



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:40 PM UTC

PDB ID : 7RFH / pdb_00007rfh
EMDB ID : EMD-24442
Title : HUMAN RETINAL VARIANT IMPDH1(595) TREATED WITH ATP,
OCTAMER-CENTERED
Authors : Burrell, A.L.; Kollman, J.M.
Deposited on : 2021-07-14
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
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:

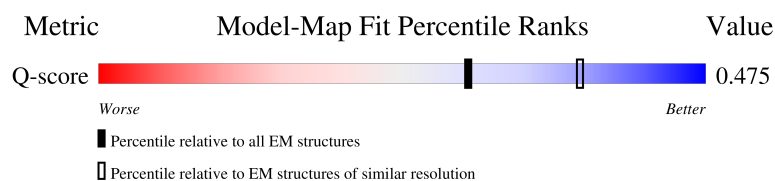
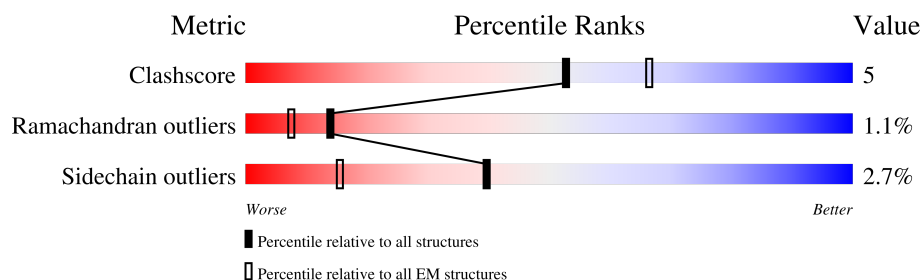
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	9% 66% 9% 25%
1	B	595	9% 65% 10% 25%
1	C	595	9% 68% 7% 25%
1	D	595	8% 68% 8% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	595	
1	F	595	
1	G	595	
1	H	595	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55333 atoms, of which 27795 are hydrogens and 0 are deuteriums.

In the tables below, 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 Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	B	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	C	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	D	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	E	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	F	449	Total	C	H	N	O	S	0	0
			6823	2136	3446	579	641	21		
1	G	450	Total	C	H	N	O	S	0	0
			6845	2142	3459	581	642	21		
1	H	451	Total	C	H	N	O	S	0	0
			6862	2147	3468	582	643	22		

