



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID : 1KYI  
Title : HslUV (H. influenzae)-NLVS Vinyl Sulfone Inhibitor Complex  
Authors : Sousa, M.C.; Kessler, B.M.; Overkleeft, H.S.; McKay, D.B.  
Deposited on : 2002-02-04  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

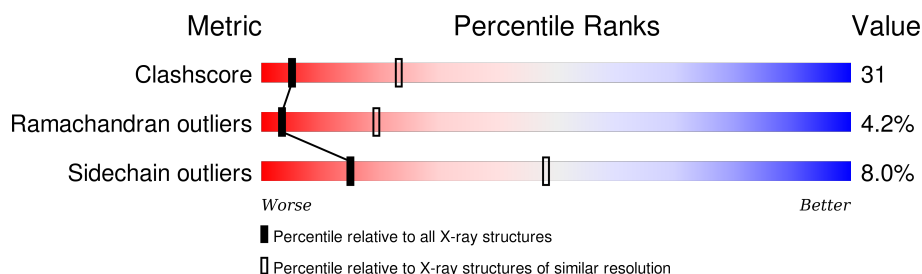
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

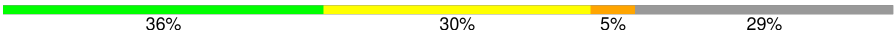
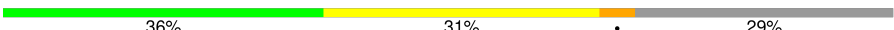
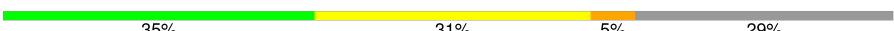
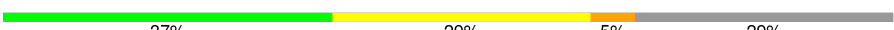
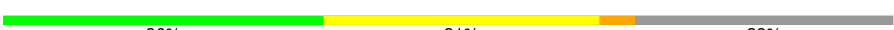





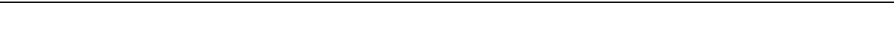

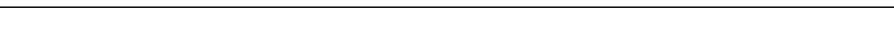
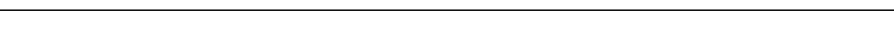
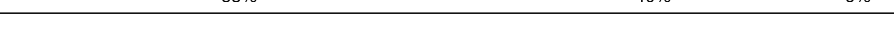


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	
1	S	444	

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Mol	Chain	Length	Quality of chain
1	T	444	
1	U	444	
1	V	444	
1	W	444	
1	X	444	
2	G	174	
2	H	174	
2	I	174	
2	J	174	
2	K	174	
2	L	174	
2	M	174	
2	N	174	
2	O	174	
2	P	174	
2	Q	174	
2	R	174	

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	LVS	J	175	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 45756 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 hsl protease ATP-binding subunit hslU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	B	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	C	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	D	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	E	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	F	321	Total	C	N	O	S	0	0	0
			2488	1557	444	477	10			
1	S	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	T	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	U	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	V	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	W	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			
1	X	317	Total	C	N	O	S	0	0	0
			2469	1543	444	472	10			

- Molecule 2 is a protein called ATP-dependent protease hslV.

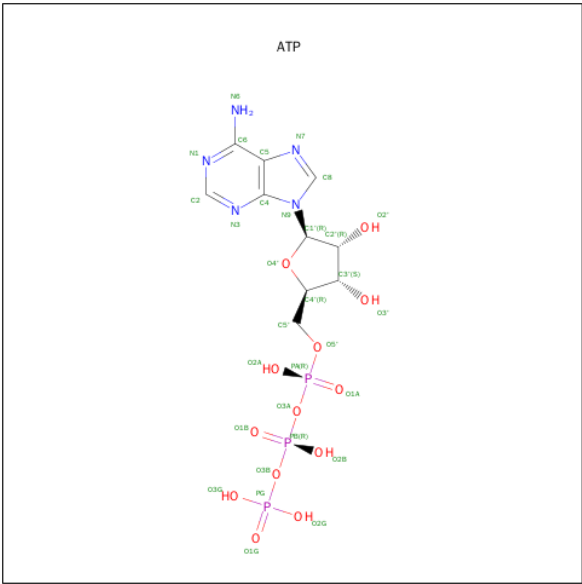
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	H	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	J	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	K	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	L	173	Total	C	N	O	S	0	0	0
			1290	809	228	249	4			
2	M	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	N	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	O	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	P	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	Q	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	R	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			

