



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:39 am GMT

PDB ID : 1OFH  
Title : ASYMMETRIC COMPLEX BETWEEN HSLV AND I-DOMAIN DELETED  
HSLU (H. INFLUENZAE)  
Authors : Kwon, A.R.; Kessler, B.M.; Overkleeft, H.S.; Mckay, D.B.  
Deposited on : 2003-04-14  
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

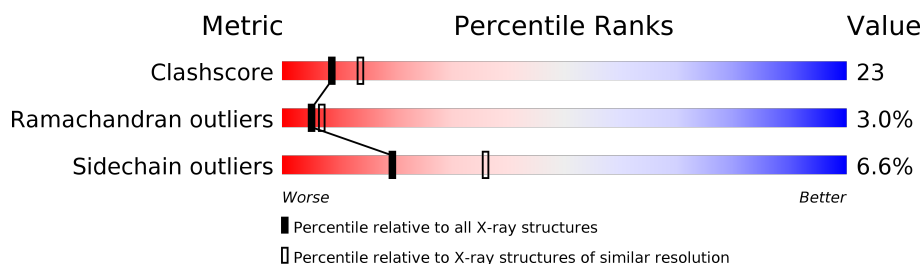
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)



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	310	<div> <div>65%</div> <div>28%</div> <div>7%</div> </div>
1	B	310	<div> <div>67%</div> <div>28%</div> <div>5%</div> </div>
1	C	310	<div> <div>72%</div> <div>23%</div> <div>5%</div> </div>
2	G	174	<div> <div>56%</div> <div>36%</div> <div>7%</div> </div>
2	H	174	<div> <div>60%</div> <div>34%</div> <div>6%</div> </div>
2	I	174	<div> <div>67%</div> <div>26%</div> <div>7%</div> </div>
2	L	174	<div> <div>54%</div> <div>41%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	M	174	 55% 41% .
2	N	174	 55% 40% 5%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15254 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 SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			
1	B	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			
1	C	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	H	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	I	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	L	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	M	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	N	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

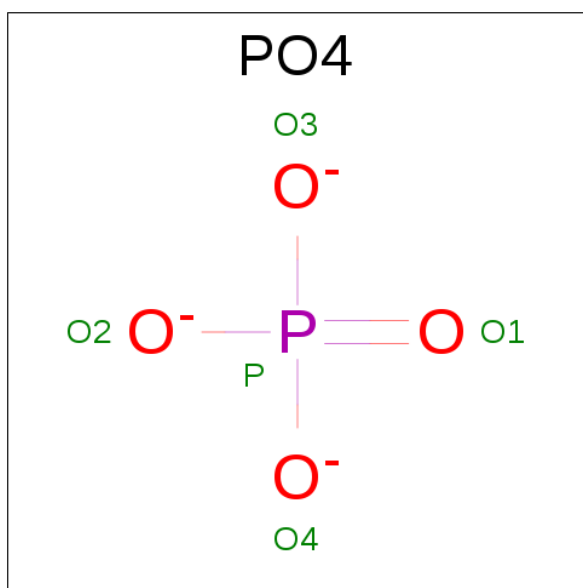


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	I	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	N	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

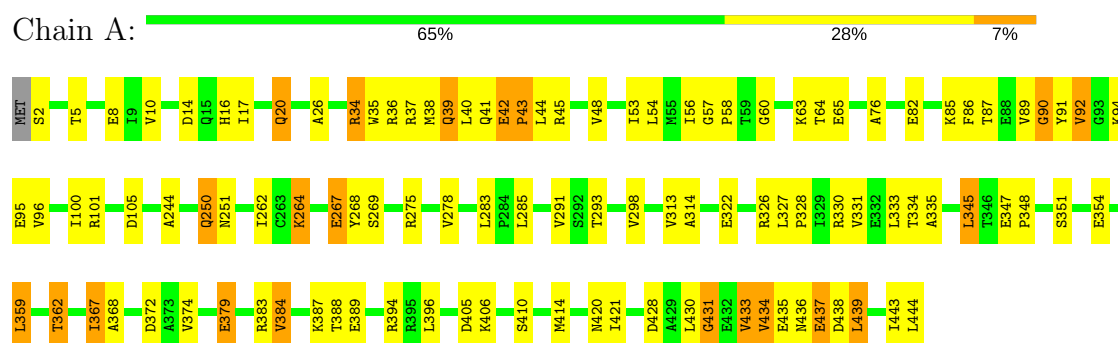
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	28	Total	O	0	0
			28	28		
6	C	31	Total	O	0	0
			31	31		
6	M	1	Total	O	0	0
			1	1		

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

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

Note EDS was not executed.

