



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:14 PM UTC

PDB ID : 1DO2 / pdb_00001do2
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

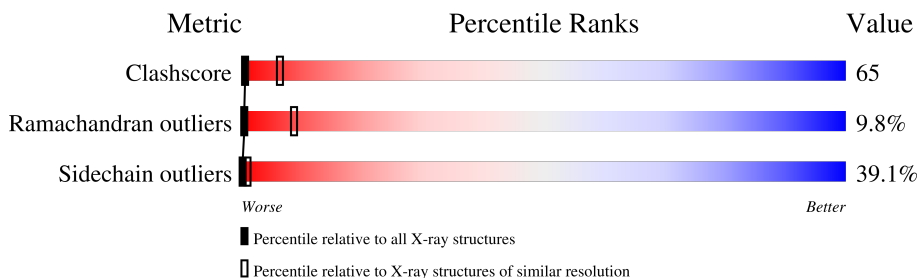
1 Overall quality at a glance

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	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	442	14% 52% 22% 8%
1	B	442	20% 49% 22% 8%
1	C	442	14% 49% 26% 8%
1	D	442	18% 52% 21% 8%

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](#)

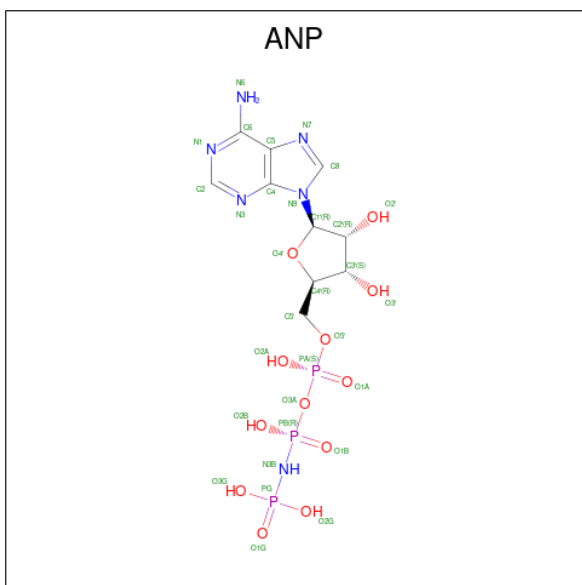
There are 2 unique types of molecules in this entry. The entry contains 12926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	407	Total 3216	C 2008	N 574	O 624	S 10	126	0	0
1	B	407	Total 3216	C 2008	N 574	O 624	S 10	492	0	0
1	C	407	Total 3216	C 2008	N 574	O 624	S 10	103	0	0
1	D	407	Total 3216	C 2008	N 574	O 624	S 10	484	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



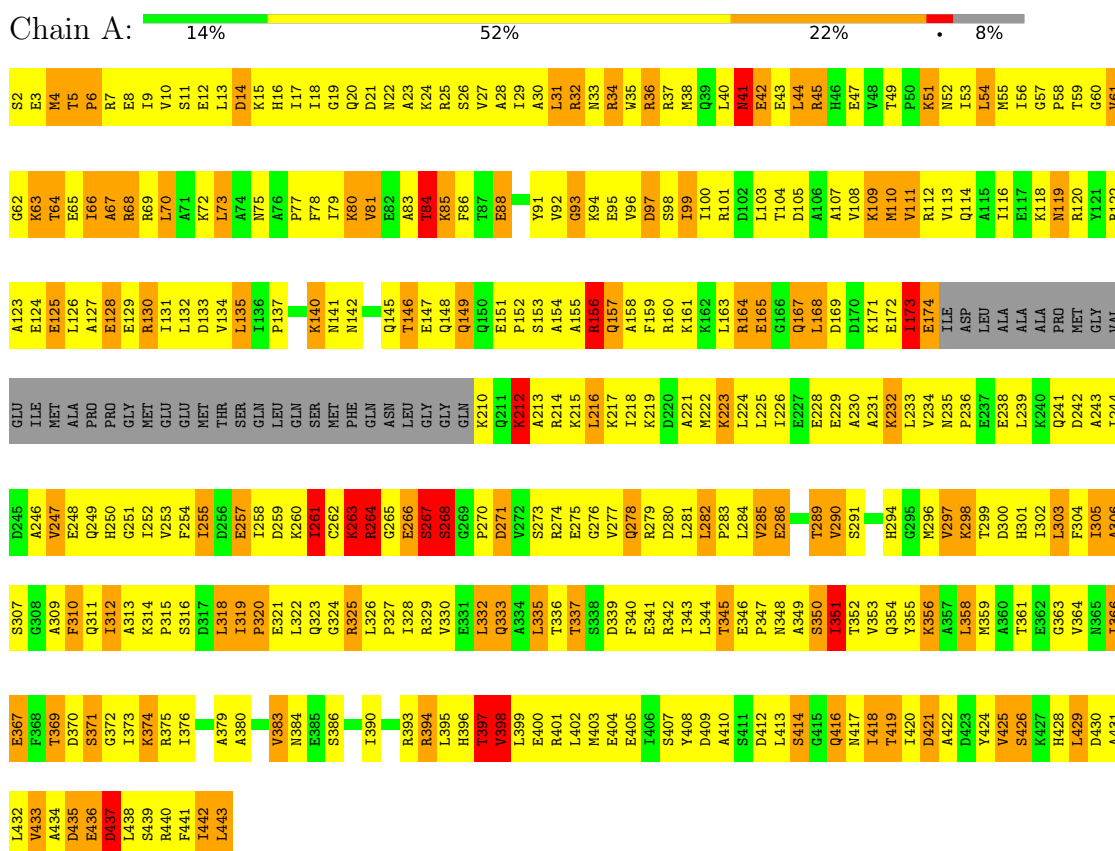
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