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



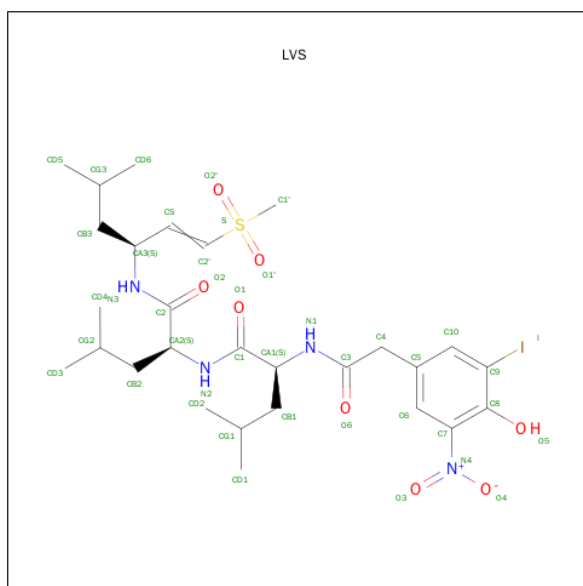
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	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	T	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	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	W	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 4-IODO-3-NITROPHENYL ACETYL-LEUCINYL-LEUCINYL-LEUCINYLVINYLSULFONE (three-letter code: LVS) (formula:  $C_{28}H_{43}IN_4O_8S$ ).

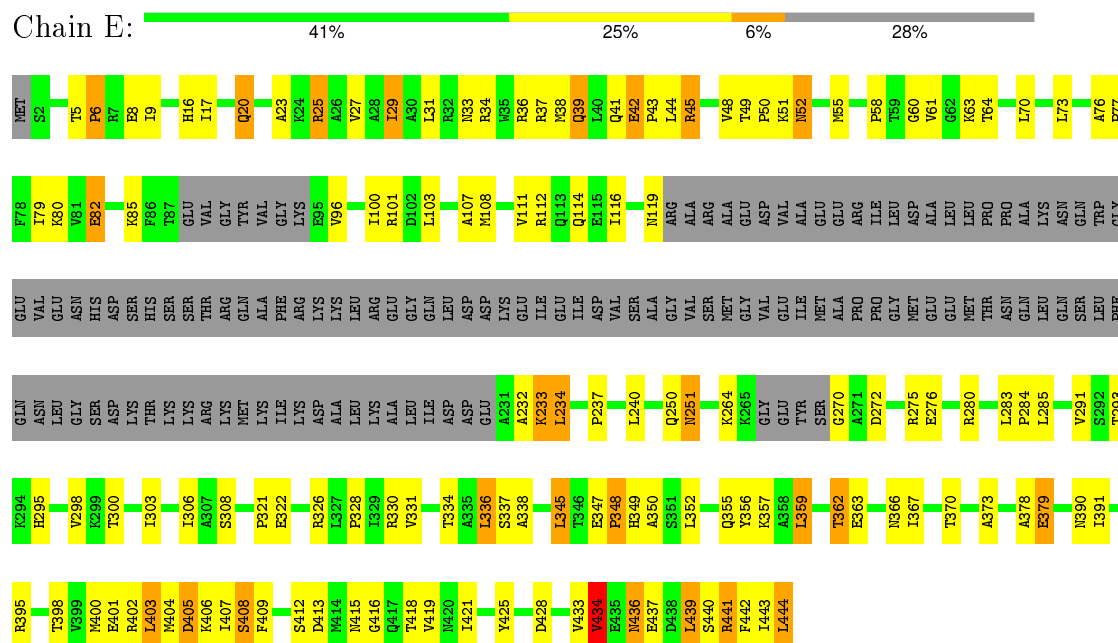


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	H	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	I	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	J	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	K	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	L	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	M	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	N	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	O	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	P	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	Q	1	Total 28	C 20	N 3	O 4	S 1	0	0
4	R	1	Total 28	C 20	N 3	O 4	S 1	0	0