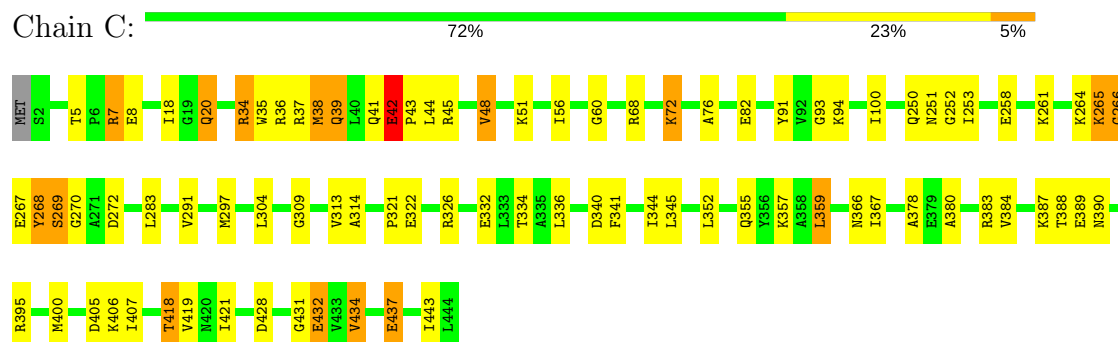
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



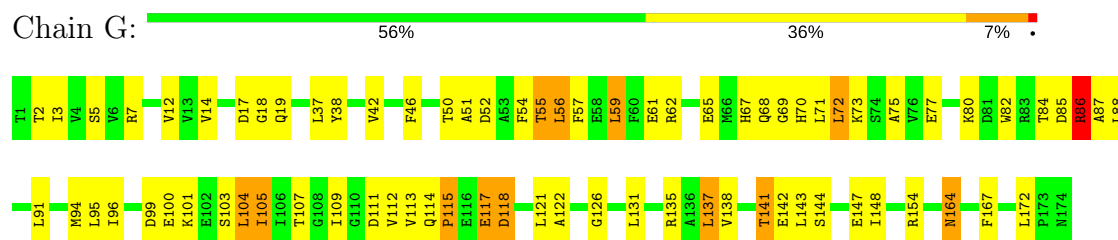
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



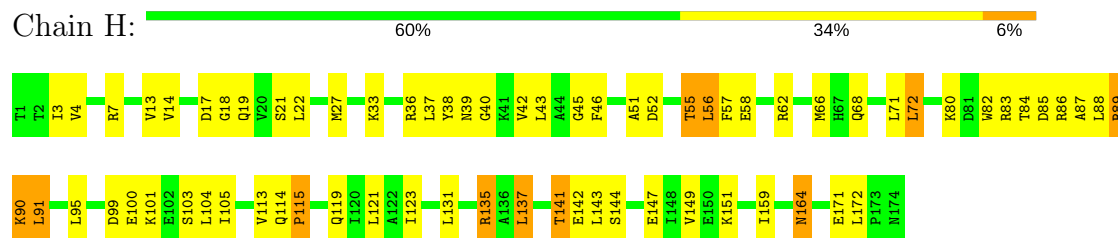
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



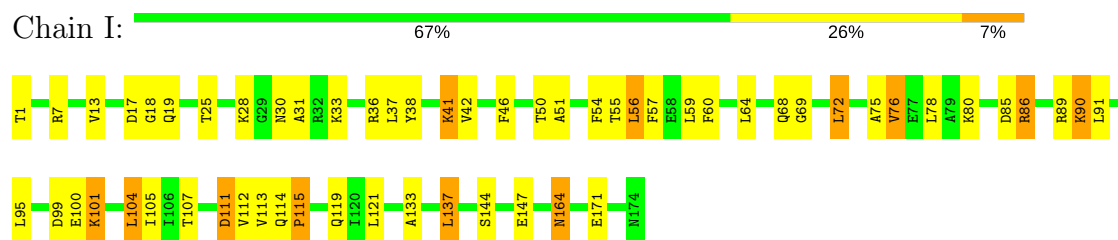
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