3 Residue-property plots

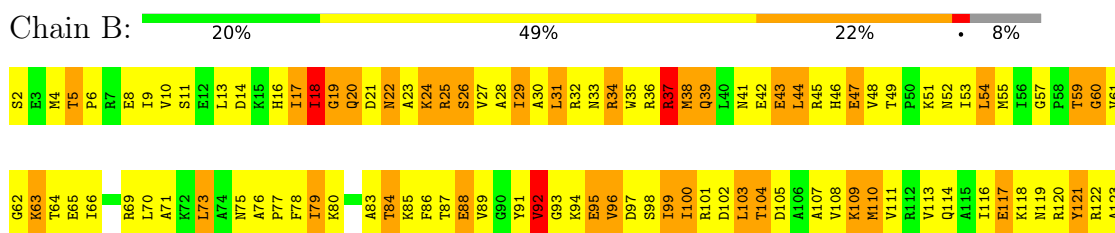
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

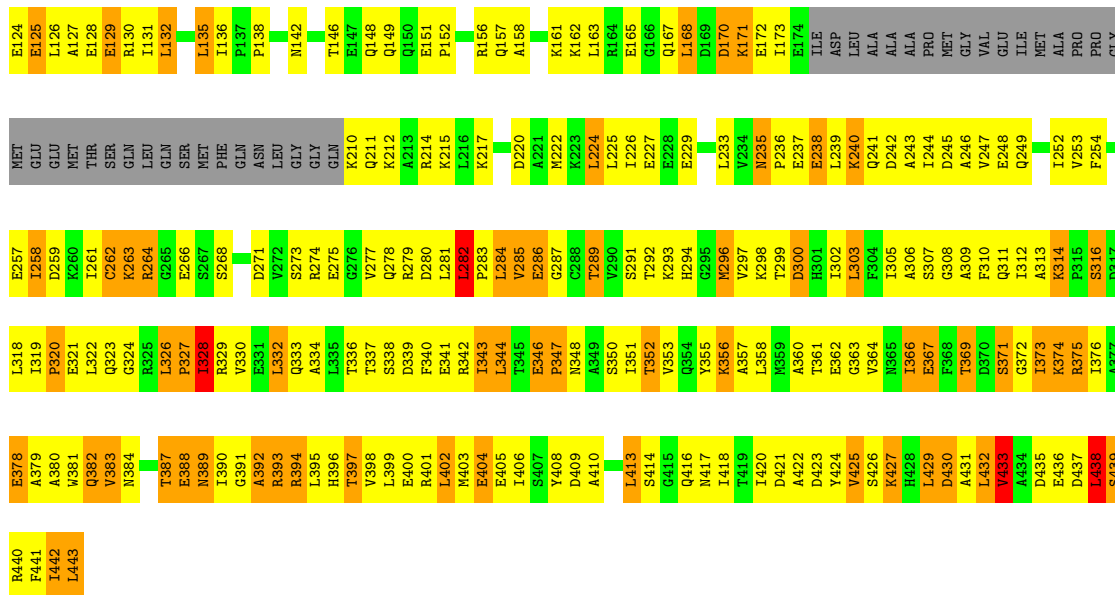
Note EDS was not executed.

- Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

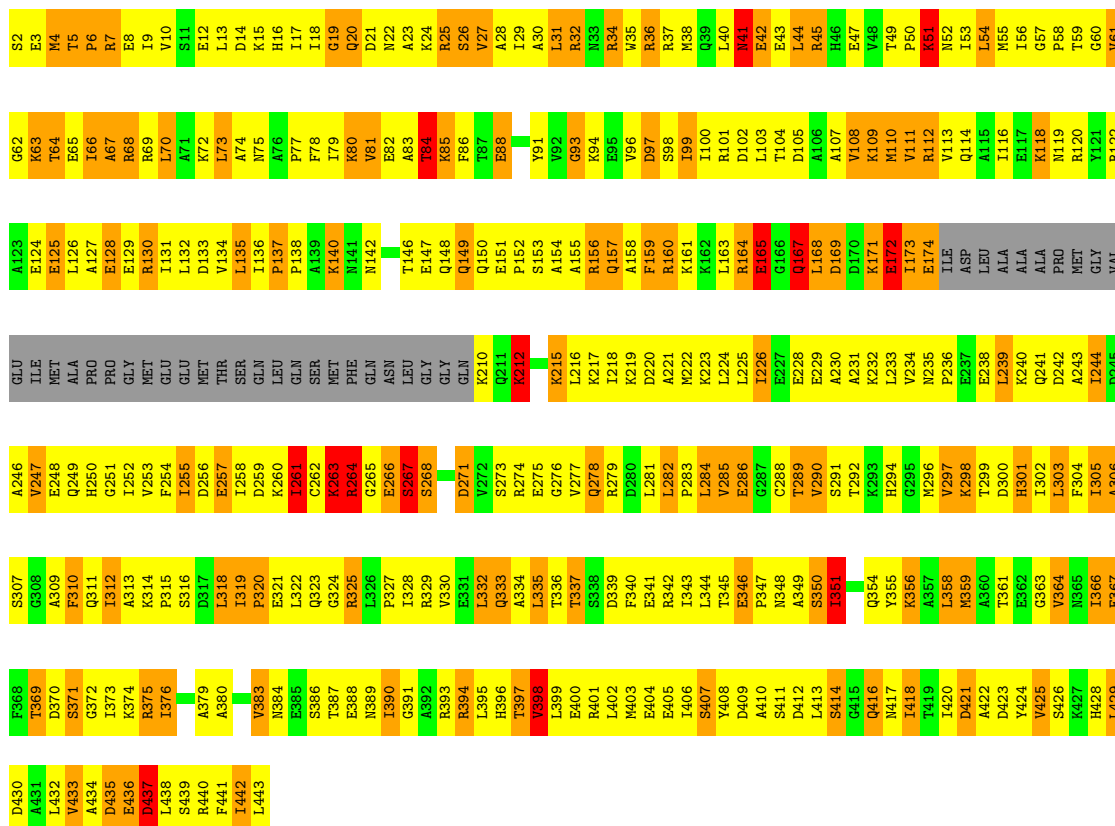
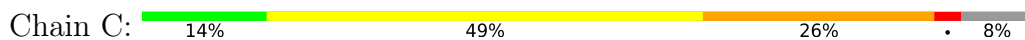


- Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)

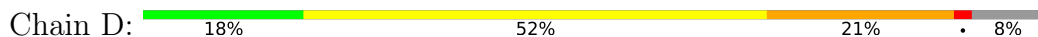




• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)



• Molecule 1: PROTEIN (HEAT SHOCK LOCUS U)