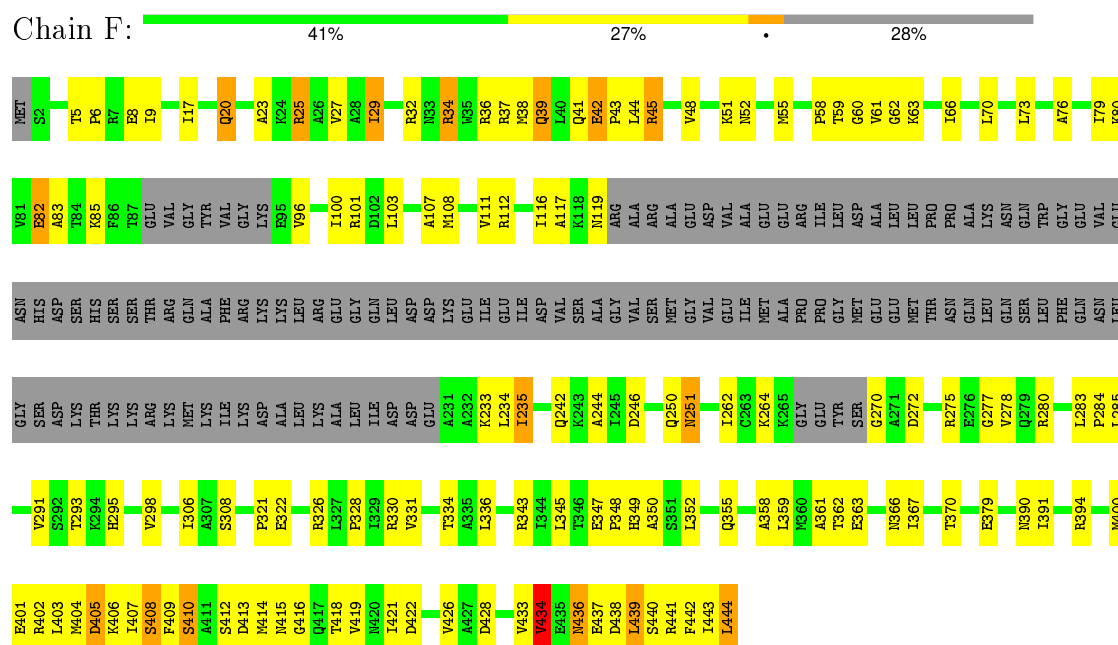




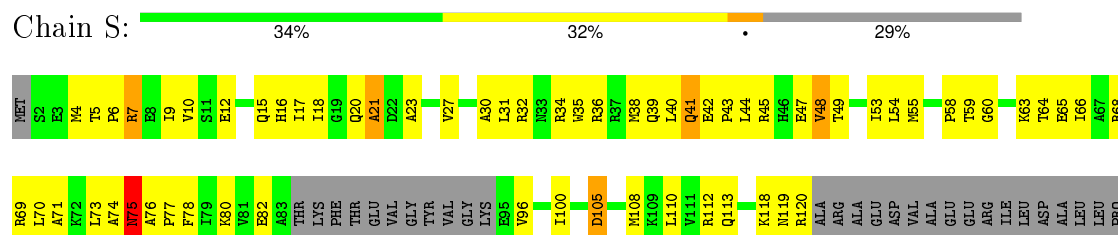


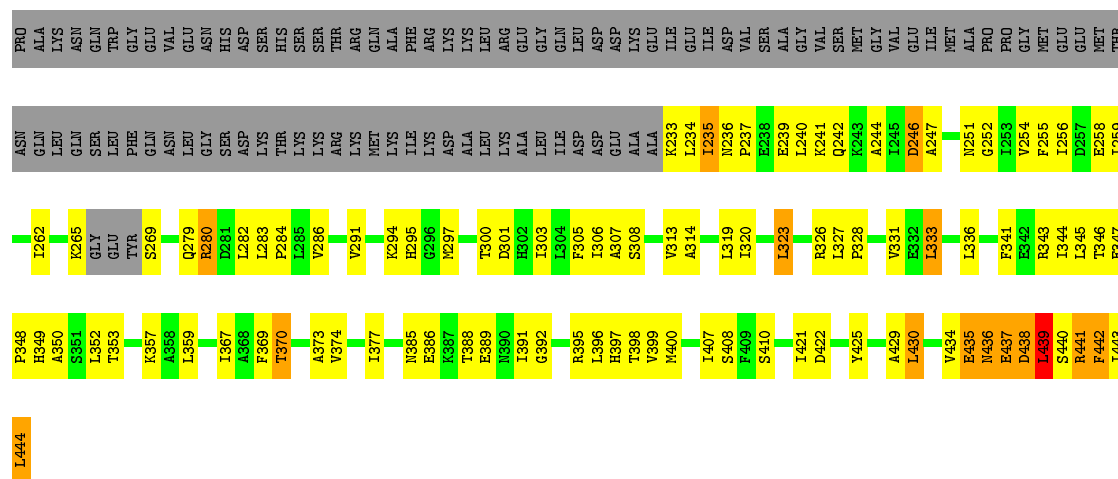


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

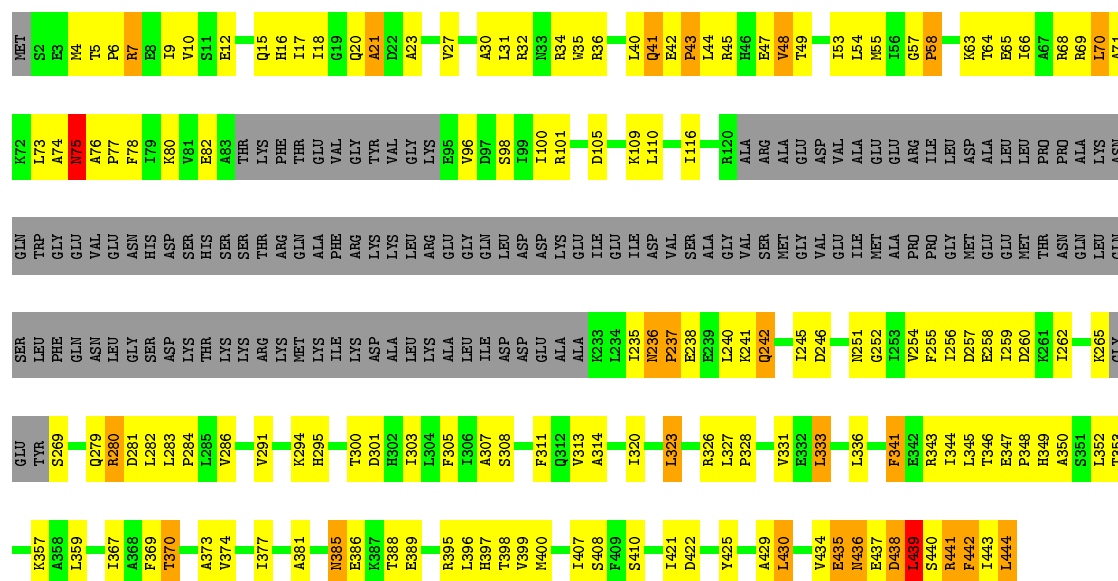


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU

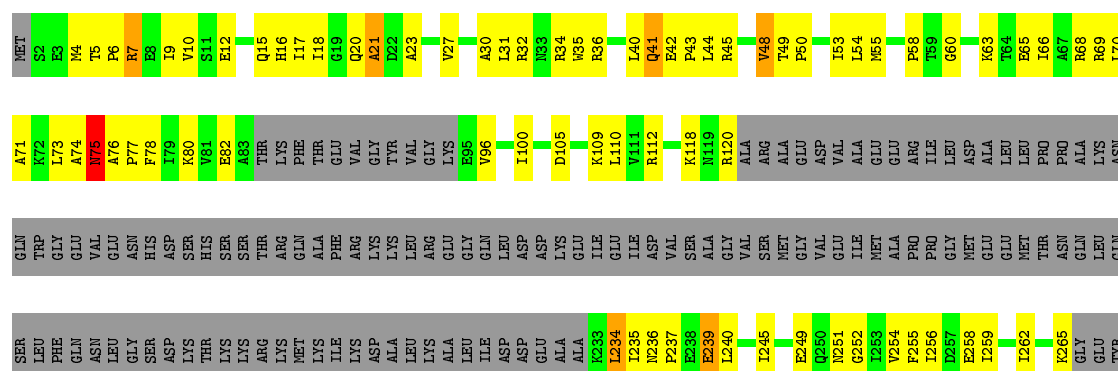


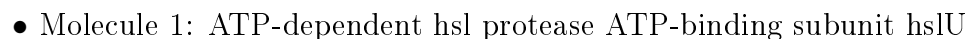


- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU



- Molecule 1: ATP-dependent hsl protease ATP-binding subunit hslU





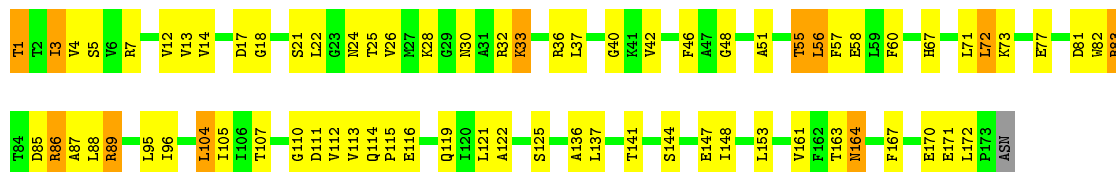
9%





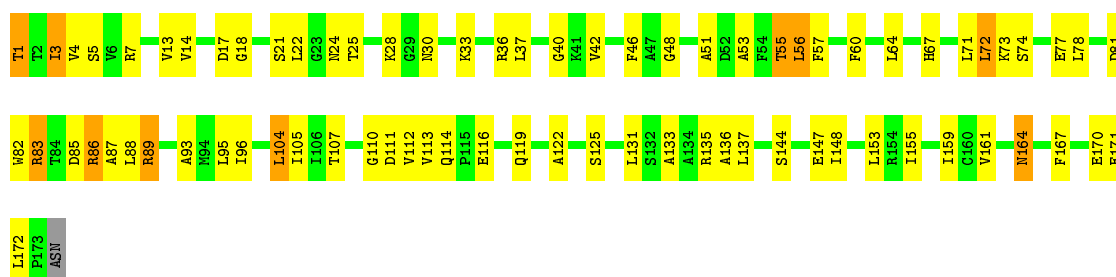
- Molecule 2: ATP-dependent protease hslV

Chain J: 57% 36% 6% .



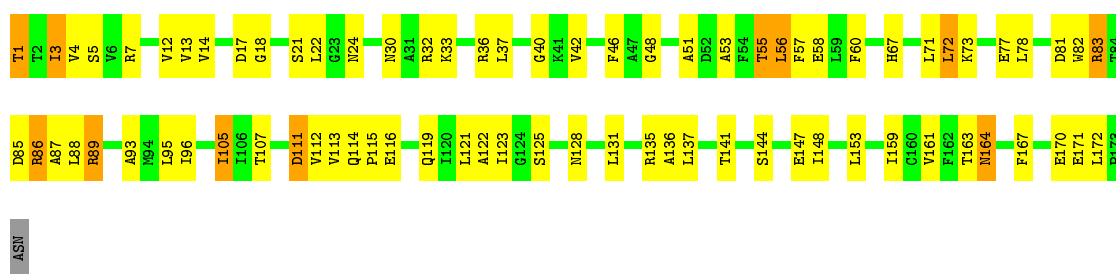
- Molecule 2: ATP-dependent protease hslV

Chain K: 56% 38% 6% .



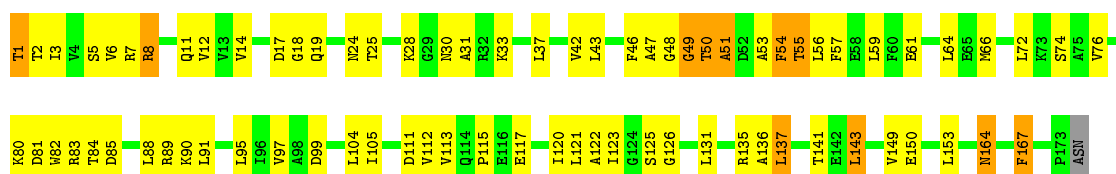
- Molecule 2: ATP-dependent protease hslV

Chain L: 55% 38% 6% .