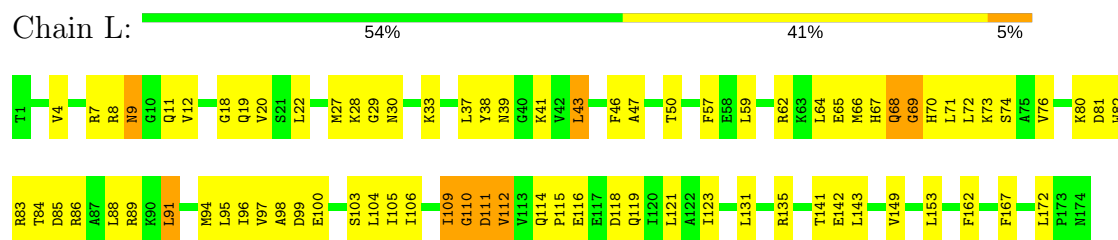
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



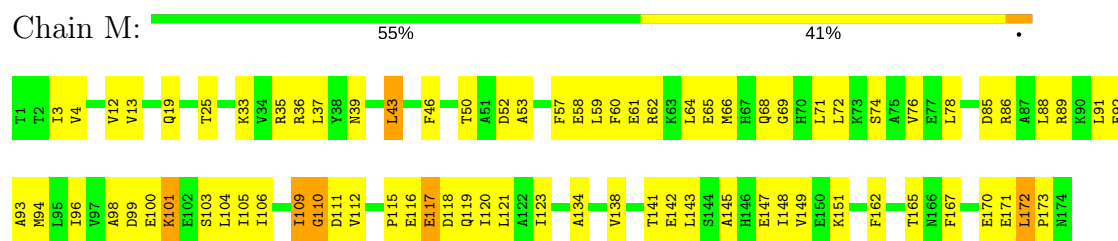
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV





T1	T2	I3	V4	R7	V12	V13	G16	Q19	N30	K33	R36	L37	Y38	K41	V42	G45	F46	T50	A51	D52	A53	F54	T55	L56	F60	L64	Q68	G69	H70	L71	L72	K73	S74	A75	V76	E77	L78	A79	K80	D81	N82	R83	T84	D85	R86	A87
L88	R89	K90	L91	E92	A93	I96	D99	E100	S103	L104	I105	G110	D111	Q114	P115	E116	E117	D118	Q119	I120	L121	A122	A133	A136	L137	V138	E139	N140	S144	E147	I148	V149	L153	I159	F162	T163	N164	T165	N166	F167	E171	L172	P173	N174		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.22Å 192.22Å 115.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.0 (40.00-2.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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: PO4, MG, 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	0.39	0/2415	0.62	0/3261
1	B	0.42	0/2415	0.64	0/3261
1	C	0.41	0/2415	0.63	0/3261
2	G	0.35	0/1333	0.60	0/1798
2	H	0.34	0/1333	0.61	0/1798
2	I	0.34	0/1333	0.62	0/1798
2	L	0.30	0/1333	0.54	0/1798
2	M	0.32	0/1333	0.55	0/1798
2	N	0.31	0/1333	0.58	0/1798
All	All	0.37	0/15243	0.61	0/20571

There are no bond length outliers.

There are no bond angle outliers.

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	2384	0	2425	98	0
1	B	2384	0	2425	88	0
1	C	2384	0	2425	86	0
2	G	1319	0	1348	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1319	0	1348	80	0
2	I	1319	0	1348	57	0
2	L	1319	0	1348	91	0
2	M	1319	0	1348	78	0
2	N	1319	0	1348	77	0
3	A	27	0	12	4	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	20	0	0	0	0
6	B	28	0	0	3	0
6	C	31	0	0	0	0
6	M	1	0	0	0	0
All	All	15254	0	15399	692	0

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 23.

