



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DO2
Title : TRIGONAL CRYSTAL FORM OF HEAT SHOCK LOCUS U (HSLU) FROM
ESCHERICHIA COLI
Authors : Bochtler, M.; Hartmann, C.; Song, H.K.; Bourenkov, G.P.; Bartunik, H.D.
Deposited on : 1999-12-18
Resolution : 4.00 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
<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 (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

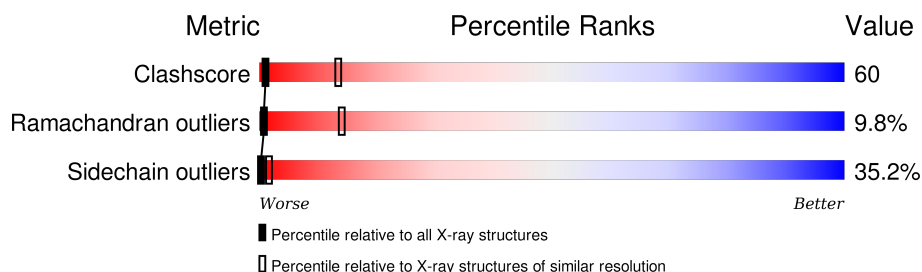
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	442	
1	B	442	
1	C	442	
1	D	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	ANP	A	900	-	-	X	-
2	ANP	C	905	-	-	X	-

2 Entry composition [i](#)

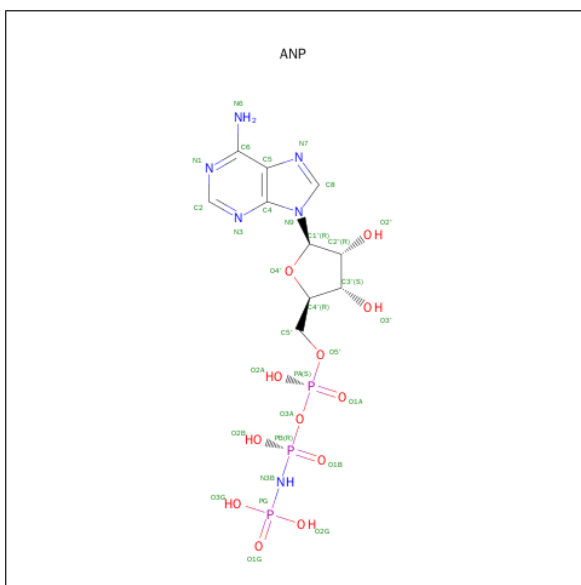
There are 2 unique types of molecules in this entry. The entry contains 12926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (HEAT SHOCK LOCUS U).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	126	0	0
			3216	2008	574	624	10			
1	B	407	Total	C	N	O	S	492	0	0
			3216	2008	574	624	10			
1	C	407	Total	C	N	O	S	103	0	0
			3216	2008	574	624	10			
1	D	407	Total	C	N	O	S	484	0	0
			3216	2008	574	624	10			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

