ASN:HD21	1:A:44:LEU:HD12	1.84	0.41
1:K:59:THR:HG21	1:L:320:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:16:HIS:O	1:T:347:PRO:HB3	2.20	0.41
1:B:421:ASP:OD1	1:B:424:TYR:N	2.49	0.41
1:D:358:LEU:O	1:D:361:THR:HB	2.19	0.41
1:E:76:ALA:HB1	1:E:250:HIS:O	2.21	0.41
1:M:440:ARG:HD3	1:N:314:LYS:HD2	2.01	0.41
1:Q:387:THR:OG1	1:Q:388:GLU:N	2.52	0.41
1:M:6:PRO:HD2	1:R:408:TYR:CD1	2.54	0.41
1:S:95:GLU:OE1	1:S:95:GLU:N	2.49	0.41
1:B:354:GLN:O	1:B:358:LEU:HG	2.20	0.41
1:B:408:TYR:CE2	1:C:7:ARG:HG2	2.56	0.41
1:F:421:ASP:OD1	1:F:424:TYR:N	2.49	0.41
1:F:27:VAL:HB	1:F:70:LEU:HD22	2.01	0.41
1:G:41:ASN:HD21	1:G:44:LEU:HD12	1.85	0.41
1:L:155:ALA:HA	1:L:158:ALA:HB3	2.03	0.41
1:G:237:GLU:HG2	1:L:227:GLU:CD	2.41	0.41
1:T:384:ASN:HA	1:T:388:GLU:O	2.20	0.41
1:X:258:ILE:HG21	1:X:306:ALA:HB1	2.01	0.41
1:C:316:SER:O	1:C:323:GLN:NE2	2.53	0.41
1:K:258:ILE:HG21	1:K:306:ALA:HB1	2.01	0.41
1:K:358:LEU:HA	1:L:40:LEU:HD21	2.02	0.41
1:Q:12:GLU:HG2	1:Q:73:LEU:HD13	2.02	0.41
1:S:41:ASN:HD21	1:S:44:LEU:HD12	1.86	0.41
1:U:316:SER:O	1:U:323:GLN:NE2	2.53	0.41
1:E:387:THR:OG1	1:E:388:GLU:N	2.54	0.41
1:I:34:ARG:NH1	1:I:250:HIS:HA	2.36	0.41
1:S:39:GLN:HB2	1:X:361:THR:OG1	2.20	0.41
1:X:34:ARG:NH1	1:X:250:HIS:HA	2.35	0.41
1:F:261:ILE:O	1:F:274:ARG:HB3	2.20	0.41
1:G:63:LYS:NZ	2:G:501:ADP:O2B	2.37	0.41
1:H:316:SER:O	1:H:323:GLN:NE2	2.54	0.41
1:K:421:ASP:OD1	1:K:424:TYR:N	2.44	0.41
1:L:128:GLU:HA	1:L:131:ILE:HG22	2.02	0.41
1:N:400:GLU:HG3	1:O:327:PRO:HB2	2.03	0.41
1:R:258:ILE:HG21	1:R:306:ALA:HB1	2.01	0.41
1:A:109:LYS:CE	1:B:298:LYS:HB2	2.50	0.41
1:I:258:ILE:HG21	1:I:306:ALA:HB1	2.03	0.41
1:M:25:ARG:O	1:M:29:ILE:HG13	2.21	0.41
1:N:384:ASN:HA	1:N:388:GLU:O	2.20	0.41
1:N:408:TYR:O	1:O:6:PRO:HG2	2.21	0.41
1:O:95:GLU:N	1:O:95:GLU:OE1	2.52	0.41
1:Q:231:ALA:HA	1:Q:234:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:128:GLU:OE1	1:R:164:ARG:NH2	2.53	0.41
1:S:5:THR:HG22	1:X:411:SER:CB	2.51	0.41
1:U:408:TYR:CE2	1:V:7:ARG:HG2	2.56	0.41
1:O:34:ARG:NH1	1:O:250:HIS:HA	2.36	0.41
1:Q:123:ALA:HA	1:Q:229:GLU:HG2	2.02	0.41
1:Q:52:ASN:HB2	1:Q:325:ARG:O	2.21	0.41
1:Q:65:GLU:HG3	2:Q:501:ADP:H2'	2.03	0.41
1:M:65:GLU:HG3	2:M:501:ADP:H2'	2.02	0.40
1:V:20:GLN:NE2	1:V:333:GLN:O	2.51	0.40
1:B:59:THR:HG21	1:C:320:PRO:HB2	2.04	0.40
1:D:411:SER:OG	1:E:32:ARG:NH2	2.54	0.40
1:H:411:SER:OG	1:I:6:PRO:HD2	2.21	0.40
1:H:408:TYR:CE2	1:I:25:ARG:CZ	3.04	0.40
1:J:234:VAL:CG2	1:J:235:ASN:N	2.84	0.40
1:M:51:LYS:HE2	1:R:400:GLU:CD	2.40	0.40
1:N:357:ALA:HB3	1:O:44:LEU:HD13	2.03	0.40
1:V:60:GLY:N	2:V:501:ADP:O1B	2.49	0.40
1:D:231:ALA:HA	1:D:234:VAL:HG12	2.02	0.40
1:H:128:GLU:OE1	1:H:164:ARG:NH2	2.54	0.40
1:K:55:MET:O	1:K:307:SER:HA	2.22	0.40
1:K:342:ARG:O	1:K:347:PRO:HD3	2.22	0.40
1:K:408:TYR:CD1	1:L:6:PRO:HB2	2.57	0.40
1:M:95:GLU:N	1:M:95:GLU:OE1	2.52	0.40
1:O:15:LYS:HB3	1:O:348:ASN:ND2	2.36	0.40
1:S:261:ILE:O	1:S:274:ARG:HB3	2.21	0.40
1:S:40:LEU:HD21	1:X:358:LEU:HA	2.03	0.40
1:T:82:GLU:HG3	1:U:279:ARG:O	2.21	0.40
1:V:387:THR:OG1	1:V:388:GLU:N	2.53	0.40
1:W:361:THR:OG1	1:X:40:LEU:HD23	2.22	0.40
1:B:409:ASP:O	1:B:413:LEU:HG	2.21	0.40