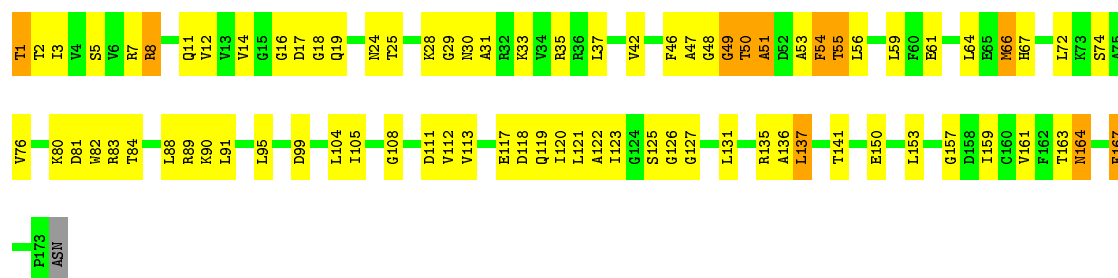
- Molecule 2: ATP-dependent protease hslV

Chain M: 55% 38% 6% .



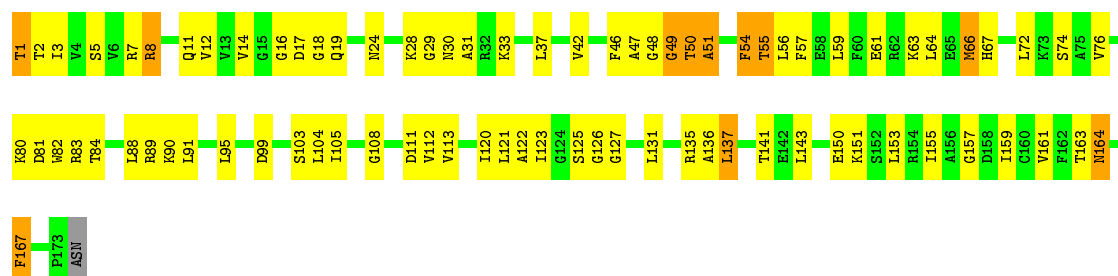
- Molecule 2: ATP-dependent protease hslV

Chain N: 53% 40% 6% .



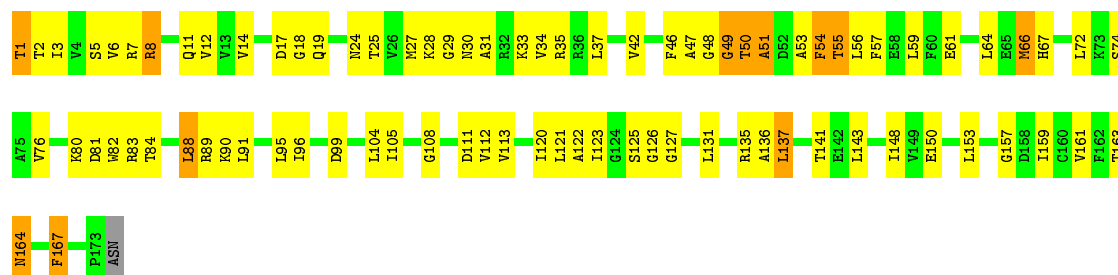
- Molecule 2: ATP-dependent protease hslV

Chain O: 53% 40% 6%



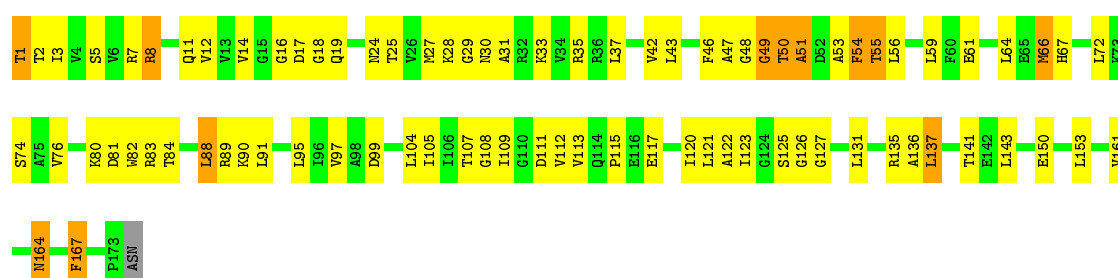
- Molecule 2: ATP-dependent protease hslV

Chain P: 51% 41% 7%



- Molecule 2: ATP-dependent protease hslV

Chain Q: 52% 41% 7%



- Molecule 2: ATP-dependent protease hslV

Chain R: 55% 38% 6%

T1	T2	T3	V4	S5	V6	R7	R8		Q11	V12	V13	V14		D17	G18	Q19		N24	T25		K28	G29	N30	A31	R32	R33	V34		L37		V42	L43		F46	A47	G48	G49	T50	A51	D52	A53	F54	T55	L56	F57	E58	L59	F60	E61		L64	E65	M66	H67		L72	K73	S74		A75
V76		K80	D81	W82	R83	T84		L88	R89	K90	L91		L95	T96	V97	A98	D99		L104	I105		G108			D111	V112	V113	Q114	P115		I120	L121	A122	I123	G124	S125	G126	G127		L131		R135	A136	L137		T141	E142	L143		E150		V161		N164	F167		P173	ASN		