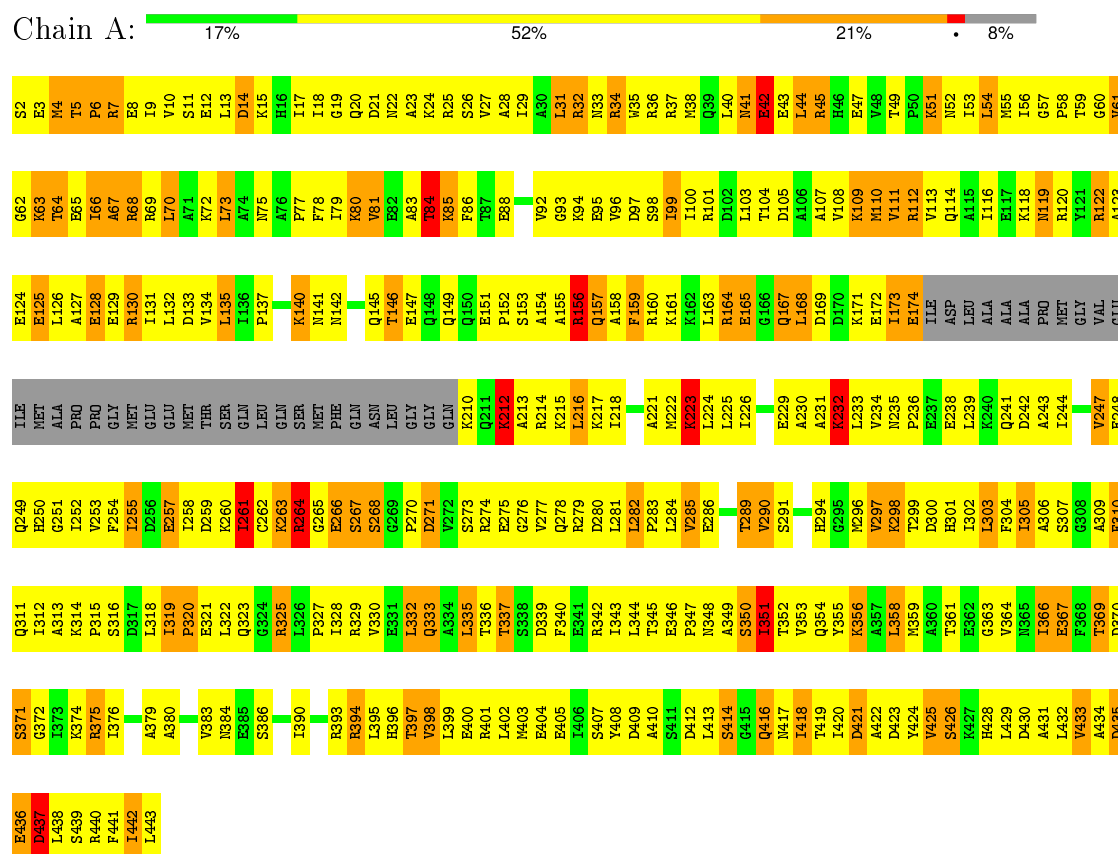


3 Residue-property plots

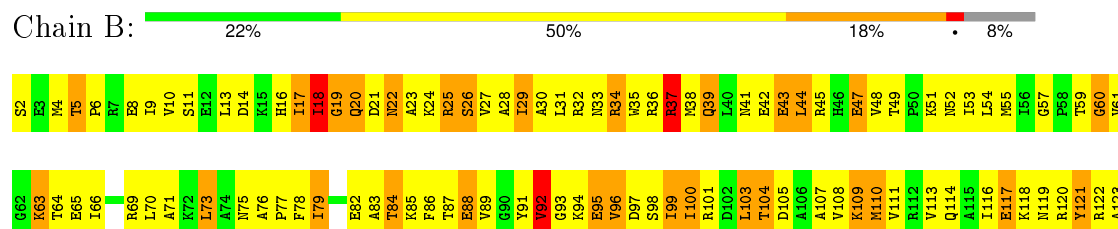
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

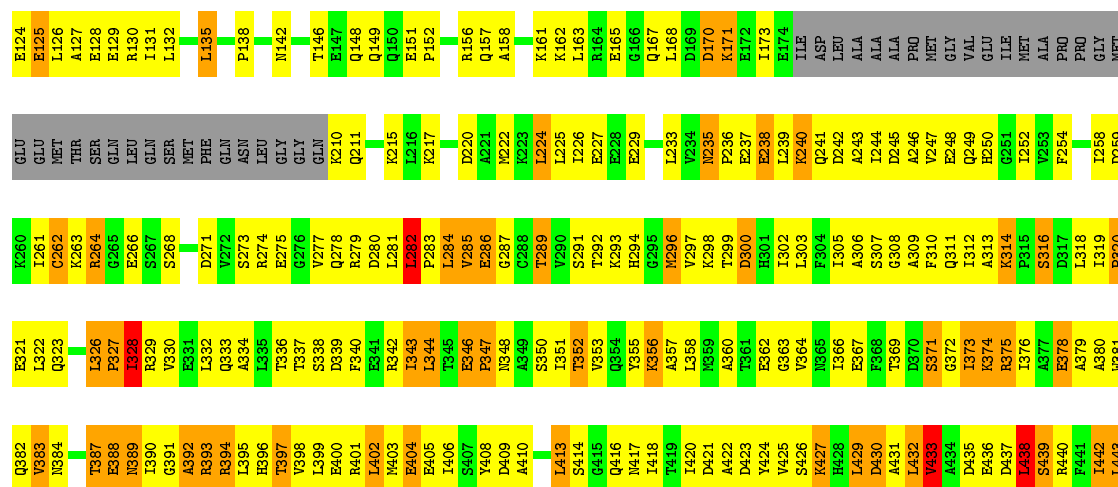
Note EDS was not executed.

• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)



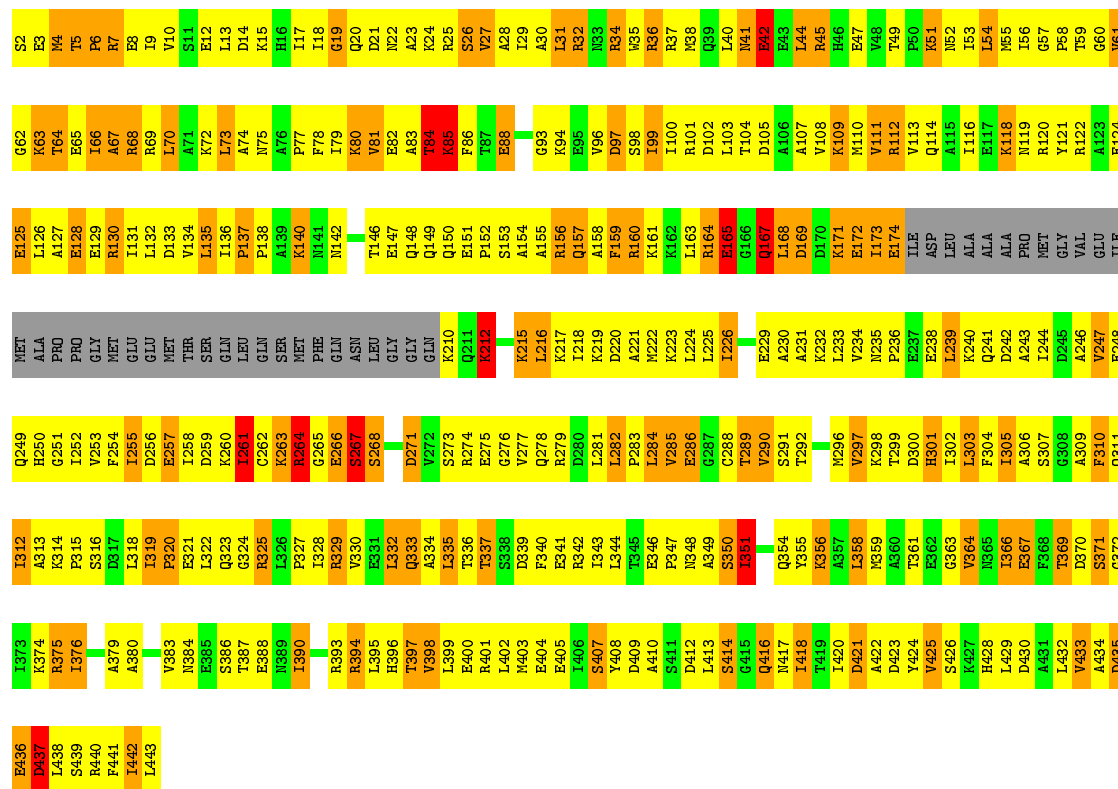
• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)





• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

Chain C: 16% 50% 24% 8%



• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

Chain D: 21% 53% 16% 8%



A379	A380	H381	Q382	V383	N384	T387	E388	N389	I390	G391	A392	R393	R394	L395	H396	T397	V398	L399	E400	R401	L402	M403	E404	E405	Y408	L413	S414	G415	Q416	N417	I418	T419	I420	D421	A422	D423	Y424	V425	S426	K427	H428	L429	D430	A431	L432	V433	E436	D437	L438	S439	R440	F441	I442	L443							
I318	I319	F320	E321	I322	Q323	G324	R325	I326	F327	I328	R329	V330	E331	Q332	Q333	A334	T335	T336	T337	S338	D339	F340	E341	R342	T343	L344	T345	E346	P347	N348	G349	S350	T351	V352	Q353	Q354	V355	K356	A357	L358	V359	A360	T361	E362	G363	V364	N365	I366	T369	D370	S371	G372	I373	K374	R375	I376	G377	E378			
E257	I258	D259	K260	I261	C262	K263	K264	G265	E266	S267	S268	D271	V272	S273	R274	E275	G276	V277	Q278	R279	D280	K281	L282	P283	L284	V285	E286	G287	C288	T289	V290	S291	T292	K293	H294	G295	M296	V297	K298	T299	D300	H301	I302	L303	F304	I305	A306	S307	G308	A309	F310	Q311	I312	G313	A314	F315	S316	D317			
MET	THR	SER	GLN	LEU	GLN	SER	MET	PHE	GLN	ASN	LEU	GLY	GLY	GLN	K210	Q211	K215	L216	K217	I218	K219	D220	A221	K222	K223	L224	L225	I226	G227	E228	E229	A230	A231	K232	L233	V234	N235	P236	E237	E238	L239	K240	Q241	D242	A243	I244	D245	A246	V247	E248	Q249	H250	G251	I252	V253	F254	I255	D256			
L126	A127	E128	E129	R130	I131	L132	D133	V134	L135	P138	N142	Q145	T146	E147	Q148	Q149	Q150	E151	R156	Q157	A158	K161	K162	L163	R164	E165	G166	Q167	L168	D169	I100	R101	D102	L103	T104	D105	ASP	LEU	ALA	V108	ALA	ALA	ALA	PRU	MET	GLY	VAL	GLU	ILE	MET	ALA	PRU	GLU	GLY	MET	GLU	E125				
T64	E65	I66	R69	L70	A71	K72	L73	A74	N75	A76	P77	F78	I79	R80	H81	E82	A83	H84	R85	F86	T87	E88	R156	Q157	H89	Y91	K161	K162	K163	K164	E165	G166	Q167	L168	D169	I100	R101	D102	L103	T104	D105	A106	LEU	ALA	V108	K109	A110	V111	MET	R112	V113	Q114	A115	I116	E117	R120	Y121	R122	A123	GLU	E125

