



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2018 – 04:47 PM EDT

PDB ID : 1HQY
Title : Nucleotide-Dependent Conformational Changes in a Protease-Associated ATPase HslU
Authors : Wang, J.; Song, J.J.; Seong, I.S.; Franklin, M.C.; Kamtekar, S.; Eom, S.H.; Chung, C.H.
Deposited on : 2000-12-20
Resolution : 2.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

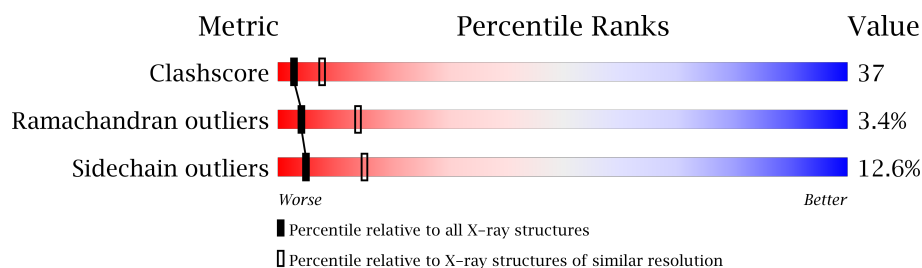
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	C	175	
1	D	175	
2	E	449	
2	F	449	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11818 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 HEAT SHOCK LOCUS HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	B	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	C	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	D	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			

- Molecule 2 is a protein called HEAT SHOCK LOCUS HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	F	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			

There are 14 discrepancies between the modelled and reference sequences:

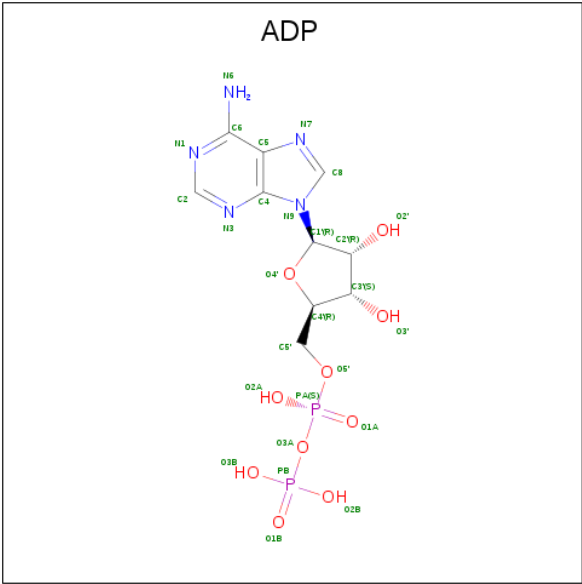
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	1	HIS	-	EXPRESSION TAG	UNP P0A6H5