The worst 5 of 692 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:G:141:THR:HG23	2:G:143:LEU:H	1.17	1.08
1:A:406:LYS:HD2	1:A:406:LYS:H	1.21	1.04
2:H:83:ARG:HG3	2:I:55:THR:HG22	1.42	0.98
1:C:406:LYS:H	1:C:406:LYS:HD2	1.25	0.98
1:C:443:ILE:HD11	2:I:72:LEU:HD11	1.48	0.96

There are no symmetry-related clashes.

## 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	307/310 (99%)	277 (90%)	19 (6%)	11 (4%)	4	5
1	B	307/310 (99%)	283 (92%)	16 (5%)	8 (3%)	6	9
1	C	307/310 (99%)	281 (92%)	18 (6%)	8 (3%)	6	9
2	G	172/174 (99%)	153 (89%)	15 (9%)	4 (2%)	7	11
2	H	172/174 (99%)	157 (91%)	12 (7%)	3 (2%)	11	18
2	I	172/174 (99%)	158 (92%)	13 (8%)	1 (1%)	28	48
2	L	172/174 (99%)	144 (84%)	21 (12%)	7 (4%)	3	4
2	M	172/174 (99%)	149 (87%)	15 (9%)	8 (5%)	3	3
2	N	172/174 (99%)	144 (84%)	20 (12%)	8 (5%)	3	3
All	All	1953/1974 (99%)	1746 (89%)	149 (8%)	58 (3%)	5	7

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	VAL
1	A	434	VAL
1	A	437	GLU
1	A	439	LEU
1	B	267	GLU

### 5.3.2 Protein sidechains [i](#)

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	255/256 (100%)	235 (92%)	20 (8%)	15	28
1	B	255/256 (100%)	234 (92%)	21 (8%)	13	25
1	C	255/256 (100%)	237 (93%)	18 (7%)	17	32
2	G	139/140 (99%)	127 (91%)	12 (9%)	12	23
2	H	139/140 (99%)	129 (93%)	10 (7%)	17	31
2	I	139/140 (99%)	125 (90%)	14 (10%)	9	17
2	L	139/140 (99%)	137 (99%)	2 (1%)	71	90
2	M	139/140 (99%)	136 (98%)	3 (2%)	57	82
2	N	139/140 (99%)	134 (96%)	5 (4%)	40	67
All	All	1599/1608 (99%)	1494 (93%)	105 (7%)	19	36

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	VAL
1	C	437	GLU
2	M	39	ASN
1	C	72	LYS
1	C	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	GLN
2	G	19	GLN
2	N	70	HIS
1	C	41	GLN
1	C	52	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	ADP	A	450	4	25,29,29	2.55	9 (36%)	24,45,45	2.24	3 (12%)
5	PO4	A	452	4	4,4,4	1.13	0	6,6,6	0.40	0
3	ADP	B	450	4	25,29,29	2.43	8 (32%)	24,45,45	2.26	2 (8%)
5	PO4	B	452	4	4,4,4	1.17	0	6,6,6	0.39	0
3	ADP	C	450	4	25,29,29	2.53	9 (36%)	24,45,45	2.33	3 (12%)
5	PO4	C	452	4	4,4,4	1.05	0	6,6,6	0.43	0

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	ADP	A	450	4	-	0/12/32/32	0/3/3/3
5	PO4	A	452	4	-	0/0/0/0	0/0/0/0
3	ADP	B	450	4	-	0/12/32/32	0/3/3/3
5	PO4	B	452	4	-	0/0/0/0	0/0/0/0
3	ADP	C	450	4	-	0/12/32/32	0/3/3/3
5	PO4	C	452	4	-	0/0/0/0	0/0/0/0

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	450	ADP	C8-N7	-3.47	1.28	1.34
3	B	450	ADP	C8-N7	-3.09	1.28	1.34
3	A	450	ADP	C8-N7	-2.96	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	450	ADP	C5-C4	-2.35	1.35	1.40
3	A	450	ADP	C5-C4	-2.02	1.35	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	450	ADP	N3-C2-N1	-10.01	120.14	128.86
3	B	450	ADP	N3-C2-N1	-9.77	120.35	128.86
3	A	450	ADP	N3-C2-N1	-9.69	120.42	128.86
3	C	450	ADP	O5'-PA-O1A	-2.25	100.15	109.25
3	A	450	ADP	O5'-PA-O1A	-2.02	101.09	109.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	ADP	4	0
3	B	450	ADP	1	0
3	C	450	ADP	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.