S439	K374	K314	V253	GLU	E124	K63	S2
R440	R375	F315	F254	GLU	E125	T64	E3
F441	I376	D317	D255	THR	L126	E65	M4
L443	A377	D316	D256	SER	A127	I66	T5
	E378	L318	E257	SER	E128	R69	P6
	A379	I319	I258	GLN	E129	L70	R7
	A380	P320	D259	LEU	R130	A71	E8
	W381	E321	K260	GLN	L131	L71	I9
	Q382	L322	I261	SER	L132	K72	V10
	V383	Q323	C262	NET	D133	L73	S11
	N384	G324	K263	PHE	V134	A74	
	T387	R325	R264	GLN	L135	N75	D14
	E388	L326	G265	ASN	I136	A76	K15
	N389	P327	E266	LEU	F137	F77	H16
	I390	R328	S267	GLY	P138	F78	I17
	G391	V330	S268	GLY		I79	I18
	R392	E331	D271	GLN	Q145	K80	G19
	R393	L332	V272	GLN	T146	V81	Q20
	R394	Q333	S273	K210	E147	E82	D21
	L395	A334	R274	K212	Q148	A83	M22
	H396	L335	E275	A213	Q149	T84	A23
	T397	T336	G276	K214	Q150	K85	K24
	V398	T337	V277	K215	E151	F86	R25
	L399	S338	Q278	K216		T87	S26
	E400	D339	R279	K217	R156	E88	V27
	R401	F340	D280	E218	Q157	V89	A28
	L402	E341	L281	K219	A158	G90	I29
	M403	R342	L282	A221	K161	Y91	A30
	E404	I343	P283	M222	K162	V92	L31
	E405	L344	L284	K223	L163	K94	R32
	I406	T345	V285	L224	E164	E95	N33
	S407	E346	E286	L225	E165	V96	R34
	Y408	P347	G287	I226	Q166	D97	W35
		N348	C288	E227	Q167	R36	R36
		A349	T289	E228	L168	I99	M38
		S350	V290	A230	D169	I100	Q39
		I351	S291	A230	D170	R101	L40
		T352	T292	A231	K171	D102	M41
		Q353	K293	K232	E172	L103	E42
		I418	H294	L233	I173	T104	E43
		T419	G295	V234	E174	D105	L44
		I420	M296	M235	ILE	A106	R45
		A357	V297	P236	ASP	A107	H46
		L358	K298	E237	LEU	V108	E47
		M359	T299	E238	ALA	K109	V48
		A360	D300	L239	ALA	M110	T49
		T361	H301	K240	ALA	V111	P50
		E362	I302	D241	PRO	R112	M51
		G363	L303	D242	MET	V113	M52
		V364	F304	A243	GLY	Q114	I53
		N365	I305	L244	VAL	A115	L54
		O366	A306	D245	GLU	I116	M55
		E367	S307	A246	ILE	E117	I56
		F368	G308	V247	MET	K118	G57
		T369	A309	E248	ALA	M119	P58
		B370	F310	Q249	PRO	R120	T59
		S371	Q311	H250	PRO	Y121	G60
		G372	I312	G251	GLY	R122	V61
		I373	A313	I252	MET	A123	G62

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
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	0.37	0/3255	0.88	9/4385 (0.2%)
1	B	0.35	0/3255	0.82	4/4385 (0.1%)
1	C	0.34	0/3255	0.81	4/4385 (0.1%)
1	D	0.34	0/3255	0.82	6/4385 (0.1%)
All	All	0.35	0/13020	0.83	23/17540 (0.1%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	CB-CG-CD	13.73	142.87	111.30
1	A	223	LYS	CB-CG-CD	10.09	134.51	111.30
1	B	59	THR	N-CA-C	7.92	122.06	111.30
1	A	263	LYS	N-CA-C	7.25	118.17	108.38
1	D	59	THR	N-CA-C	7.20	121.09	111.30

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	3216	0	3284	412	0
1	B	3216	0	3284	317	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3216	0	3284	464	0
1	D	3216	0	3284	342	0
2	A	31	0	13	9	0
2	C	31	0	13	11	0
All	All	12926	0	13162	1521	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 65.

The worst 5 of 1521 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%)	0 9
1	B	403/442 (91%)	251 (62%)	111 (28%)	41 (10%)	0 8
1	C	403/442 (91%)	258 (64%)	104 (26%)	41 (10%)	0 8
1	D	403/442 (91%)	251 (62%)	115 (28%)	37 (9%)	0 10
All	All	1612/1768 (91%)	1022 (63%)	432 (27%)	158 (10%)	0 9

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 [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	349/376 (93%)	218 (62%)	131 (38%)	0	1
1	B	349/376 (93%)	215 (62%)	134 (38%)	0	1
1	C	349/376 (93%)	207 (59%)	142 (41%)	0	0
1	D	349/376 (93%)	210 (60%)	139 (40%)	0	1
All	All	1396/1504 (93%)	850 (61%)	546 (39%)	0	1