There are 504 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P20839-5
A	?	-	CYS	deletion	UNP P20839-5
A	?	-	PHE	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	GLU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	SER	deletion	UNP P20839-5
A	?	-	SER	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	ALA	deletion	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	GLY	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	GLN	deletion	UNP P20839-5
A	?	-	MET	deletion	UNP P20839-5
A	?	-	ASP	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	ALA	deletion	UNP P20839-5
A	510	THR	-	expression tag	UNP P20839-5
A	511	PHE	-	expression tag	UNP P20839-5
A	512	LEU	-	expression tag	UNP P20839-5
A	513	PRO	-	expression tag	UNP P20839-5
A	514	PHE	-	expression tag	UNP P20839-5
A	515	THR	-	expression tag	UNP P20839-5
A	516	LYS	-	expression tag	UNP P20839-5
A	517	SER	-	expression tag	UNP P20839-5
A	518	GLY	-	expression tag	UNP P20839-5
A	519	CYS	-	expression tag	UNP P20839-5
A	520	THR	-	expression tag	UNP P20839-5
A	521	GLU	-	expression tag	UNP P20839-5
A	522	ASP	-	expression tag	UNP P20839-5
A	523	SER	-	expression tag	UNP P20839-5
A	524	GLY	-	expression tag	UNP P20839-5
A	525	GLY	-	expression tag	UNP P20839-5
A	526	GLY	-	expression tag	UNP P20839-5
A	527	ARG	-	expression tag	UNP P20839-5
A	528	GLY	-	expression tag	UNP P20839-5
A	529	GLY	-	expression tag	UNP P20839-5
A	530	GLY	-	expression tag	UNP P20839-5
A	531	GLY	-	expression tag	UNP P20839-5
A	532	ASP	-	expression tag	UNP P20839-5
A	533	ALA	-	expression tag	UNP P20839-5
A	534	PRO	-	expression tag	UNP P20839-5
A	535	GLN	-	expression tag	UNP P20839-5
A	536	CYS	-	expression tag	UNP P20839-5
A	537	PRO	-	expression tag	UNP P20839-5
A	538	LEU	-	expression tag	UNP P20839-5
A	539	LEU	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	GLY	-	expression tag	UNP P20839-5
A	541	THR	-	expression tag	UNP P20839-5
A	542	ALA	-	expression tag	UNP P20839-5
A	543	SER	-	expression tag	UNP P20839-5
A	544	LEU	-	expression tag	UNP P20839-5
A	545	HIS	-	expression tag	UNP P20839-5
A	546	ASN	-	expression tag	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	CYS	deletion	UNP P20839-5
B	?	-	PHE	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	GLU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	ALA	deletion	UNP P20839-5
B	?	-	GLY	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	GLY	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	GLN	deletion	UNP P20839-5
B	?	-	MET	deletion	UNP P20839-5
B	?	-	ASP	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	ALA	deletion	UNP P20839-5
B	510	THR	-	expression tag	UNP P20839-5
B	511	PHE	-	expression tag	UNP P20839-5
B	512	LEU	-	expression tag	UNP P20839-5
B	513	PRO	-	expression tag	UNP P20839-5
B	514	PHE	-	expression tag	UNP P20839-5
B	515	THR	-	expression tag	UNP P20839-5
B	516	LYS	-	expression tag	UNP P20839-5
B	517	SER	-	expression tag	UNP P20839-5
B	518	GLY	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	519	CYS	-	expression tag	UNP P20839-5
B	520	THR	-	expression tag	UNP P20839-5
B	521	GLU	-	expression tag	UNP P20839-5
B	522	ASP	-	expression tag	UNP P20839-5
B	523	SER	-	expression tag	UNP P20839-5
B	524	GLY	-	expression tag	UNP P20839-5
B	525	GLY	-	expression tag	UNP P20839-5
B	526	GLY	-	expression tag	UNP P20839-5
B	527	ARG	-	expression tag	UNP P20839-5
B	528	GLY	-	expression tag	UNP P20839-5
B	529	GLY	-	expression tag	UNP P20839-5
B	530	GLY	-	expression tag	UNP P20839-5
B	531	GLY	-	expression tag	UNP P20839-5
B	532	ASP	-	expression tag	UNP P20839-5
B	533	ALA	-	expression tag	UNP P20839-5
B	534	PRO	-	expression tag	UNP P20839-5
B	535	GLN	-	expression tag	UNP P20839-5
B	536	CYS	-	expression tag	UNP P20839-5
B	537	PRO	-	expression tag	UNP P20839-5
B	538	LEU	-	expression tag	UNP P20839-5
B	539	LEU	-	expression tag	UNP P20839-5
B	540	GLY	-	expression tag	UNP P20839-5
B	541	THR	-	expression tag	UNP P20839-5
B	542	ALA	-	expression tag	UNP P20839-5
B	543	SER	-	expression tag	UNP P20839-5
B	544	LEU	-	expression tag	UNP P20839-5
B	545	HIS	-	expression tag	UNP P20839-5
B	546	ASN	-	expression tag	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	CYS	deletion	UNP P20839-5
C	?	-	PHE	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	GLU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	ALA	deletion	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	GLY	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	GLN	deletion	UNP P20839-5
C	?	-	MET	deletion	UNP P20839-5
C	?	-	ASP	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	ALA	deletion	UNP P20839-5
C	510	THR	-	expression tag	UNP P20839-5
C	511	PHE	-	expression tag	UNP P20839-5
C	512	LEU	-	expression tag	UNP P20839-5
C	513	PRO	-	expression tag	UNP P20839-5
C	514	PHE	-	expression tag	UNP P20839-5
C	515	THR	-	expression tag	UNP P20839-5
C	516	LYS	-	expression tag	UNP P20839-5
C	517	SER	-	expression tag	UNP P20839-5
C	518	GLY	-	expression tag	UNP P20839-5
C	519	CYS	-	expression tag	UNP P20839-5
C	520	THR	-	expression tag	UNP P20839-5
C	521	GLU	-	expression tag	UNP P20839-5
C	522	ASP	-	expression tag	UNP P20839-5
C	523	SER	-	expression tag	UNP P20839-5
C	524	GLY	-	expression tag	UNP P20839-5
C	525	GLY	-	expression tag	UNP P20839-5
C	526	GLY	-	expression tag	UNP P20839-5
C	527	ARG	-	expression tag	UNP P20839-5
C	528	GLY	-	expression tag	UNP P20839-5
C	529	GLY	-	expression tag	UNP P20839-5
C	530	GLY	-	expression tag	UNP P20839-5
C	531	GLY	-	expression tag	UNP P20839-5
C	532	ASP	-	expression tag	UNP P20839-5
C	533	ALA	-	expression tag	UNP P20839-5
C	534	PRO	-	expression tag	UNP P20839-5
C	535	GLN	-	expression tag	UNP P20839-5
C	536	CYS	-	expression tag	UNP P20839-5
C	537	PRO	-	expression tag	UNP P20839-5
C	538	LEU	-	expression tag	UNP P20839-5
C	539	LEU	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	540	GLY	-	expression tag	UNP P20839-5
C	541	THR	-	expression tag	UNP P20839-5
C	542	ALA	-	expression tag	UNP P20839-5
C	543	SER	-	expression tag	UNP P20839-5
C	544	LEU	-	expression tag	UNP P20839-5
C	545	HIS	-	expression tag	UNP P20839-5
C	546	ASN	-	expression tag	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	CYS	deletion	UNP P20839-5
D	?	-	PHE	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	GLU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	ALA	deletion	UNP P20839-5
D	?	-	GLY	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	GLY	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	GLN	deletion	UNP P20839-5
D	?	-	MET	deletion	UNP P20839-5
D	?	-	ASP	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	ALA	deletion	UNP P20839-5
D	510	THR	-	expression tag	UNP P20839-5
D	511	PHE	-	expression tag	UNP P20839-5
D	512	LEU	-	expression tag	UNP P20839-5
D	513	PRO	-	expression tag	UNP P20839-5
D	514	PHE	-	expression tag	UNP P20839-5
D	515	THR	-	expression tag	UNP P20839-5
D	516	LYS	-	expression tag	UNP P20839-5
D	517	SER	-	expression tag	UNP P20839-5