1:G:409:ASP:OD1	1:H:7:ARG:NH2	2.53	0.40
1:H:429:LEU:O	1:H:432:LEU:N	2.51	0.40
1:I:76:ALA:HB1	1:I:250:HIS:O	2.21	0.40
1:I:335:LEU:O	1:I:381:TRP:HZ3	2.05	0.40
1:M:47:GLU:HG3	1:R:349:ALA:CB	2.52	0.40
1:N:65:GLU:HG3	2:N:501:ADP:H2'	2.02	0.40
1:T:63:LYS:NZ	2:T:501:ADP:O2B	2.33	0.40
1:X:12:GLU:HG2	1:X:73:LEU:HD13	2.03	0.40
1:E:153:SER:HB2	1:E:156:ARG:HB2	2.04	0.40
1:F:34:ARG:NH1	1:F:250:HIS:HA	2.37	0.40
1:I:318:LEU:HD22	1:I:322:LEU:HD23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASP:OD1	1:L:427:LYS:HE3	2.21	0.40
1:R:261:ILE:O	1:R:274:ARG:HB3	2.22	0.40
1:T:59:THR:HG21	1:U:320:PRO:CB	2.51	0.40
1:U:359:MET:HG3	1:U:366:ILE:HG13	2.03	0.40
1:U:65:GLU:HG3	2:U:501:ADP:H2'	2.03	0.40
1:X:37:ARG:O	1:X:45:ARG:HG2	2.21	0.40

All (7) 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:419:THR:OG1	1:X:122:ARG:NH1[1_455]	1.55	0.65
1:K:418:ILE:CD1	1:X:121:TYR:CE2[1_455]	1.81	0.39
1:K:418:ILE:CD1	1:X:121:TYR:CZ[1_455]	1.84	0.36
1:J:419:THR:O	1:Q:122:ARG:NH1[2_454]	1.88	0.32
1:F:419:THR:OG1	1:O:122:ARG:NH1[1_655]	1.93	0.27
1:P:417:ASN:ND2	1:T:419:THR:O[2_545]	2.09	0.11
1:B:165:GLU:OE1	1:M:342:ARG:NH1[1_656]	2.13	0.07

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	322/442 (73%)	315 (98%)	7 (2%)	0	100	100
1	B	327/442 (74%)	321 (98%)	6 (2%)	0	100	100
1	C	356/442 (80%)	350 (98%)	6 (2%)	0	100	100
1	D	325/442 (74%)	318 (98%)	7 (2%)	0	100	100
1	E	348/442 (79%)	341 (98%)	7 (2%)	0	100	100
1	F	330/442 (75%)	323 (98%)	7 (2%)	0	100	100
1	G	319/442 (72%)	312 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	361/442 (82%)	355 (98%)	6 (2%)	0	100	100
1	I	337/442 (76%)	330 (98%)	7 (2%)	0	100	100
1	J	323/442 (73%)	317 (98%)	6 (2%)	0	100	100
1	K	329/442 (74%)	322 (98%)	7 (2%)	0	100	100
1	L	361/442 (82%)	355 (98%)	6 (2%)	0	100	100
1	M	332/442 (75%)	325 (98%)	7 (2%)	0	100	100
1	N	320/442 (72%)	313 (98%)	7 (2%)	0	100	100
1	O	338/442 (76%)	331 (98%)	7 (2%)	0	100	100
1	P	297/442 (67%)	291 (98%)	6 (2%)	0	100	100
1	Q	360/442 (81%)	355 (99%)	5 (1%)	0	100	100
1	R	328/442 (74%)	321 (98%)	7 (2%)	0	100	100
1	S	302/442 (68%)	296 (98%)	6 (2%)	0	100	100
1	T	310/442 (70%)	303 (98%)	7 (2%)	0	100	100
1	U	313/442 (71%)	306 (98%)	7 (2%)	0	100	100
1	V	342/442 (77%)	335 (98%)	7 (2%)	0	100	100
1	W	328/442 (74%)	321 (98%)	7 (2%)	0	100	100
1	X	350/442 (79%)	344 (98%)	6 (2%)	0	100	100
All	All	7958/10608 (75%)	7800 (98%)	158 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	283/376 (75%)	282 (100%)	1 (0%)	93	96
1	B	286/376 (76%)	285 (100%)	1 (0%)	94	96
1	C	310/376 (82%)	309 (100%)	1 (0%)	94	96
1	D	285/376 (76%)	284 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	305/376 (81%)	304 (100%)	1 (0%)	94	96
1	F	290/376 (77%)	289 (100%)	1 (0%)	94	96
1	G	281/376 (75%)	280 (100%)	1 (0%)	93	96
1	H	316/376 (84%)	315 (100%)	1 (0%)	94	96
1	I	297/376 (79%)	296 (100%)	1 (0%)	94	96
1	J	286/376 (76%)	285 (100%)	1 (0%)	94	96
1	K	289/376 (77%)	288 (100%)	1 (0%)	94	96
1	L	316/376 (84%)	315 (100%)	1 (0%)	94	96
1	M	293/376 (78%)	292 (100%)	1 (0%)	94	96
1	N	282/376 (75%)	280 (99%)	2 (1%)	88	94