5 of 546 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	167	GLN
1	D	219	LYS
1	D	165	GLU
1	D	371	SER
1	B	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	384	ASN
1	D	323	GLN
1	C	396	HIS
1	D	22	ASN
1	D	382	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	33,33,33	1.13	4 (12%)	45,52,52	1.19	2 (4%)
2	ANP	C	905	-	33,33,33	1.11	4 (12%)	45,52,52	1.18	2 (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	ANP	A	900	-	-	8/18/38/38	0/3/3/3
2	ANP	C	905	-	-	8/18/38/38	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-O1G	2.92	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	905	ANP	PG-O1G	2.68	1.50	1.46
2	A	900	ANP	PG-O2G	-2.64	1.49	1.56
2	C	905	ANP	PG-O2G	-2.63	1.49	1.56
2	C	905	ANP	PB-O1B	2.43	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ANP	O2B-PB-O1B	4.79	120.14	109.87
2	C	905	ANP	O2B-PB-O1B	4.79	120.14	109.87
2	A	900	ANP	O1G-PG-N3B	-4.23	105.55	111.77
2	C	905	ANP	O1G-PG-N3B	-4.19	105.61	111.77

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

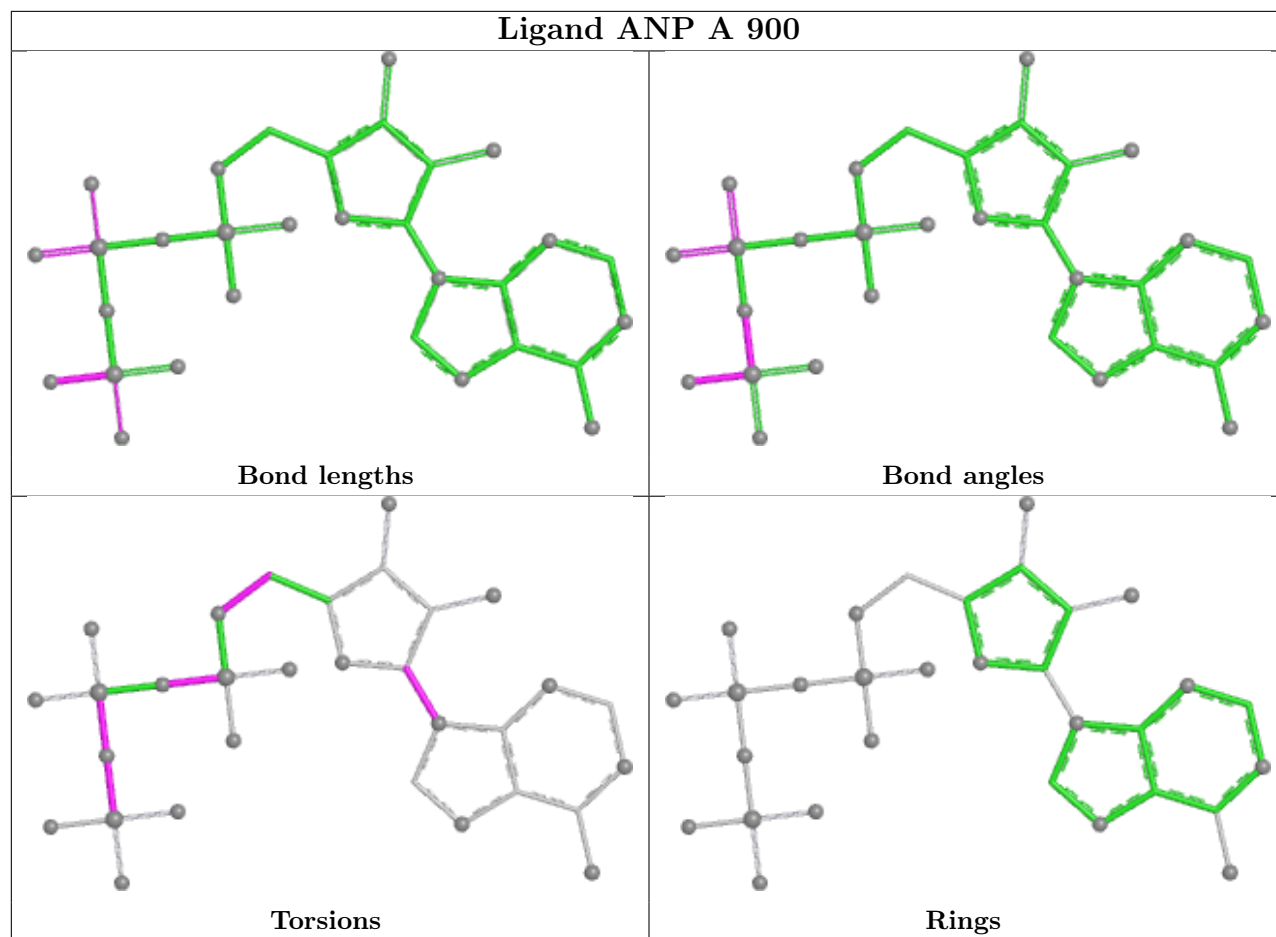
Mol	Chain	Res	Type	Atoms
2	A	900	ANP	PB-N3B-PG-O1G
2	A	900	ANP	PG-N3B-PB-O1B
2	A	900	ANP	PG-N3B-PB-O3A
2	A	900	ANP	O4'-C1'-N9-C8
2	A	900	ANP	O4'-C1'-N9-C4