D	518	GLY	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	519	CYS	-	expression tag	UNP P20839-5
D	520	THR	-	expression tag	UNP P20839-5
D	521	GLU	-	expression tag	UNP P20839-5
D	522	ASP	-	expression tag	UNP P20839-5
D	523	SER	-	expression tag	UNP P20839-5
D	524	GLY	-	expression tag	UNP P20839-5
D	525	GLY	-	expression tag	UNP P20839-5
D	526	GLY	-	expression tag	UNP P20839-5
D	527	ARG	-	expression tag	UNP P20839-5
D	528	GLY	-	expression tag	UNP P20839-5
D	529	GLY	-	expression tag	UNP P20839-5
D	530	GLY	-	expression tag	UNP P20839-5
D	531	GLY	-	expression tag	UNP P20839-5
D	532	ASP	-	expression tag	UNP P20839-5
D	533	ALA	-	expression tag	UNP P20839-5
D	534	PRO	-	expression tag	UNP P20839-5
D	535	GLN	-	expression tag	UNP P20839-5
D	536	CYS	-	expression tag	UNP P20839-5
D	537	PRO	-	expression tag	UNP P20839-5
D	538	LEU	-	expression tag	UNP P20839-5
D	539	LEU	-	expression tag	UNP P20839-5
D	540	GLY	-	expression tag	UNP P20839-5
D	541	THR	-	expression tag	UNP P20839-5
D	542	ALA	-	expression tag	UNP P20839-5
D	543	SER	-	expression tag	UNP P20839-5
D	544	LEU	-	expression tag	UNP P20839-5
D	545	HIS	-	expression tag	UNP P20839-5
D	546	ASN	-	expression tag	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	CYS	deletion	UNP P20839-5
E	?	-	PHE	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	GLU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	ALA	deletion	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	GLY	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	GLN	deletion	UNP P20839-5
E	?	-	MET	deletion	UNP P20839-5
E	?	-	ASP	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	ALA	deletion	UNP P20839-5
E	510	THR	-	expression tag	UNP P20839-5
E	511	PHE	-	expression tag	UNP P20839-5
E	512	LEU	-	expression tag	UNP P20839-5
E	513	PRO	-	expression tag	UNP P20839-5
E	514	PHE	-	expression tag	UNP P20839-5
E	515	THR	-	expression tag	UNP P20839-5
E	516	LYS	-	expression tag	UNP P20839-5
E	517	SER	-	expression tag	UNP P20839-5
E	518	GLY	-	expression tag	UNP P20839-5
E	519	CYS	-	expression tag	UNP P20839-5
E	520	THR	-	expression tag	UNP P20839-5
E	521	GLU	-	expression tag	UNP P20839-5
E	522	ASP	-	expression tag	UNP P20839-5
E	523	SER	-	expression tag	UNP P20839-5
E	524	GLY	-	expression tag	UNP P20839-5
E	525	GLY	-	expression tag	UNP P20839-5
E	526	GLY	-	expression tag	UNP P20839-5
E	527	ARG	-	expression tag	UNP P20839-5
E	528	GLY	-	expression tag	UNP P20839-5
E	529	GLY	-	expression tag	UNP P20839-5
E	530	GLY	-	expression tag	UNP P20839-5
E	531	GLY	-	expression tag	UNP P20839-5
E	532	ASP	-	expression tag	UNP P20839-5
E	533	ALA	-	expression tag	UNP P20839-5
E	534	PRO	-	expression tag	UNP P20839-5
E	535	GLN	-	expression tag	UNP P20839-5
E	536	CYS	-	expression tag	UNP P20839-5
E	537	PRO	-	expression tag	UNP P20839-5
E	538	LEU	-	expression tag	UNP P20839-5
E	539	LEU	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	540	GLY	-	expression tag	UNP P20839-5
E	541	THR	-	expression tag	UNP P20839-5
E	542	ALA	-	expression tag	UNP P20839-5
E	543	SER	-	expression tag	UNP P20839-5
E	544	LEU	-	expression tag	UNP P20839-5
E	545	HIS	-	expression tag	UNP P20839-5
E	546	ASN	-	expression tag	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	CYS	deletion	UNP P20839-5
F	?	-	PHE	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	GLU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	ALA	deletion	UNP P20839-5
F	?	-	GLY	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	GLY	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	GLN	deletion	UNP P20839-5
F	?	-	MET	deletion	UNP P20839-5
F	?	-	ASP	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	ALA	deletion	UNP P20839-5
F	510	THR	-	expression tag	UNP P20839-5
F	511	PHE	-	expression tag	UNP P20839-5
F	512	LEU	-	expression tag	UNP P20839-5
F	513	PRO	-	expression tag	UNP P20839-5
F	514	PHE	-	expression tag	UNP P20839-5
F	515	THR	-	expression tag	UNP P20839-5
F	516	LYS	-	expression tag	UNP P20839-5
F	517	SER	-	expression tag	UNP P20839-5
F	518	GLY	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	519	CYS	-	expression tag	UNP P20839-5
F	520	THR	-	expression tag	UNP P20839-5
F	521	GLU	-	expression tag	UNP P20839-5
F	522	ASP	-	expression tag	UNP P20839-5
F	523	SER	-	expression tag	UNP P20839-5
F	524	GLY	-	expression tag	UNP P20839-5
F	525	GLY	-	expression tag	UNP P20839-5
F	526	GLY	-	expression tag	UNP P20839-5
F	527	ARG	-	expression tag	UNP P20839-5
F	528	GLY	-	expression tag	UNP P20839-5
F	529	GLY	-	expression tag	UNP P20839-5
F	530	GLY	-	expression tag	UNP P20839-5
F	531	GLY	-	expression tag	UNP P20839-5
F	532	ASP	-	expression tag	UNP P20839-5
F	533	ALA	-	expression tag	UNP P20839-5
F	534	PRO	-	expression tag	UNP P20839-5
F	535	GLN	-	expression tag	UNP P20839-5
F	536	CYS	-	expression tag	UNP P20839-5
F	537	PRO	-	expression tag	UNP P20839-5
F	538	LEU	-	expression tag	UNP P20839-5
F	539	LEU	-	expression tag	UNP P20839-5
F	540	GLY	-	expression tag	UNP P20839-5
F	541	THR	-	expression tag	UNP P20839-5
F	542	ALA	-	expression tag	UNP P20839-5
F	543	SER	-	expression tag	UNP P20839-5
F	544	LEU	-	expression tag	UNP P20839-5
F	545	HIS	-	expression tag	UNP P20839-5
F	546	ASN	-	expression tag	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	CYS	deletion	UNP P20839-5
G	?	-	PHE	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	GLU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	ALA	deletion	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLY	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	GLY	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	GLN	deletion	UNP P20839-5
G	?	-	MET	deletion	UNP P20839-5
G	?	-	ASP	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	ALA	deletion	UNP P20839-5
G	510	THR	-	expression tag	UNP P20839-5
G	511	PHE	-	expression tag	UNP P20839-5
G	512	LEU	-	expression tag	UNP P20839-5
G	513	PRO	-	expression tag	UNP P20839-5
G	514	PHE	-	expression tag	UNP P20839-5
G	515	THR	-	expression tag	UNP P20839-5
G	516	LYS	-	expression tag	UNP P20839-5
G	517	SER	-	expression tag	UNP P20839-5
G	518	GLY	-	expression tag	UNP P20839-5
G	519	CYS	-	expression tag	UNP P20839-5
G	520	THR	-	expression tag	UNP P20839-5
G	521	GLU	-	expression tag	UNP P20839-5
G	522	ASP	-	expression tag	UNP P20839-5
G	523	SER	-	expression tag	UNP P20839-5
G	524	GLY	-	expression tag	UNP P20839-5
G	525	GLY	-	expression tag	UNP P20839-5
G	526	GLY	-	expression tag	UNP P20839-5
G	527	ARG	-	expression tag	UNP P20839-5
G	528	GLY	-	expression tag	UNP P20839-5
G	529	GLY	-	expression tag	UNP P20839-5
G	530	GLY	-	expression tag	UNP P20839-5
G	531	GLY	-	expression tag	UNP P20839-5
G	532	ASP	-	expression tag	UNP P20839-5
G	533	ALA	-	expression tag	UNP P20839-5
G	534	PRO	-	expression tag	UNP P20839-5
G	535	GLN	-	expression tag	UNP P20839-5
G	536	CYS	-	expression tag	UNP P20839-5
G	537	PRO	-	expression tag	UNP P20839-5
G	538	LEU	-	expression tag	UNP P20839-5
G	539	LEU	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