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.78Å 201.78Å 171.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 4.00	Depositor
% Data completeness (in resolution range)	95.8 (15.00-4.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	10.50	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.229 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12926	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: ANP

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	0.30	0/3255	0.58	3/4385 (0.1%)
1	B	0.28	0/3255	0.50	0/4385
1	C	0.29	0/3255	0.51	0/4385
1	D	0.28	0/3255	0.52	0/4385
All	All	0.29	0/13020	0.53	3/17540 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	CB-CG-CD	12.03	142.87	111.60
1	A	223	LYS	CB-CG-CD	8.81	134.51	111.60
1	A	232	LYS	N-CA-CB	5.85	121.13	110.60

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	3216	0	3284	386	0
1	B	3216	0	3284	289	0
1	C	3216	0	3284	434	0
1	D	3216	0	3284	316	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	13	9	0
2	C	31	0	13	11	0
All	All	12926	0	13162	1411	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 60.

The worst 5 of 1411 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:A:356:LYS:HA	1:A:366:ILE:HD11	1.38	1.01
1:C:54:LEU:HD13	1:C:56:ILE:HD11	1.39	1.01
1:A:366:ILE:HD13	1:A:366:ILE:H	1.28	0.98
1:A:54:LEU:HD13	1:A:56:ILE:HD11	1.43	0.97
1:A:282:LEU:HD21	1:A:321:GLU:HB3	1.46	0.97

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	403/442 (91%)	262 (65%)	102 (25%)	39 (10%)	1	14
1	B	403/442 (91%)	251 (62%)	111 (28%)	41 (10%)	1	13
1	C	403/442 (91%)	258 (64%)	104 (26%)	41 (10%)	1	13
1	D	403/442 (91%)	251 (62%)	115 (28%)	37 (9%)	1	16
All	All	1612/1768 (91%)	1022 (63%)	432 (27%)	158 (10%)	1	14

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	63	LYS
1	A	110	MET
1	A	268	SER
1	A	398	VAL

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	349/376 (93%)	226 (65%)	123 (35%)	0	1
1	B	349/376 (93%)	227 (65%)	122 (35%)	0	2
1	C	349/376 (93%)	220 (63%)	129 (37%)	0	1
1	D	349/376 (93%)	231 (66%)	118 (34%)	0	2
All	All	1396/1504 (93%)	904 (65%)	492 (35%)	0	1

5 of 492 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	374	LYS
1	C	94	LYS
1	D	316	SER
1	B	389	ASN
1	C	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	323	GLN
1	C	39	GLN
1	D	235	ASN
1	B	384	ASN
1	C	75	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 ⓘ

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	$\# Z > 2$
2	ANP	A	900	-	27,33,33	1.37	4 (14%)	30,52,52	1.48	2 (6%)
2	ANP	C	905	-	27,33,33	1.35	4 (14%)	30,52,52	1.45	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
2	ANP	A	900	-	-	0/12/38/38	0/3/3/3
2	ANP	C	905	-	-	0/12/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ANP	PG-O2G	-2.48	1.49	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	905	ANP	PG-O2G	-2.46	1.49	1.56
2	A	900	ANP	PB-O2B	-2.25	1.50	1.56
2	C	905	ANP	PB-O2B	-2.24	1.50	1.56
2	A	900	ANP	PB-O1B	2.74	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ANP	O1G-PG-N3B	-4.14	105.55	111.90
2	C	905	ANP	O1G-PG-N3B	-4.10	105.61	111.90
2	C	905	ANP	O2B-PB-O1B	4.86	120.14	110.00
2	A	900	ANP	O2B-PB-O1B	4.86	120.14	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	ANP	9	0
2	C	905	ANP	11	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.