1	O	298/376 (79%)	297 (100%)	1 (0%)	94	96
1	P	263/376 (70%)	262 (100%)	1 (0%)	93	96
1	Q	314/376 (84%)	313 (100%)	1 (0%)	94	96
1	R	290/376 (77%)	289 (100%)	1 (0%)	94	96
1	S	267/376 (71%)	266 (100%)	1 (0%)	93	96
1	T	274/376 (73%)	273 (100%)	1 (0%)	93	96
1	U	274/376 (73%)	273 (100%)	1 (0%)	93	96
1	V	300/376 (80%)	299 (100%)	1 (0%)	94	96
1	W	289/376 (77%)	288 (100%)	1 (0%)	94	96
1	X	310/376 (82%)	308 (99%)	2 (1%)	90	95
All	All	6998/9024 (78%)	6972 (100%)	26 (0%)	93	96

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	TYR
1	B	355	TYR
1	C	355	TYR
1	D	355	TYR
1	E	355	TYR
1	F	355	TYR
1	G	355	TYR
1	H	355	TYR
1	I	355	TYR
1	J	355	TYR

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Mol	Chain	Res	Type
1	K	355	TYR
1	L	355	TYR
1	M	355	TYR
1	N	355	TYR
1	N	361	THR
1	O	355	TYR
1	P	355	TYR
1	Q	355	TYR
1	R	355	TYR
1	S	355	TYR
1	T	355	TYR
1	U	355	TYR
1	V	355	TYR
1	W	355	TYR
1	X	355	TYR
1	X	361	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
1	C	75	ASN
1	C	114	GLN
1	C	301	HIS
1	D	33	ASN
1	D	75	ASN
1	D	114	GLN
1	D	365	ASN
1	D	417	ASN
1	E	75	ASN
1	E	114	GLN
1	F	75	ASN
1	F	114	GLN
1	G	75	ASN
1	G	114	GLN
1	H	75	ASN
1	H	114	GLN
1	H	301	HIS
1	I	75	ASN
1	I	114	GLN
1	J	75	ASN
1	J	114	GLN

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Mol	Chain	Res	Type
1	J	301	HIS
1	K	75	ASN
1	K	114	GLN
1	K	416	GLN
1	L	41	ASN
1	L	75	ASN
1	L	114	GLN
1	L	428	HIS
1	M	75	ASN
1	M	114	GLN
1	N	75	ASN
1	N	114	GLN
1	O	75	ASN
1	O	114	GLN
1	P	75	ASN
1	P	114	GLN
1	Q	301	HIS
1	R	75	ASN
1	R	114	GLN
1	R	157	GLN
1	R	301	HIS
1	S	22	ASN
1	S	75	ASN
1	S	114	GLN
1	S	301	HIS
1	T	75	ASN
1	T	114	GLN
1	U	75	ASN
1	U	114	GLN
1	U	301	HIS
1	V	75	ASN
1	V	114	GLN
1	W	75	ASN
1	W	114	GLN
1	X	75	ASN
1	X	114	GLN
1	X	301	HIS

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 ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	A	501	-	24,29,29	0.97	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	B	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.67	1 (4%)
2	ADP	C	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.63	1 (4%)
2	ADP	D	501	-	24,29,29	1.04	1 (4%)	23,45,45	1.65	1 (4%)
2	ADP	E	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.64	2 (8%)
2	ADP	F	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.69	2 (8%)
2	ADP	G	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.64	1 (4%)
2	ADP	H	501	-	24,29,29	0.98	1 (4%)	23,45,45	1.71	2 (8%)
2	ADP	I	501	-	24,29,29	0.99	1 (4%)	23,45,45	1.69	1 (4%)
2	ADP	J	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.67	1 (4%)
2	ADP	K	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.64	1 (4%)
2	ADP	L	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.66	1 (4%)
2	ADP	M	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	N	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.63	1 (4%)
2	ADP	O	501	-	24,29,29	1.02	1 (4%)	23,45,45	1.65	1 (4%)
2	ADP	P	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.62	1 (4%)