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.51Å 219.97Å 242.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	92.9 (30.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.266 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.55	1/2515 (0.0%)	0.80	4/3391 (0.1%)
1	B	0.55	0/2515	0.75	2/3391 (0.1%)
1	C	0.56	0/2515	0.76	2/3391 (0.1%)
1	D	0.56	0/2515	0.75	2/3391 (0.1%)
1	E	0.57	0/2515	0.75	2/3391 (0.1%)
1	F	0.54	0/2515	0.74	3/3391 (0.1%)
1	S	0.29	0/2495	0.57	0/3360
1	T	0.30	0/2495	0.57	0/3360
1	U	0.30	0/2495	0.57	0/3360
1	V	0.30	0/2495	0.58	0/3360
1	W	0.30	0/2495	0.57	0/3360
1	X	0.29	0/2495	0.57	1/3360 (0.0%)
2	G	0.55	0/1304	0.77	0/1765
2	H	0.55	0/1304	0.77	0/1765
2	I	0.57	0/1304	0.79	0/1765
2	J	0.60	0/1304	0.80	0/1765
2	K	0.54	0/1304	0.77	0/1765
2	L	0.57	0/1304	0.79	0/1765
2	M	0.45	0/1275	0.70	0/1732
2	N	0.48	0/1275	0.72	0/1732
2	O	0.47	0/1275	0.70	0/1732
2	P	0.48	0/1275	0.72	0/1732
2	Q	0.46	0/1275	0.72	0/1732
2	R	0.48	1/1275 (0.1%)	0.71	0/1732
All	All	0.47	2/45534 (0.0%)	0.70	16/61488 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	1	THR	C-N	8.01	1.52	1.34
1	A	263	CYS	CB-SG	-5.19	1.73	1.81

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LEU	CA-CB-CG	10.08	138.48	115.30
1	A	234	LEU	N-CA-C	-8.40	88.32	111.00
1	A	436	ASN	N-CA-C	6.53	128.63	111.00
1	C	436	ASN	N-CA-C	6.45	128.41	111.00
1	B	436	ASN	N-CA-C	6.24	127.86	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2488	0	2546	148	0
1	B	2488	0	2546	150	0
1	C	2488	0	2546	144	0
1	D	2488	0	2546	142	0
1	E	2488	0	2546	136	0
1	F	2488	0	2546	142	0
1	S	2469	0	2540	159	0
1	T	2469	0	2540	148	0
1	U	2469	0	2540	155	0
1	V	2469	0	2540	154	0
1	W	2469	0	2540	144	0
1	X	2469	0	2540	154	1
2	G	1290	0	1288	98	0
2	H	1290	0	1288	103	0
2	I	1290	0	1288	108	0
2	J	1290	0	1288	108	0
2	K	1290	0	1288	99	0
2	L	1290	0	1288	103	0
2	M	1261	0	1239	105	0
2	N	1261	0	1239	106	0
2	O	1261	0	1239	106	0
2	P	1261	0	1239	122	0
2	Q	1261	0	1239	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1261	0	1239	106	0
3	A	31	0	12	3	0
3	B	31	0	12	5	0
3	C	31	0	12	8	0
3	D	31	0	12	5	0
3	E	31	0	12	6	0
3	F	31	0	12	4	0
3	S	31	0	12	3	0
3	T	31	0	12	4	0
3	U	31	0	12	5	0
3	V	31	0	12	2	0
3	W	31	0	12	4	0
3	X	31	0	12	3	0
4	G	28	0	36	15	0
4	H	28	0	36	14	0
4	I	28	0	36	16	0
4	J	28	0	36	22	0
4	K	28	0	36	17	0
4	L	28	0	36	14	0
4	M	28	0	36	12	0
4	N	28	0	36	15	0
4	O	28	0	36	11	0
4	P	28	0	36	12	0
4	Q	28	0	36	13	0
4	R	28	0	36	12	0
All	All	45756	0	46254	2818	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 31.

The worst 5 of 2818 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)
2:P:1:THR:HG21	2:P:33:LYS:CD	1.47	1.44
2:G:1:THR:CG2	2:G:33:LYS:CE	1.98	1.41
2:O:1:THR:HG21	2:O:33:LYS:CD	1.50	1.40
2:H:1:THR:HG21	2:H:33:LYS:CE	1.53	1.38
2:G:1:THR:HG21	2:G:33:LYS:CD	1.53	1.38

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ARG:NH2	1:X:7:ARG:NH2[2_765]	2.04	0.16