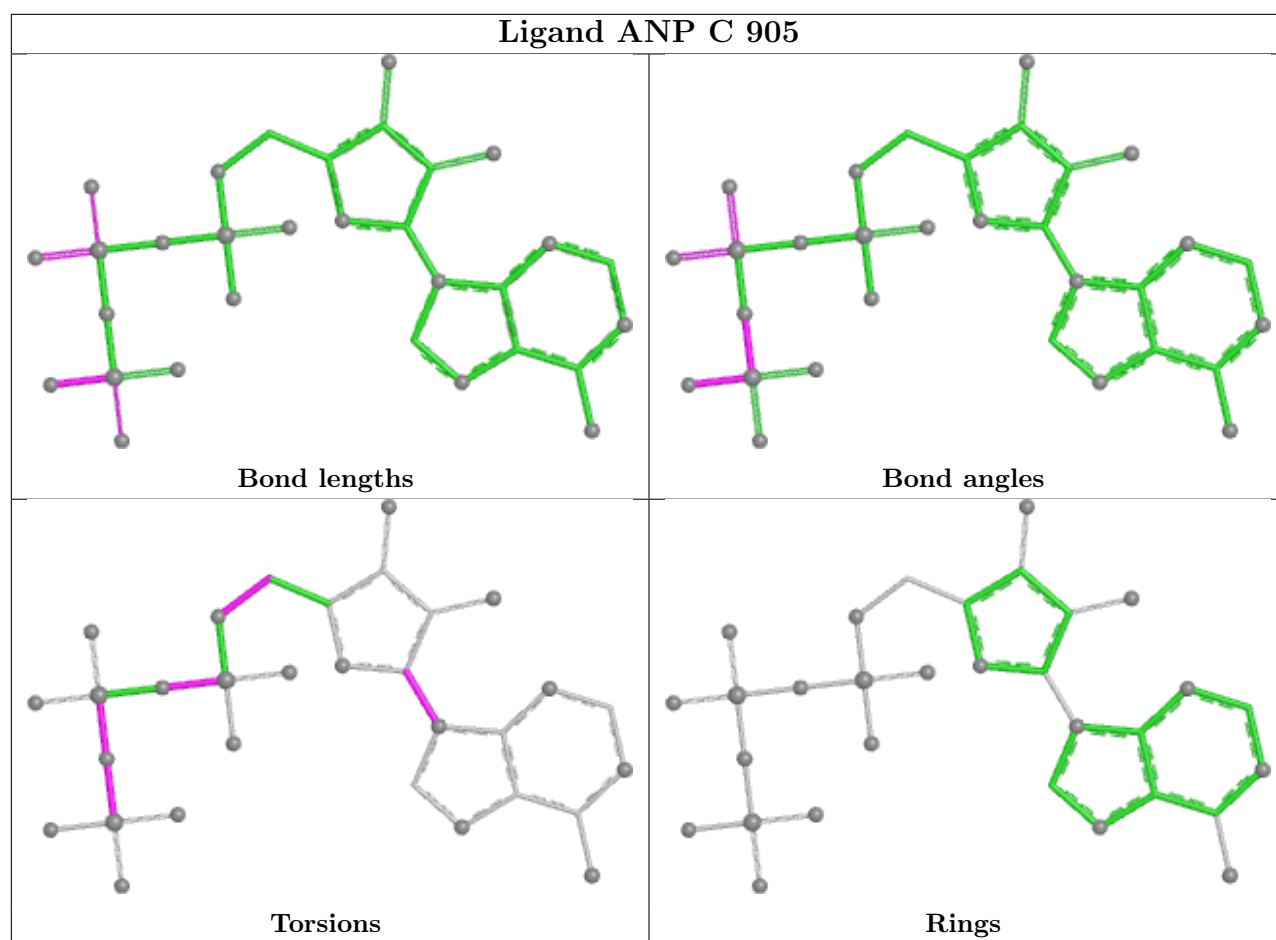
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.