2	ADP	Q	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	R	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.66	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	S	501	-	24,29,29	0.99	1 (4%)	23,45,45	1.72	1 (4%)
2	ADP	T	501	-	24,29,29	1.04	1 (4%)	23,45,45	1.63	1 (4%)
2	ADP	U	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.64	1 (4%)
2	ADP	V	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.67	1 (4%)
2	ADP	W	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.67	1 (4%)
2	ADP	X	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.61	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	501	-	-	0/12/32/32	0/3/3/3
2	ADP	B	501	-	-	0/12/32/32	0/3/3/3
2	ADP	C	501	-	-	0/12/32/32	0/3/3/3
2	ADP	D	501	-	-	0/12/32/32	0/3/3/3
2	ADP	E	501	-	-	0/12/32/32	0/3/3/3
2	ADP	F	501	-	-	0/12/32/32	0/3/3/3
2	ADP	G	501	-	-	0/12/32/32	0/3/3/3
2	ADP	H	501	-	-	0/12/32/32	0/3/3/3
2	ADP	I	501	-	-	0/12/32/32	0/3/3/3
2	ADP	J	501	-	-	0/12/32/32	0/3/3/3
2	ADP	K	501	-	-	0/12/32/32	0/3/3/3
2	ADP	L	501	-	-	0/12/32/32	0/3/3/3
2	ADP	M	501	-	-	0/12/32/32	0/3/3/3
2	ADP	N	501	-	-	0/12/32/32	0/3/3/3
2	ADP	O	501	-	-	0/12/32/32	0/3/3/3
2	ADP	P	501	-	-	0/12/32/32	0/3/3/3
2	ADP	Q	501	-	-	0/12/32/32	0/3/3/3
2	ADP	R	501	-	-	0/12/32/32	0/3/3/3
2	ADP	S	501	-	-	0/12/32/32	0/3/3/3
2	ADP	T	501	-	-	0/12/32/32	0/3/3/3
2	ADP	U	501	-	-	0/12/32/32	0/3/3/3
2	ADP	V	501	-	-	0/12/32/32	0/3/3/3
2	ADP	W	501	-	-	0/12/32/32	0/3/3/3
2	ADP	X	501	-	-	0/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ADP	C5-C4	3.07	1.47	1.40
2	S	501	ADP	C5-C4	3.09	1.47	1.40
2	H	501	ADP	C5-C4	3.15	1.47	1.40
2	I	501	ADP	C5-C4	3.16	1.47	1.40
2	M	501	ADP	C5-C4	3.16	1.47	1.40
2	V	501	ADP	C5-C4	3.17	1.47	1.40
2	Q	501	ADP	C5-C4	3.18	1.47	1.40
2	L	501	ADP	C5-C4	3.21	1.47	1.40
2	F	501	ADP	C5-C4	3.21	1.47	1.40
2	B	501	ADP	C5-C4	3.22	1.47	1.40
2	R	501	ADP	C5-C4	3.23	1.47	1.40
2	J	501	ADP	C5-C4	3.25	1.47	1.40
2	N	501	ADP	C5-C4	3.25	1.47	1.40
2	P	501	ADP	C5-C4	3.26	1.47	1.40
2	C	501	ADP	C5-C4	3.26	1.47	1.40
2	E	501	ADP	C5-C4	3.26	1.47	1.40
2	W	501	ADP	C5-C4	3.27	1.47	1.40
2	K	501	ADP	C5-C4	3.27	1.47	1.40
2	G	501	ADP	C5-C4	3.28	1.47	1.40
2	U	501	ADP	C5-C4	3.28	1.47	1.40
2	X	501	ADP	C5-C4	3.29	1.47	1.40
2	D	501	ADP	C5-C4	3.30	1.47	1.40
2	O	501	ADP	C5-C4	3.31	1.48	1.40
2	T	501	ADP	C5-C4	3.31	1.48	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	501	ADP	N3-C2-N1	-6.73	123.58	128.87
2	M	501	ADP	N3-C2-N1	-6.62	123.67	128.87
2	A	501	ADP	N3-C2-N1	-6.61	123.68	128.87
2	H	501	ADP	N3-C2-N1	-6.59	123.69	128.87
2	I	501	ADP	N3-C2-N1	-6.54	123.73	128.87
2	Q	501	ADP	N3-C2-N1	-6.54	123.74	128.87
2	J	501	ADP	N3-C2-N1	-6.42	123.83	128.87
2	F	501	ADP	N3-C2-N1	-6.41	123.84	128.87
2	B	501	ADP	N3-C2-N1	-6.40	123.84	128.87
2	V	501	ADP	N3-C2-N1	-6.37	123.87	128.87
2	U	501	ADP	N3-C2-N1	-6.36	123.87	128.87
2	G	501	ADP	N3-C2-N1	-6.34	123.89	128.87
2	W	501	ADP	N3-C2-N1	-6.34	123.89	128.87
2	K	501	ADP	N3-C2-N1	-6.32	123.91	128.87
2	R	501	ADP	N3-C2-N1	-6.31	123.91	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	501	ADP	N3-C2-N1	-6.29	123.93	128.87
2	N	501	ADP	N3-C2-N1	-6.28	123.94	128.87
2	E	501	ADP	N3-C2-N1	-6.28	123.94	128.87