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	313/444 (70%)	261 (83%)	41 (13%)	11 (4%)	4	24
1	B	313/444 (70%)	258 (82%)	43 (14%)	12 (4%)	4	22
1	C	313/444 (70%)	261 (83%)	43 (14%)	9 (3%)	6	29
1	D	313/444 (70%)	270 (86%)	32 (10%)	11 (4%)	4	24
1	E	313/444 (70%)	266 (85%)	37 (12%)	10 (3%)	5	26
1	F	313/444 (70%)	264 (84%)	39 (12%)	10 (3%)	5	26
1	S	309/444 (70%)	235 (76%)	57 (18%)	17 (6%)	2	13
1	T	309/444 (70%)	238 (77%)	51 (16%)	20 (6%)	1	9
1	U	309/444 (70%)	235 (76%)	55 (18%)	19 (6%)	2	11
1	V	309/444 (70%)	237 (77%)	54 (18%)	18 (6%)	2	12
1	W	309/444 (70%)	233 (75%)	57 (18%)	19 (6%)	2	11
1	X	309/444 (70%)	237 (77%)	55 (18%)	17 (6%)	2	13
2	G	171/174 (98%)	157 (92%)	9 (5%)	5 (3%)	6	29
2	H	171/174 (98%)	153 (90%)	13 (8%)	5 (3%)	6	29
2	I	171/174 (98%)	154 (90%)	11 (6%)	6 (4%)	4	24
2	J	171/174 (98%)	154 (90%)	12 (7%)	5 (3%)	6	29
2	K	171/174 (98%)	154 (90%)	13 (8%)	4 (2%)	8	35
2	L	171/174 (98%)	155 (91%)	12 (7%)	4 (2%)	8	35
2	M	171/174 (98%)	145 (85%)	19 (11%)	7 (4%)	3	20
2	N	171/174 (98%)	143 (84%)	21 (12%)	7 (4%)	3	20
2	O	171/174 (98%)	141 (82%)	24 (14%)	6 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	171/174 (98%)	143 (84%)	22 (13%)	6 (4%)	4	24
2	Q	171/174 (98%)	142 (83%)	21 (12%)	8 (5%)	3	17
2	R	171/174 (98%)	144 (84%)	20 (12%)	7 (4%)	3	20
All	All	5784/7416 (78%)	4780 (83%)	761 (13%)	243 (4%)	3	19

5 of 243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	233	LYS
1	A	434	VAL
1	A	436	ASN
1	A	439	LEU

### 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	267/373 (72%)	241 (90%)	26 (10%)	10	36
1	B	267/373 (72%)	242 (91%)	25 (9%)	11	39
1	C	267/373 (72%)	248 (93%)	19 (7%)	18	54
1	D	267/373 (72%)	244 (91%)	23 (9%)	13	45
1	E	267/373 (72%)	242 (91%)	25 (9%)	11	39
1	F	267/373 (72%)	248 (93%)	19 (7%)	18	54
1	S	267/373 (72%)	253 (95%)	14 (5%)	29	65
1	T	267/373 (72%)	250 (94%)	17 (6%)	22	57
1	U	267/373 (72%)	255 (96%)	12 (4%)	34	70
1	V	267/373 (72%)	253 (95%)	14 (5%)	29	65
1	W	267/373 (72%)	249 (93%)	18 (7%)	20	56
1	X	267/373 (72%)	252 (94%)	15 (6%)	26	62
2	G	132/140 (94%)	116 (88%)	16 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	132/140 (94%)	118 (89%)	14 (11%)	8	31
2	I	132/140 (94%)	118 (89%)	14 (11%)	8	31
2	J	132/140 (94%)	116 (88%)	16 (12%)	6	24
2	K	132/140 (94%)	119 (90%)	13 (10%)	10	36
2	L	132/140 (94%)	117 (89%)	15 (11%)	7	28
2	M	125/140 (89%)	114 (91%)	11 (9%)	12	43
2	N	125/140 (89%)	115 (92%)	10 (8%)	15	48
2	O	125/140 (89%)	115 (92%)	10 (8%)	15	48
2	P	125/140 (89%)	114 (91%)	11 (9%)	12	43
2	Q	125/140 (89%)	114 (91%)	11 (9%)	12	43
2	R	125/140 (89%)	114 (91%)	11 (9%)	12	43
All	All	4746/6156 (77%)	4367 (92%)	379 (8%)	15	48

5 of 379 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	55	THR
2	L	21	SER
1	W	109	LYS
2	I	85	ASP
2	J	86	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	24	ASN
1	S	279	GLN
1	X	16	HIS
2	L	146	HIS
2	Q	164	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 ⓘ