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

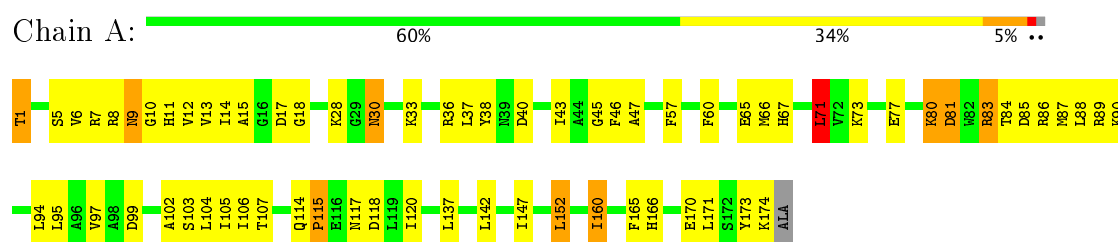


3 Residue-property plots

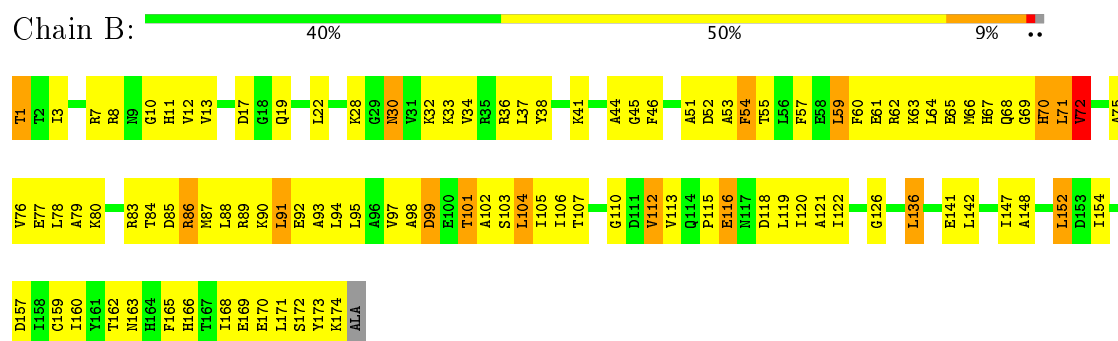
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