2	P	501	ADP	N3-C2-N1	-6.28	123.94	128.87
2	L	501	ADP	N3-C2-N1	-6.27	123.94	128.87
2	C	501	ADP	N3-C2-N1	-6.27	123.95	128.87
2	D	501	ADP	N3-C2-N1	-6.21	123.99	128.87
2	T	501	ADP	N3-C2-N1	-6.19	124.01	128.87
2	X	501	ADP	N3-C2-N1	-6.10	124.08	128.87
2	H	501	ADP	O3B-PB-O2B	2.01	114.83	107.44
2	E	501	ADP	O3B-PB-O2B	2.02	114.87	107.44
2	F	501	ADP	O3B-PB-O2B	2.05	114.96	107.44
2	Q	501	ADP	O3B-PB-O2B	2.06	115.02	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	4	0
2	B	501	ADP	2	0
2	C	501	ADP	4	0
2	D	501	ADP	1	0
2	E	501	ADP	4	0
2	F	501	ADP	2	0
2	G	501	ADP	5	0
2	H	501	ADP	5	0
2	I	501	ADP	4	0
2	J	501	ADP	3	0
2	K	501	ADP	4	0
2	L	501	ADP	3	0
2	M	501	ADP	5	0
2	N	501	ADP	2	0
2	O	501	ADP	3	0
2	P	501	ADP	5	0
2	Q	501	ADP	4	0
2	R	501	ADP	3	0
2	S	501	ADP	4	0
2	T	501	ADP	4	0
2	U	501	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	501	ADP	3	0
2	W	501	ADP	1	0
2	X	501	ADP	4	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	330/442 (74%)	0.44	22 (6%)	21 23	348, 386, 520, 579	0
1	B	337/442 (76%)	0.46	24 (7%)	19 22	359, 407, 523, 668	0
1	C	366/442 (82%)	0.33	14 (3%)	44 42	338, 364, 431, 475	0
1	D	333/442 (75%)	0.43	24 (7%)	18 21	324, 387, 495, 545	0
1	E	359/442 (81%)	0.31	14 (3%)	43 41	349, 404, 477, 537	0
1	F	338/442 (76%)	0.39	18 (5%)	30 31	312, 365, 465, 546	0
1	G	327/442 (73%)	0.45	23 (7%)	19 22	342, 388, 491, 572	0
1	H	371/442 (83%)	0.16	3 (0%)	87 84	329, 368, 418, 450	0
1	I	348/442 (78%)	0.49	29 (8%)	14 18	321, 398, 501, 526	0
1	J	332/442 (75%)	0.31	17 (5%)	32 32	355, 395, 477, 581	0
1	K	337/442 (76%)	0.35	15 (4%)	37 36	327, 380, 455, 532	0
1	L	371/442 (83%)	0.37	10 (2%)	58 54	335, 370, 437, 506	0
1	M	342/442 (77%)	0.45	23 (6%)	21 23	377, 426, 490, 553	0
1	N	328/442 (74%)	0.69	32 (9%)	10 14	371, 471, 572, 699	0
1	O	348/442 (78%)	0.29	11 (3%)	51 47	367, 405, 458, 526	0
1	P	305/442 (69%)	0.53	22 (7%)	18 21	342, 380, 436, 479	0
1	Q	370/442 (83%)	0.54	43 (11%)	6 12	327, 378, 565, 603	0
1	R	338/442 (76%)	0.40	13 (3%)	44 42	394, 427, 522, 610	0
1	S	310/442 (70%)	0.43	23 (7%)	17 21	415, 467, 563, 658	0
1	T	318/442 (71%)	0.47	12 (3%)	44 42	359, 429, 516, 594	0
1	U	321/442 (72%)	0.39	11 (3%)	49 46	358, 387, 446, 534	0
1	V	352/442 (79%)	0.69	30 (8%)	13 18	375, 439, 573, 616	0
1	W	336/442 (76%)	0.66	43 (12%)	5 11	406, 444, 509, 548	0
1	X	360/442 (81%)	0.22	10 (2%)	56 52	412, 448, 493, 543	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	8177/10608 (77%)	0.42	486 (5%)	26 26	312, 406, 515, 699	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	124	GLU	10.0
1	I	410	ALA	7.8
1	I	362	GLU	6.8
1	G	120	ARG	6.5
1	I	411	SER	6.4
1	W	235	ASN	5.8
1	B	232	LYS	5.7
1	Q	398	VAL	5.7
1	G	125	GLU	5.7
1	W	233	LEU	5.6
1	Q	403	MET	5.6
1	J	93	GLY	5.4
1	W	234	VAL	5.4
1	V	220	ASP	5.3
1	N	228	GLU	5.3
1	W	403	MET	5.2
1	I	128	GLU	5.1
1	W	232	LYS	5.1
1	W	93	GLY	5.1
1	C	18	ILE	5.0
1	M	387	THR	4.9
1	P	367	GLU	4.8
1	I	124	GLU	4.7
1	M	443	LEU	4.7
1	W	231	ALA	4.7
1	V	77	PRO	4.7
1	M	366	ILE	4.6
1	N	232	LYS	4.6
1	G	119	ASN	4.6
1	D	125	GLU	4.5
1	Q	399	LEU	4.5
1	M	386	SER	4.4