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	$\# Z  > 2$
3	ATP	A	450	-	24,33,33	0.74	0	31,52,52	1.10	2 (6%)
3	ATP	B	451	-	24,33,33	0.70	0	31,52,52	1.17	4 (12%)
3	ATP	C	452	-	24,33,33	0.64	0	31,52,52	1.36	4 (12%)
3	ATP	D	453	-	24,33,33	0.66	0	31,52,52	1.37	4 (12%)
3	ATP	E	454	-	24,33,33	0.82	1 (4%)	31,52,52	1.36	2 (6%)
3	ATP	F	455	-	24,33,33	0.79	1 (4%)	31,52,52	1.08	2 (6%)
4	LVS	G	175	2	25,27,42	3.07	4 (16%)	31,37,59	1.14	2 (6%)
4	LVS	H	175	2	25,27,42	2.86	4 (16%)	31,37,59	1.02	2 (6%)
4	LVS	I	175	2	25,27,42	2.69	3 (12%)	31,37,59	1.23	2 (6%)
4	LVS	J	175	2	25,27,42	3.01	4 (16%)	31,37,59	1.22	3 (9%)
4	LVS	K	175	2	25,27,42	3.06	3 (12%)	31,37,59	1.22	2 (6%)
4	LVS	L	175	2	25,27,42	2.90	4 (16%)	31,37,59	1.06	2 (6%)
4	LVS	M	175	2	25,27,42	3.02	4 (16%)	31,37,59	1.35	5 (16%)
4	LVS	N	175	2	25,27,42	3.25	3 (12%)	31,37,59	1.38	5 (16%)
4	LVS	O	175	2	25,27,42	3.12	3 (12%)	31,37,59	1.39	5 (16%)
4	LVS	P	175	2	25,27,42	3.23	4 (16%)	31,37,59	1.37	5 (16%)
4	LVS	Q	175	2	25,27,42	3.03	4 (16%)	31,37,59	1.33	5 (16%)
4	LVS	R	175	2	25,27,42	3.17	4 (16%)	31,37,59	1.43	5 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	S	456	-	24,33,33	0.61	0	31,52,52	0.91	1 (3%)
3	ATP	T	457	-	24,33,33	0.58	0	31,52,52	0.84	1 (3%)
3	ATP	U	458	-	24,33,33	0.58	0	31,52,52	0.89	1 (3%)
3	ATP	V	459	-	24,33,33	0.62	0	31,52,52	0.91	1 (3%)
3	ATP	W	460	-	24,33,33	0.61	0	31,52,52	0.91	1 (3%)
3	ATP	X	461	-	24,33,33	0.58	0	31,52,52	0.93	2 (6%)

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	450	-	-	0/18/38/38	0/3/3/3
3	ATP	B	451	-	-	0/18/38/38	0/3/3/3
3	ATP	C	452	-	-	0/18/38/38	0/3/3/3
3	ATP	D	453	-	-	0/18/38/38	0/3/3/3
3	ATP	E	454	-	-	0/18/38/38	0/3/3/3
3	ATP	F	455	-	-	0/18/38/38	0/3/3/3
4	LVS	G	175	2	-	1/33/34/46	0/0/0/1
4	LVS	H	175	2	-	1/33/34/46	0/0/0/1
4	LVS	I	175	2	-	1/33/34/46	0/0/0/1
4	LVS	J	175	2	-	1/33/34/46	0/0/0/1
4	LVS	K	175	2	-	1/33/34/46	0/0/0/1
4	LVS	L	175	2	-	1/33/34/46	0/0/0/1
4	LVS	M	175	2	-	1/33/34/46	0/0/0/1
4	LVS	N	175	2	-	1/33/34/46	0/0/0/1
4	LVS	O	175	2	-	1/33/34/46	0/0/0/1
4	LVS	P	175	2	-	1/33/34/46	0/0/0/1
4	LVS	Q	175	2	-	1/33/34/46	0/0/0/1
4	LVS	R	175	2	-	1/33/34/46	0/0/0/1
3	ATP	S	456	-	-	0/18/38/38	0/3/3/3
3	ATP	T	457	-	-	0/18/38/38	0/3/3/3
3	ATP	U	458	-	-	0/18/38/38	0/3/3/3
3	ATP	V	459	-	-	0/18/38/38	0/3/3/3
3	ATP	W	460	-	-	0/18/38/38	0/3/3/3
3	ATP	X	461	-	-	0/18/38/38	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	454	ATP	C8-N7	-2.27	1.30	1.34
3	F	455	ATP	C8-N7	-2.13	1.30	1.34
4	R	175	LVS	O1'-S	2.23	1.46	1.44
4	O	175	LVS	O1'-S	2.50	1.47	1.44
4	M	175	LVS	C1'-S	2.65	1.79	1.76

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	454	ATP	C2'-C1'-N9	-5.45	105.97	114.29
3	D	453	ATP	C2'-C1'-N9	-4.68	107.14	114.29
3	C	452	ATP	C2'-C1'-N9	-4.51	107.40	114.29
4	I	175	LVS	O2'-S-O1'	-4.20	107.18	117.56
4	J	175	LVS	O2'-S-O1'	-3.98	107.71	117.56

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	175	LVS	CA3-CS-C2'-S
4	Q	175	LVS	CA3-CS-C2'-S
4	O	175	LVS	CA3-CS-C2'-S
4	M	175	LVS	CA3-CS-C2'-S
4	P	175	LVS	CA3-CS-C2'-S

There are no ring outliers.

24 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	ATP	3	0
3	B	451	ATP	5	0
3	C	452	ATP	8	0
3	D	453	ATP	5	0
3	E	454	ATP	6	0
3	F	455	ATP	4	0
4	G	175	LVS	15	0
4	H	175	LVS	14	0
4	I	175	LVS	16	0
4	J	175	LVS	22	0
4	K	175	LVS	17	0
4	L	175	LVS	14	0
4	M	175	LVS	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	175	LVS	15	0
4	O	175	LVS	11	0
4	P	175	LVS	12	0
4	Q	175	LVS	13	0
4	R	175	LVS	12	0
3	S	456	ATP	3	0
3	T	457	ATP	4	0
3	U	458	ATP	5	0
3	V	459	ATP	2	0
3	W	460	ATP	4	0
3	X	461	ATP	3	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.