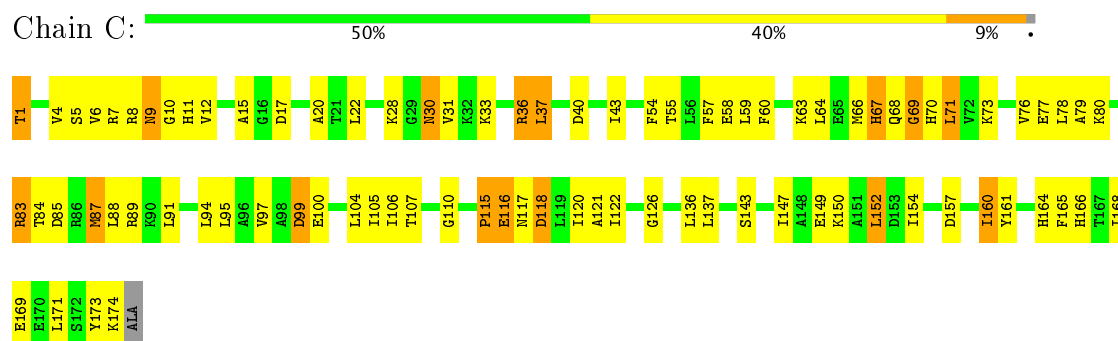
• Molecule 1: HEAT SHOCK LOCUS HSLV



• Molecule 1: HEAT SHOCK LOCUS HSLV

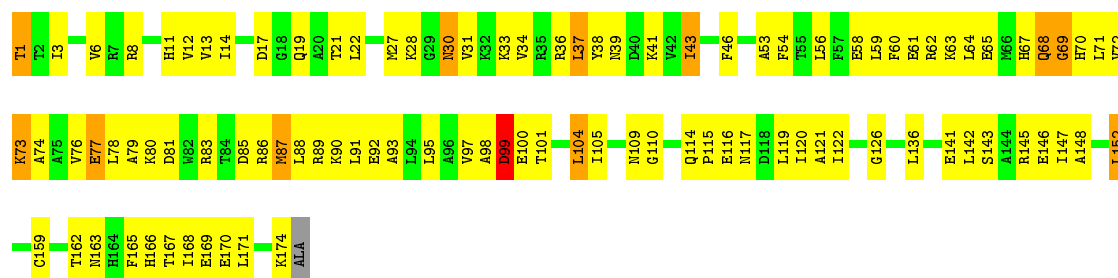


• Molecule 1: HEAT SHOCK LOCUS HSLV



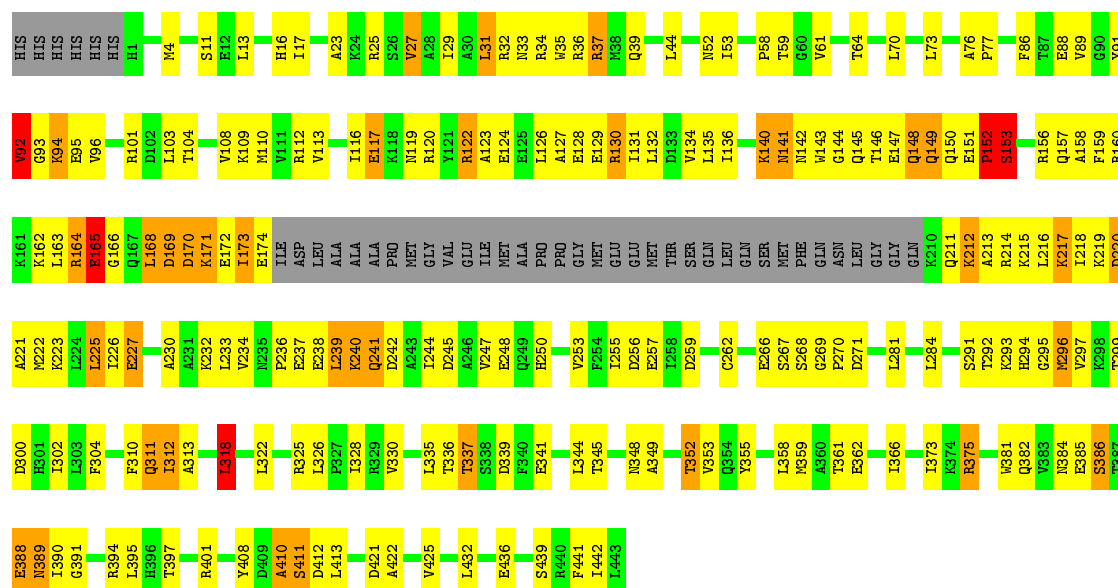
• Molecule 1: HEAT SHOCK LOCUS HSLV





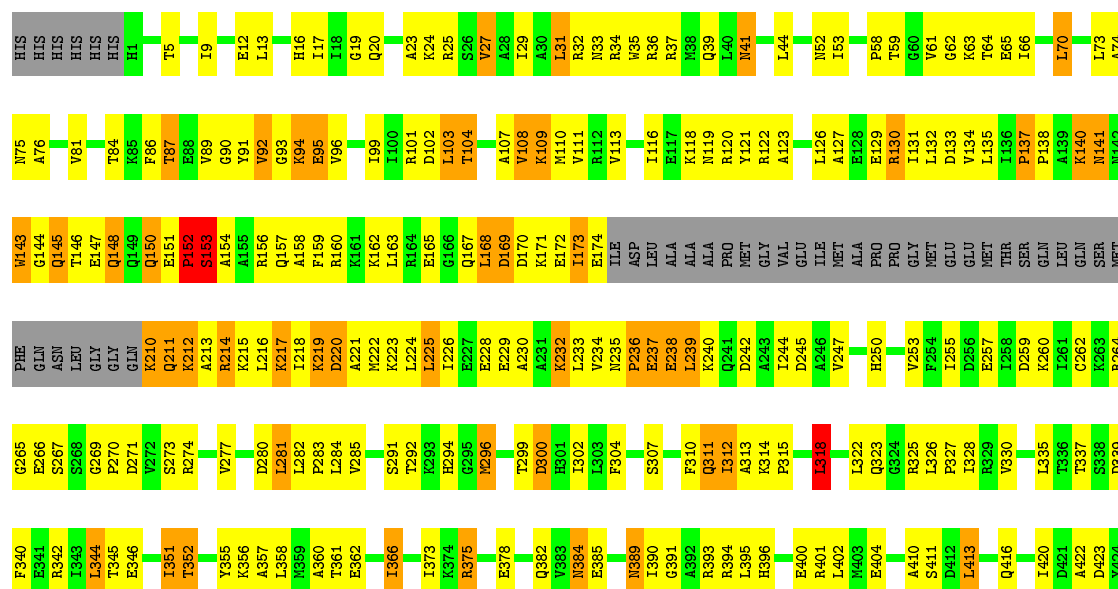
• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain E: 45% 37% 8% 9%



• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain F: 39% 40% 11% 9%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.02Å 172.02Å 276.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.62 – 2.80	Depositor
% Data completeness (in resolution range)	92.2 (29.62-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.287 , 0.333	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11818	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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: 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	0.47	0/1345	0.72	0/1817
1	B	0.43	0/1345	0.69	0/1817
1	C	0.38	0/1345	0.68	0/1817
1	D	0.38	0/1345	0.64	0/1817
2	E	0.46	2/3266 (0.1%)	0.72	4/4400 (0.1%)
2	F	0.48	2/3266 (0.1%)	0.72	5/4400 (0.1%)
All	All	0.45	4/11912 (0.0%)	0.70	9/16068 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	152	PRO	CA-C	-7.24	1.38	1.52
2	F	152	PRO	CA-C	-6.39	1.40	1.52
2	E	153	SER	N-CA	-6.12	1.34	1.46
2	F	152	PRO	C-N	-5.72	1.21	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	152	PRO	CA-N-CD	-8.50	99.61	111.50
2	E	152	PRO	C-N-CA	-7.76	102.31	121.70
2	F	153	SER	CB-CA-C	7.51	124.38	110.10
2	F	153	SER	C-N-CA	6.99	139.17	121.70
2	E	153	SER	CB-CA-C	6.80	123.03	110.10