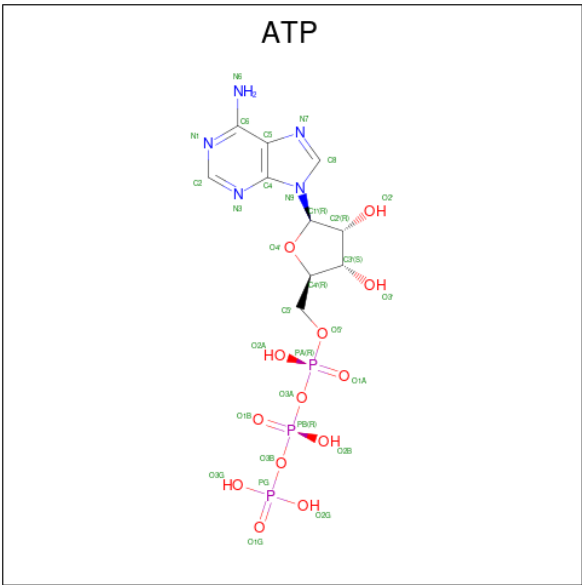
Chain	Residue	Modelled	Actual	Comment	Reference
G	540	GLY	-	expression tag	UNP P20839-5
G	541	THR	-	expression tag	UNP P20839-5
G	542	ALA	-	expression tag	UNP P20839-5
G	543	SER	-	expression tag	UNP P20839-5
G	544	LEU	-	expression tag	UNP P20839-5
G	545	HIS	-	expression tag	UNP P20839-5
G	546	ASN	-	expression tag	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	CYS	deletion	UNP P20839-5
H	?	-	PHE	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	GLU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	ALA	deletion	UNP P20839-5
H	?	-	GLY	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	GLY	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	GLN	deletion	UNP P20839-5
H	?	-	MET	deletion	UNP P20839-5
H	?	-	ASP	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	ALA	deletion	UNP P20839-5
H	510	THR	-	expression tag	UNP P20839-5
H	511	PHE	-	expression tag	UNP P20839-5
H	512	LEU	-	expression tag	UNP P20839-5
H	513	PRO	-	expression tag	UNP P20839-5
H	514	PHE	-	expression tag	UNP P20839-5
H	515	THR	-	expression tag	UNP P20839-5
H	516	LYS	-	expression tag	UNP P20839-5
H	517	SER	-	expression tag	UNP P20839-5
H	518	GLY	-	expression tag	UNP P20839-5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	519	CYS	-	expression tag	UNP P20839-5
H	520	THR	-	expression tag	UNP P20839-5
H	521	GLU	-	expression tag	UNP P20839-5
H	522	ASP	-	expression tag	UNP P20839-5
H	523	SER	-	expression tag	UNP P20839-5
H	524	GLY	-	expression tag	UNP P20839-5
H	525	GLY	-	expression tag	UNP P20839-5
H	526	GLY	-	expression tag	UNP P20839-5
H	527	ARG	-	expression tag	UNP P20839-5
H	528	GLY	-	expression tag	UNP P20839-5
H	529	GLY	-	expression tag	UNP P20839-5
H	530	GLY	-	expression tag	UNP P20839-5
H	531	GLY	-	expression tag	UNP P20839-5
H	532	ASP	-	expression tag	UNP P20839-5
H	533	ALA	-	expression tag	UNP P20839-5
H	534	PRO	-	expression tag	UNP P20839-5
H	535	GLN	-	expression tag	UNP P20839-5
H	536	CYS	-	expression tag	UNP P20839-5
H	537	PRO	-	expression tag	UNP P20839-5
H	538	LEU	-	expression tag	UNP P20839-5
H	539	LEU	-	expression tag	UNP P20839-5
H	540	GLY	-	expression tag	UNP P20839-5
H	541	THR	-	expression tag	UNP P20839-5
H	542	ALA	-	expression tag	UNP P20839-5
H	543	SER	-	expression tag	UNP P20839-5
H	544	LEU	-	expression tag	UNP P20839-5
H	545	HIS	-	expression tag	UNP P20839-5
H	546	ASN	-	expression tag	UNP P20839-5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