1	W	227	GLU	4.4
1	P	366	ILE	4.3
1	W	230	ALA	4.3
1	N	93	GLY	4.3
1	V	163	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	235	ASN	4.2
1	Q	139	ALA	4.2
1	W	411	SER	4.2
1	M	440	ARG	4.1
1	X	220	ASP	4.1
1	K	392	ALA	4.1
1	F	49	THR	4.0
1	W	407	SER	4.0
1	Q	136	ILE	4.0
1	D	88	GLU	4.0
1	V	166	GLY	4.0
1	Q	135	LEU	3.9
1	D	376	ILE	3.9
1	X	365	ASN	3.9
1	K	124	GLU	3.9
1	P	2	SER	3.9
1	T	294	HIS	3.8
1	E	119	ASN	3.8
1	B	233	LEU	3.8
1	U	433	VAL	3.8
1	V	398	VAL	3.8
1	Q	402	LEU	3.8
1	R	87	THR	3.8
1	Q	406	ILE	3.8
1	N	376	ILE	3.7
1	R	165	GLU	3.7
1	I	221	ALA	3.7
1	V	222	MET	3.7
1	F	234	VAL	3.7
1	I	406	ILE	3.7
1	V	76	ALA	3.7
1	J	119	ASN	3.7
1	Q	397	THR	3.7
1	Q	131	ILE	3.7
1	O	387	THR	3.7
1	U	87	THR	3.6
1	L	17	ILE	3.6
1	B	235	ASN	3.6
1	Q	443	LEU	3.6
1	G	123	ALA	3.6
1	M	368	PHE	3.6
1	G	122	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	W	229	GLU	3.6
1	F	232	LYS	3.6
1	J	439	SER	3.6
1	I	93	GLY	3.5
1	W	376	ILE	3.5
1	S	33	ASN	3.5
1	G	233	LEU	3.5
1	W	2	SER	3.5
1	C	17	ILE	3.5
1	D	124	GLU	3.5
1	S	294	HIS	3.5
1	F	407	SER	3.5
1	W	414	SER	3.5
1	P	365	ASN	3.5
1	P	333	GLN	3.5
1	S	48	VAL	3.5
1	P	116	ILE	3.5
1	W	119	ASN	3.5
1	I	222	MET	3.4
1	W	412	ASP	3.4
1	I	413	LEU	3.4
1	I	120	ARG	3.4
1	J	433	VAL	3.4
1	X	366	ILE	3.4
1	V	221	ALA	3.4
1	T	243	ALA	3.4
1	R	376	ILE	3.4
1	L	18	ILE	3.3
1	Q	376	ILE	3.3
1	R	133	ASP	3.3
1	V	2	SER	3.3
1	B	220	ASP	3.3
1	S	297	VAL	3.3
1	A	87	THR	3.3
1	E	122	ARG	3.3
1	T	77	PRO	3.3
1	S	352	THR	3.3
1	M	294	HIS	3.3
1	N	230	ALA	3.3
1	T	53	ILE	3.3
1	S	75	ASN	3.2
1	V	362	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	121	TYR	3.2
1	A	356	LYS	3.2
1	V	294	HIS	3.2
1	U	124	GLU	3.2
1	R	335	LEU	3.2
1	K	407	SER	3.2
1	G	121	TYR	3.2
1	C	362	GLU	3.2
1	A	366	ILE	3.2
1	W	236	PRO	3.2
1	E	235	ASN	3.2
1	R	368	PHE	3.1
1	I	407	SER	3.1
1	K	93	GLY	3.1
1	B	107	ALA	3.1
1	I	125	GLU	3.1
1	F	366	ILE	3.1
1	W	406	ILE	3.1
1	N	332	LEU	3.1
1	M	93	GLY	3.1
1	P	77	PRO	3.1
1	M	88	GLU	3.1
1	D	379	ALA	3.1
1	A	368	PHE	3.1
1	Q	395	LEU	3.1
1	D	233	LEU	3.1
1	N	313	ALA	3.1
1	M	388	GLU	3.0
1	S	104	THR	3.0
1	A	412	ASP	3.0
1	Q	401	ARG	3.0
1	R	151	GLU	3.0
1	A	411	SER	3.0
1	N	333	GLN	3.0
1	J	434	ALA	3.0
1	E	124	GLU	3.0
1	N	317	ASP	3.0
1	W	228	GLU	3.0
1	V	251	GLY	3.0
1	N	395	LEU	3.0
1	W	32	ARG	3.0
1	N	119	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	V	75	ASN	3.0
1	J	18	ILE	3.0
1	E	233	LEU	3.0
1	B	17	ILE	2.9
1	N	20	GLN	2.9
1	Q	132	LEU	2.9
1	Q	153	SER	2.9
1	I	412	ASP	2.9
1	F	233	LEU	2.9
1	P	19	GLY	2.9
1	P	75	ASN	2.9
1	N	231	ALA	2.9
1	G	232	LYS	2.9
1	T	88	GLU	2.9
1	R	373	ILE	2.9
1	A	268	SER	2.9
1	A	235	ASN	2.9
1	B	221	ALA	2.9
1	C	368	PHE	2.9
1	N	127	ALA	2.9
1	Q	133	ASP	2.9
1	N	88	GLU	2.9
1	W	112	ARG	2.9
1	D	235	ASN	2.8
1	U	434	ALA	2.8
1	R	88	GLU	2.8
1	W	324	GLY	2.8
1	A	348	ASN	2.8
1	F	409	ASP	2.8
1	M	383	VAL	2.8
1	T	315	PRO	2.8
1	G	430	ASP	2.8
1	U	120	ARG	2.8
1	V	395	LEU	2.8
1	N	229	GLU	2.8
1	Q	436	GLU	2.8
1	Q	439	SER	2.8
1	B	231	ALA	2.8
1	J	36	ARG	2.8
1	V	3	GLU	2.8
1	W	4	MET	2.8
1	S	295	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	U	19	GLY	2.8
1	W	415	GLY	2.8
1	T	3	GLU	2.8