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	1328	0	1348	73	0
1	B	1328	0	1348	103	0
1	C	1328	0	1348	83	0
1	D	1328	0	1348	111	0
2	E	3226	0	3293	257	0
2	F	3226	0	3293	286	0
3	E	27	0	12	1	0
3	F	27	0	12	3	0
All	All	11818	0	12002	889	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 37.

The worst 5 of 889 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:F:152:PRO:HB2	2:F:156:ARG:HB2	1.30	1.11
2:E:152:PRO:HB2	2:E:156:ARG:HB2	1.27	1.10
2:E:170:ASP:HA	2:E:217:LYS:HA	1.34	1.06
2:E:174:GLU:HB3	2:E:211:GLN:HG3	1.38	1.05
2:E:312:ILE:HD13	2:E:312:ILE:H	1.20	1.02

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	172/175 (98%)	148 (86%)	19 (11%)	5 (3%)	5	17
1	B	172/175 (98%)	138 (80%)	25 (14%)	9 (5%)	2	7
1	C	172/175 (98%)	150 (87%)	18 (10%)	4 (2%)	7	23
1	D	172/175 (98%)	140 (81%)	28 (16%)	4 (2%)	7	23
2	E	404/449 (90%)	355 (88%)	36 (9%)	13 (3%)	4	15
2	F	404/449 (90%)	340 (84%)	48 (12%)	16 (4%)	3	10
All	All	1496/1598 (94%)	1271 (85%)	174 (12%)	51 (3%)	4	14

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
1	D	69	GLY
2	E	92	VAL
2	E	144	GLY
2	E	146	THR

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	136/136 (100%)	127 (93%)	9 (7%)	18	47
1	B	136/136 (100%)	119 (88%)	17 (12%)	5	15
1	C	136/136 (100%)	121 (89%)	15 (11%)	7	21
1	D	136/136 (100%)	122 (90%)	14 (10%)	8	23
2	E	350/383 (91%)	305 (87%)	45 (13%)	5	14
2	F	350/383 (91%)	293 (84%)	57 (16%)	2	8
All	All	1244/1310 (95%)	1087 (87%)	157 (13%)	5	15

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	165	GLU

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Mol	Chain	Res	Type
2	E	326	LEU
2	F	352	THR
2	E	169	ASP
2	E	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	311	GLN
2	E	416	GLN
2	F	384	ASN
2	E	382	GLN
2	E	428	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 ⓘ

2 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	ADP	E	450	-	25,29,29	1.64	6 (24%)	25,45,45	1.90	4 (16%)
3	ADP	F	1450	-	25,29,29	1.60	4 (16%)	25,45,45	1.89	3 (12%)

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	E	450	-	-	0/12/32/32	0/3/3/3
3	ADP	F	1450	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1450	ADP	C8-N7	-4.18	1.27	1.34
3	E	450	ADP	C8-N7	-4.17	1.27	1.34
3	E	450	ADP	PB-O3A	-2.94	1.55	1.60
3	F	1450	ADP	C8-N9	-2.70	1.33	1.36
3	E	450	ADP	C8-N9	-2.48	1.33	1.36

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1450	ADP	N3-C2-N1	-4.63	124.90	128.86
3	E	450	ADP	N3-C2-N1	-4.27	125.20	128.86
3	E	450	ADP	O2A-PA-O1A	2.04	122.52	112.14
3	F	1450	ADP	C2'-C3'-C4'	3.15	108.66	102.62
3	E	450	ADP	C2'-C3'-C4'	3.23	108.81	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	450	ADP	1	0
3	F	1450	ADP	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.