Continued on next page...

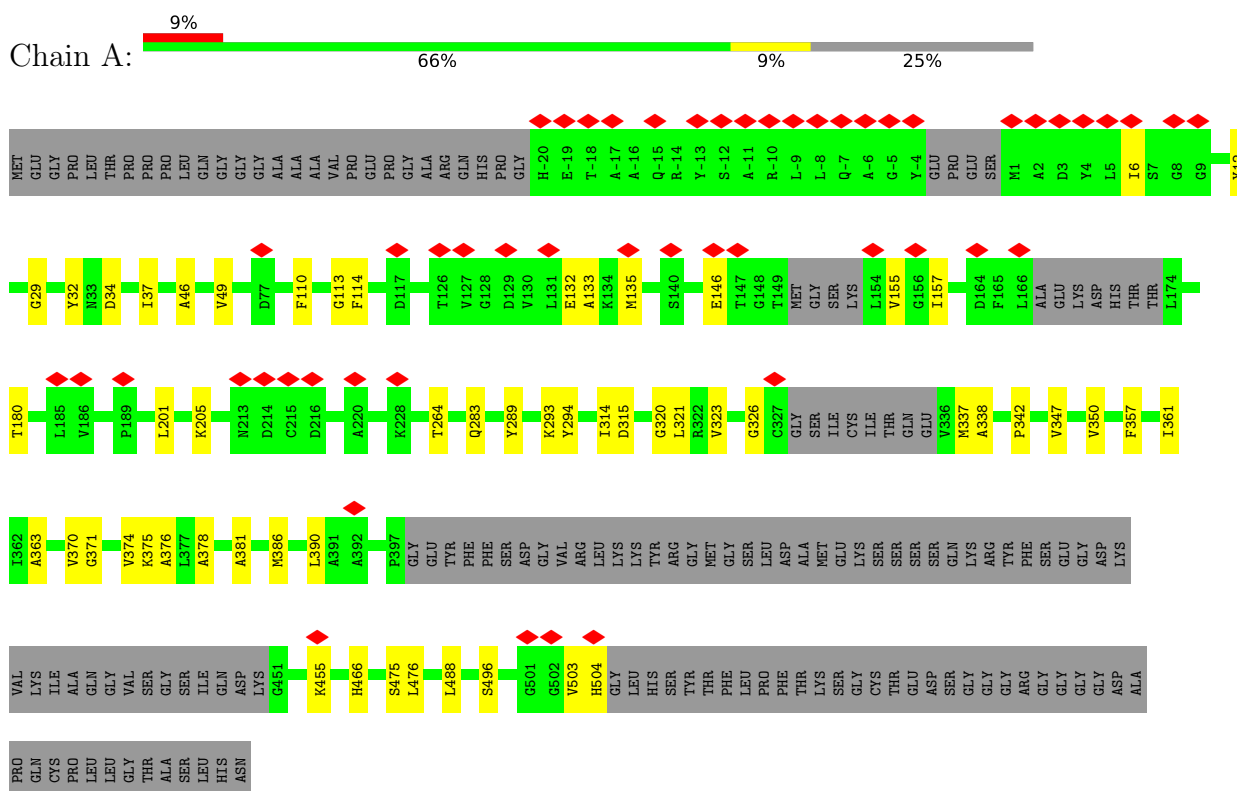
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	H	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	H	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