1	B	229	GLU	2.7
1	P	3	GLU	2.7
1	N	233	LEU	2.7
1	L	386	SER	2.7
1	W	402	LEU	2.7
1	E	366	ILE	2.7
1	S	366	ILE	2.7
1	I	220	ASP	2.7
1	B	234	VAL	2.7
1	C	373	ILE	2.7
1	K	121	TYR	2.7
1	J	436	GLU	2.7
1	I	122	ARG	2.7
1	B	16	HIS	2.7
1	G	234	VAL	2.7
1	M	297	VAL	2.7
1	M	439	SER	2.7
1	P	117	GLU	2.7
1	P	406	ILE	2.7
1	G	230	ALA	2.7
1	B	386	SER	2.7
1	F	19	GLY	2.7
1	Q	128	GLU	2.7
1	A	352	THR	2.7
1	A	226	ILE	2.6
1	O	51	LYS	2.6
1	P	376	ILE	2.6
1	V	359	MET	2.6
1	D	122	ARG	2.6
1	K	125	GLU	2.6
1	U	88	GLU	2.6
1	M	365	ASN	2.6
1	N	128	GLU	2.6
1	S	19	GLY	2.6
1	A	354	GLN	2.6
1	E	232	LYS	2.6
1	B	230	ALA	2.6
1	V	87	THR	2.6
1	N	124	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	379	ALA	2.6
1	W	57	GLY	2.6
1	K	123	ALA	2.6
1	O	386	SER	2.6
1	V	104	THR	2.6
1	Q	394	ARG	2.6
1	I	409	ASP	2.6
1	Q	416	GLN	2.6
1	I	123	ALA	2.6
1	S	18	ILE	2.6
1	Q	156	ARG	2.6
1	F	406	ILE	2.6
1	Q	121	TYR	2.6
1	I	132	LEU	2.6
1	C	122	ARG	2.5
1	F	300	ASP	2.5
1	D	380	ALA	2.5
1	E	222	MET	2.5
1	G	226	ILE	2.5
1	N	120	ARG	2.5
1	T	19	GLY	2.5
1	Q	134	VAL	2.5
1	Q	129	GLU	2.5
1	C	139	ALA	2.5
1	J	32	ARG	2.5
1	J	443	LEU	2.5
1	V	399	LEU	2.5
1	J	413	LEU	2.5
1	Q	159	PHE	2.5
1	A	16	HIS	2.5
1	I	129	GLU	2.5
1	G	235	ASN	2.5
1	N	407	SER	2.5
1	A	234	VAL	2.5
1	D	407	SER	2.5
1	R	132	LEU	2.5
1	S	243	ALA	2.5
1	A	125	GLU	2.5
1	D	395	LEU	2.5
1	L	19	GLY	2.5
1	V	162	LYS	2.5
1	A	126	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	429	LEU	2.5
1	V	218	ILE	2.5
1	K	18	ILE	2.5
1	S	74	ALA	2.5
1	B	335	LEU	2.5
1	L	436	GLU	2.5
1	F	411	SER	2.5
1	P	403	MET	2.5
1	W	33	ASN	2.5
1	C	19	GLY	2.5
1	P	360	ALA	2.5
1	E	238	GLU	2.4
1	C	392	ALA	2.4
1	C	363	GLY	2.4
1	D	127	ALA	2.4
1	B	19	GLY	2.4
1	G	222	MET	2.4
1	W	410	ALA	2.4
1	K	227	GLU	2.4
1	T	297	VAL	2.4
1	J	435	ASP	2.4
1	L	387	THR	2.4
1	E	221	ALA	2.4
1	D	93	GLY	2.4
1	G	227	GLU	2.4
1	G	431	ALA	2.4
1	W	362	GLU	2.4
1	A	225	LEU	2.4
1	O	75	ASN	2.4
1	J	297	VAL	2.4
1	I	88	GLU	2.4
1	N	392	ALA	2.4
1	O	39	GLN	2.4
1	M	87	THR	2.4
1	R	392	ALA	2.4
1	X	221	ALA	2.4
1	C	167	GLN	2.4
1	D	232	LYS	2.4
1	Q	407	SER	2.4
1	V	86	PHE	2.4
1	A	49	THR	2.4
1	G	433	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	379	ALA	2.4
1	Q	366	ILE	2.4
1	U	376	ILE	2.4
1	V	108	VAL	2.3
1	G	224	LEU	2.3
1	K	229	GLU	2.3
1	T	293	LYS	2.3
1	B	443	LEU	2.3
1	W	122	ARG	2.3
1	O	33	ASN	2.3
1	S	95	GLU	2.3
1	N	428	HIS	2.3
1	S	87	THR	2.3
1	K	256	ASP	2.3
1	T	328	ILE	2.3
1	I	376	ILE	2.3
1	M	124	GLU	2.3
1	P	76	ALA	2.3
1	W	75	ASN	2.3
1	M	417	ASN	2.3
1	F	418	ILE	2.3
1	L	321	GLU	2.3
1	J	17	ILE	2.3
1	B	165	GLU	2.3
1	G	84	THR	2.3
1	B	439	SER	2.3
1	E	120	ARG	2.3
1	F	18	ILE	2.3
1	X	95	GLU	2.3
1	K	122	ARG	2.3
1	W	22	ASN	2.3
1	A	324	GLY	2.3
1	B	387	THR	2.3
1	M	76	ALA	2.3
1	S	44	LEU	2.3
1	I	414	SER	2.3
1	Q	352	THR	2.3
1	Q	433	VAL	2.3
1	E	229	GLU	2.3
1	F	50	PRO	2.3
1	I	217	LYS	2.3
1	D	373	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	377	ALA	2.2
1	K	2	SER	2.2
1	Q	379	ALA	2.2
1	B	436	GLU	2.2
1	M	367	GLU	2.2
1	Q	163	LEU	2.2
1	R	297	VAL	2.2
1	C	335	LEU	2.2
1	N	131	ILE	2.2
1	C	365	ASN	2.2
1	G	407	SER	2.2
1	W	380	ALA	2.2
1	S	359	MET	2.2
1	B	392	ALA	2.2
1	E	123	ALA	2.2
1	W	226	ILE	2.2
1	O	346	GLU	2.2
1	P	22	ASN	2.2
1	M	403	MET	2.2
1	U	50	PRO	2.2
1	V	235	ASN	2.2
1	X	3	GLU	2.2
1	F	412	ASP	2.2
1	W	363	GLY	2.2
1	D	126	LEU	2.2
1	W	123	ALA	2.2
1	N	331	GLU	2.2
1	W	325	ARG	2.2
1	A	376	ILE	2.2
1	X	330	VAL	2.2
1	N	429	LEU	2.2
1	U	116	ILE	2.2
1	V	114	GLN	2.2
1	H	235	ASN	2.2
1	N	316	SER	2.2
1	P	407	SER	2.2
1	Q	119	ASN	2.2
1	Q	380	ALA	2.2
1	V	164	ARG	2.2
1	I	429	LEU	2.2
1	S	368	PHE	2.2
1	X	82	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	V	391	GLY	2.1
1	N	19	GLY	2.1
1	O	406	ILE	2.1
1	D	243	ALA	2.1
1	B	163	LEU	2.1
1	G	2	SER	2.1
1	V	119	ASN	2.1
1	D	403	MET	2.1
1	O	36	ARG	2.1
1	A	355	TYR	2.1
1	N	75	ASN	2.1
1	A	370	ASP	2.1
1	F	25	ARG	2.1
1	L	16	HIS	2.1
1	J	406	ILE	2.1
1	M	37	ARG	2.1
1	Q	160	ARG	2.1
1	I	119	ASN	2.1
1	P	297	VAL	2.1
1	Q	3	GLU	2.1
1	B	222	MET	2.1
1	D	121	TYR	2.1
1	D	120	ARG	2.1
1	N	130	ARG	2.1
1	N	234	VAL	2.1
1	W	36	ARG	2.1
1	D	94	LYS	2.1
1	I	402	LEU	2.1
1	K	226	ILE	2.1
1	J	332	LEU	2.1
1	Q	415	GLY	2.1
1	D	398	VAL	2.1
1	H	87	THR	2.1
1	B	429	LEU	2.1
1	H	294	HIS	2.1
1	Q	87	THR	2.1
1	V	392	ALA	2.1
1	D	294	HIS	2.1
1	P	348	ASN	2.1
1	M	243	ALA	2.1
1	S	406	ILE	2.1
1	L	365	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	230	ALA	2.1
1	Q	400	GLU	2.1
1	L	156	ARG	2.1
1	R	19	GLY	2.1
1	W	413	LEU	2.1
1	W	125	GLU	2.1
1	M	247	VAL	2.0
1	W	243	ALA	2.0
1	O	335	LEU	2.0
1	I	232	LYS	2.0
1	I	131	ILE	2.0
1	W	416	GLN	2.0
1	X	367	GLU	2.0
1	G	82	GLU	2.0
1	C	361	THR	2.0
1	Q	155	ALA	2.0
1	S	407	SER	2.0
1	V	410	ALA	2.0
1	N	352	THR	2.0
1	Q	396	HIS	2.0
1	T	51	LYS	2.0
1	Q	137	PRO	2.0
1	O	392	ALA	2.0
1	P	36	ARG	2.0
1	X	407	SER	2.0
1	S	122	ARG	2.0
1	S	355	TYR	2.0
1	F	6	PRO	2.0
1	J	49	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	I	501	27/27	0.71	0.48	0.79	372,390,412,414	0
2	ADP	T	501	27/27	0.72	0.50	0.58	363,375,385,390	0
2	ADP	D	501	27/27	0.71	0.41	0.35	367,381,393,394	0
2	ADP	M	501	27/27	0.80	0.40	0.29	405,413,424,426	0
2	ADP	V	501	27/27	0.87	0.42	0.28	381,388,395,396	0
2	ADP	K	501	27/27	0.73	0.56	0.20	345,351,360,362	0
2	ADP	J	501	27/27	0.66	0.49	0.16	352,357,367,370	0
2	ADP	E	501	27/27	0.82	0.40	0.13	381,386,388,390	0
2	ADP	H	501	27/27	0.76	0.41	0.11	356,360,364,365	0
2	ADP	R	501	27/27	0.74	0.48	0.08	400,410,414,415	0
2	ADP	A	501	27/27	0.79	0.36	0.03	357,374,384,386	0
2	ADP	O	501	27/27	0.74	0.42	0.01	381,387,392,397	0
2	ADP	B	501	27/27	0.76	0.48	-0.02	372,381,394,400	0
2	ADP	Q	501	27/27	0.83	0.38	-0.07	355,379,383,385	0
2	ADP	L	501	27/27	0.74	0.48	-0.11	337,343,347,348	0
2	ADP	S	501	27/27	0.77	0.40	-0.12	422,429,441,443	0
2	ADP	X	501	27/27	0.83	0.29	-0.17	423,430,439,442	0
2	ADP	U	501	27/27	0.81	0.37	-0.24	358,361,365,368	0
2	ADP	C	501	27/27	0.73	0.45	-0.24	348,353,357,358	0
2	ADP	P	501	27/27	0.79	0.37	-0.36	345,348,352,354	0
2	ADP	F	501	27/27	0.77	0.37	-0.37	312,321,330,331	0
2	ADP	W	501	27/27	0.83	0.30	-0.41	434,448,455,456	0
2	ADP	G	501	27/27	0.85	0.39	-0.46	348,358,372,375	0
2	ADP	N	501	27/27	0.81	0.41	-0.57	448,470,480,482	0

6.5 Other polymers ⓘ

There are no such residues in this entry.