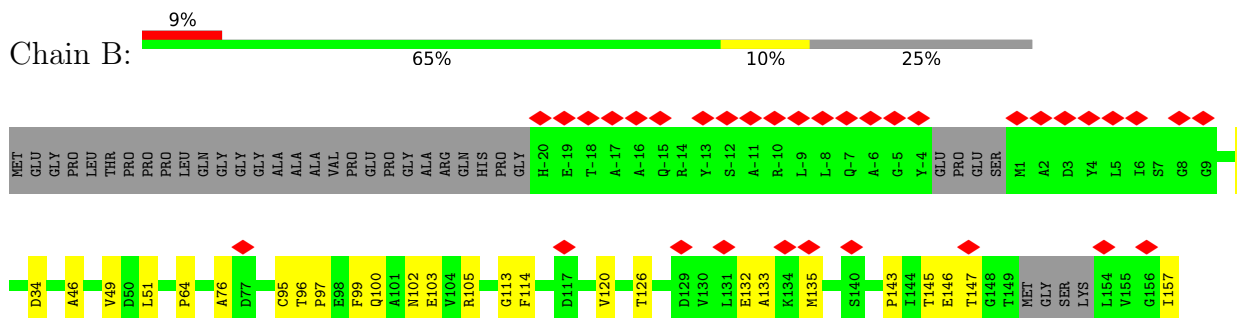
3 Residue-property plots

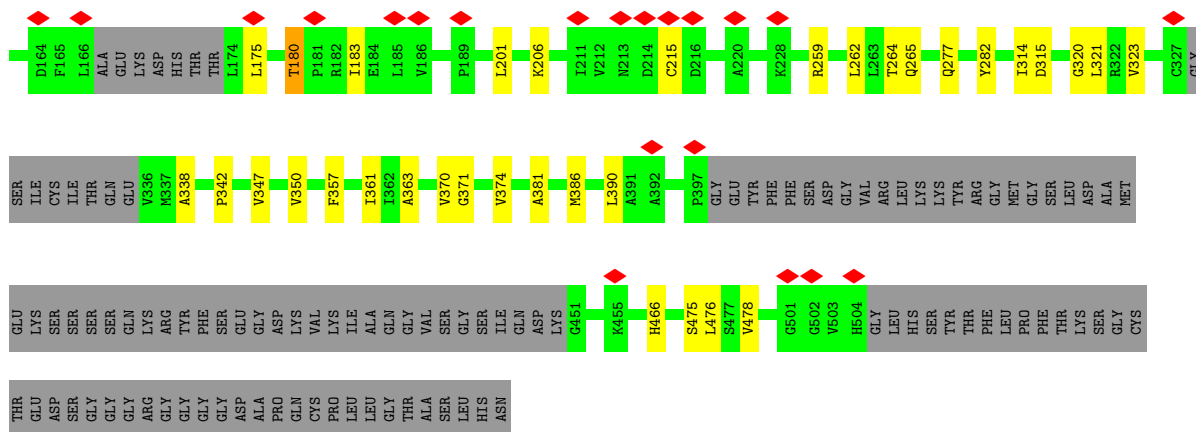
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

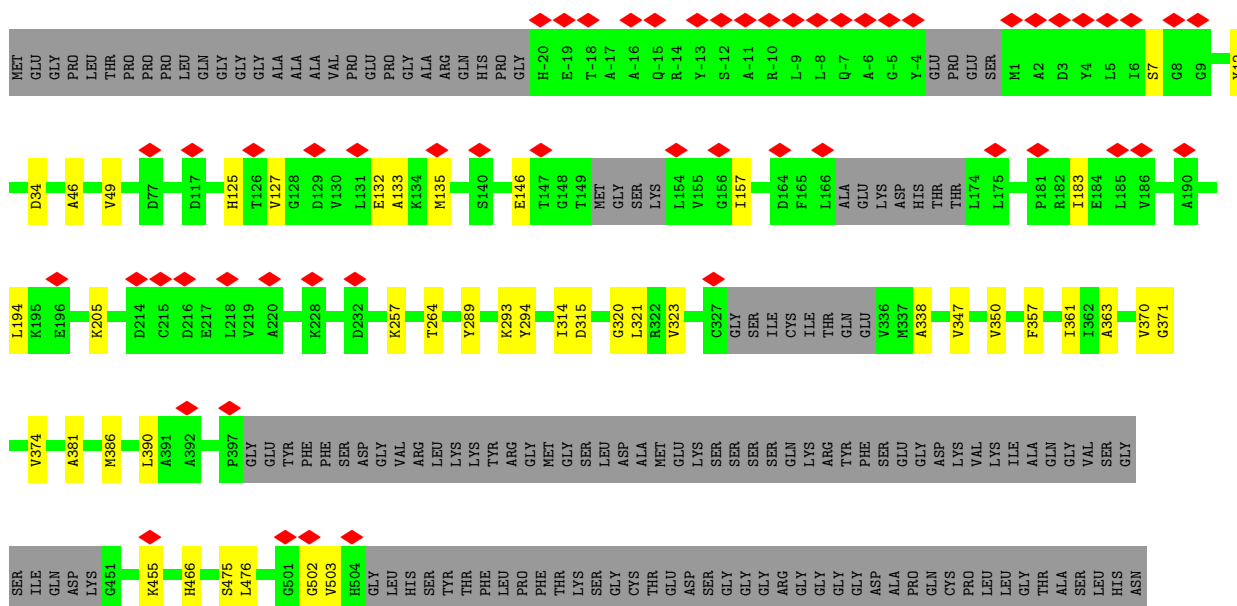


- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

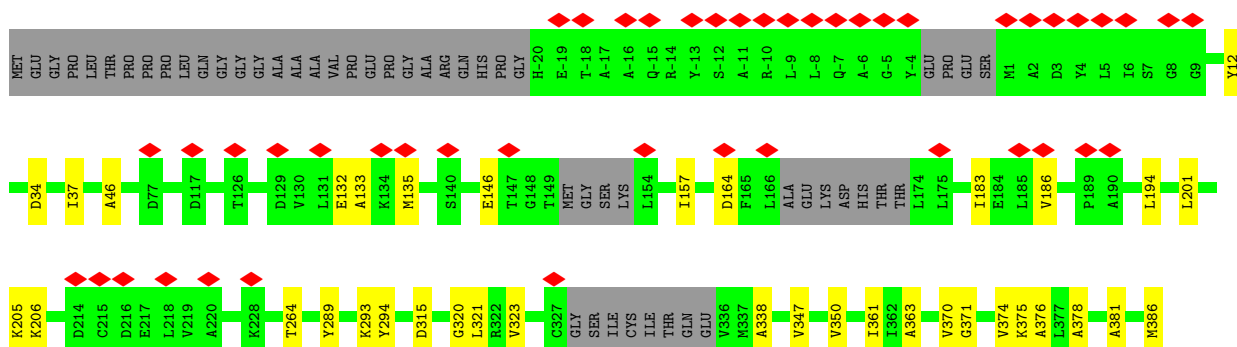




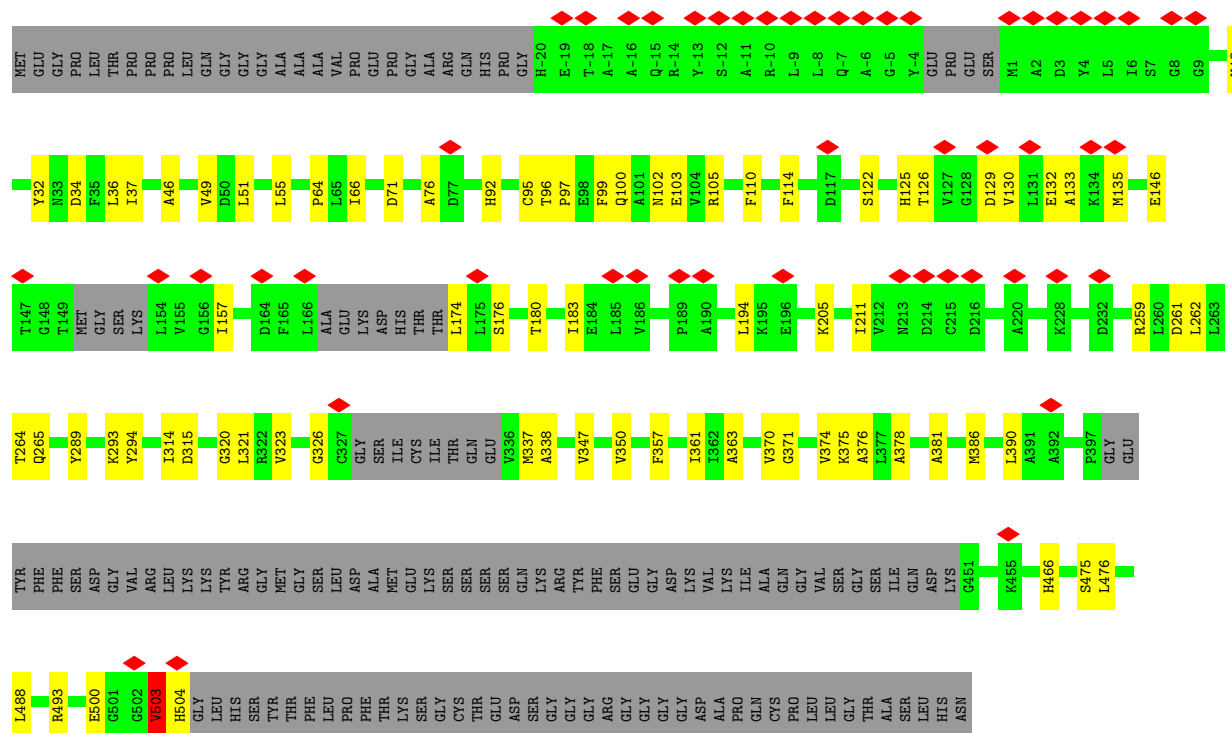
- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



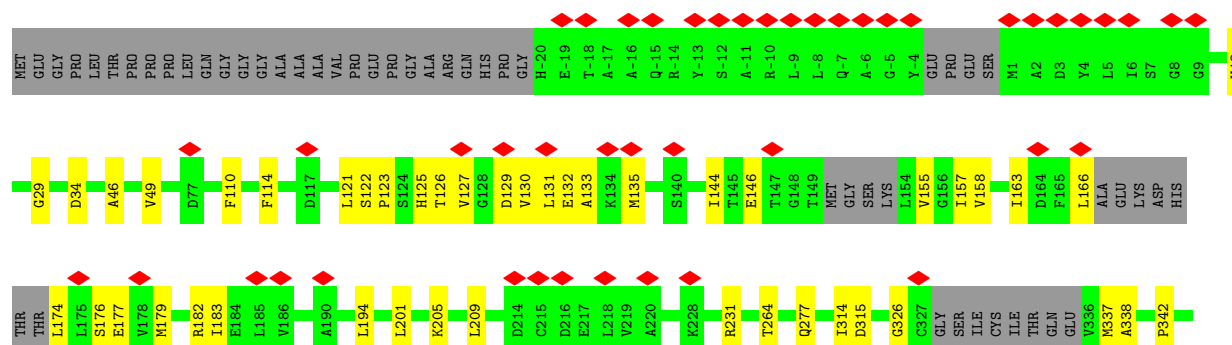
- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

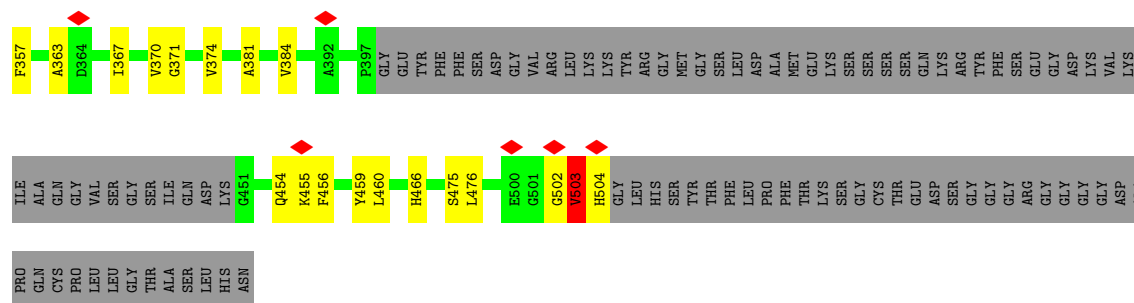


- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

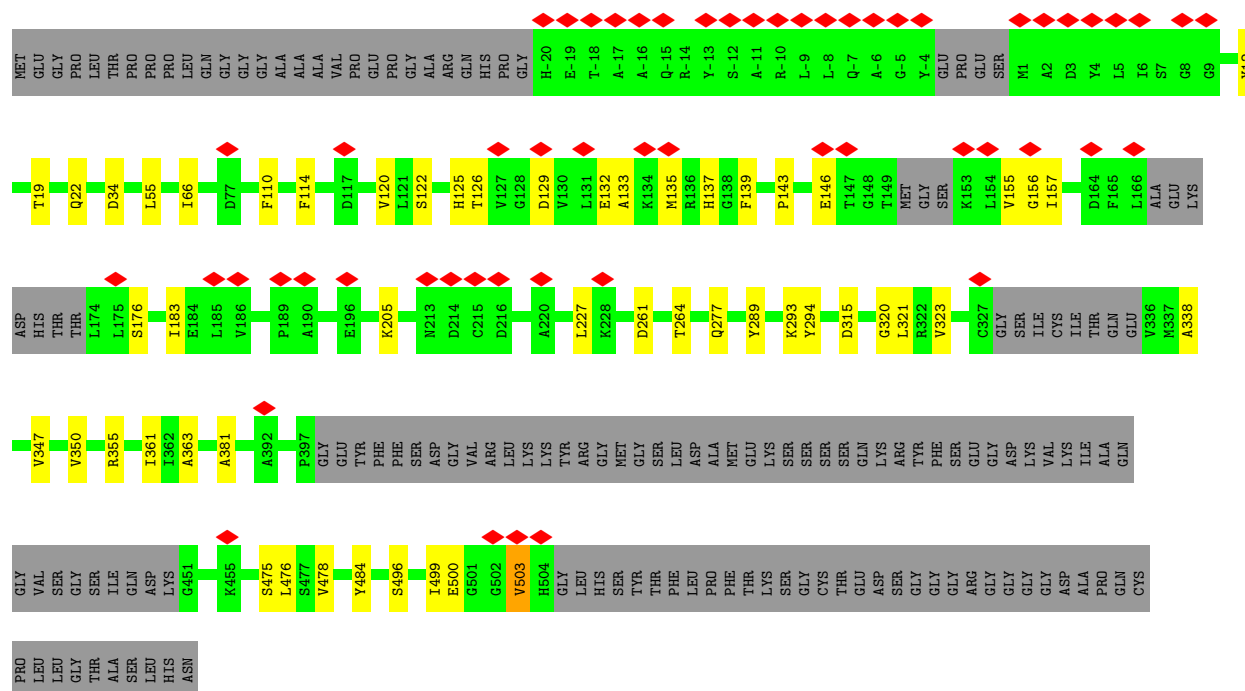


- Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1

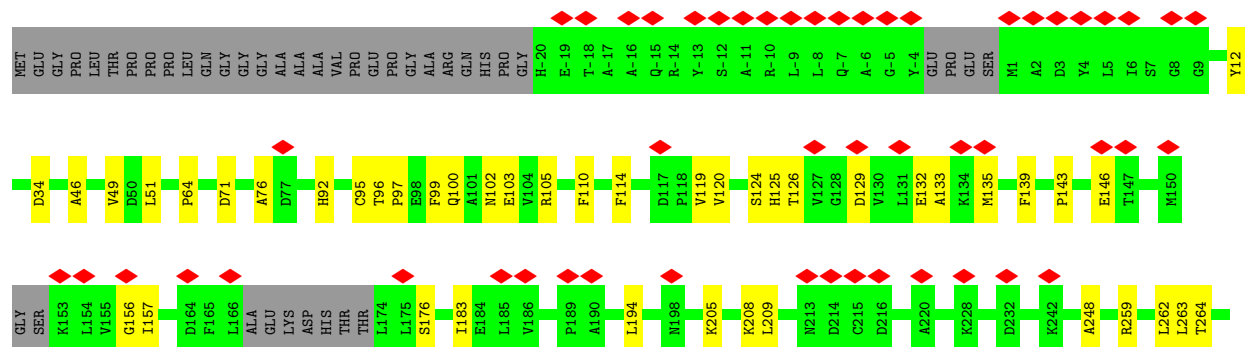


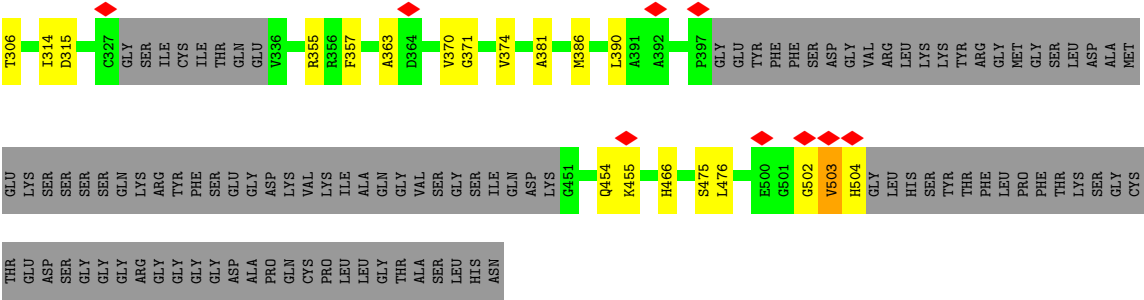


• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.224	Depositor
Minimum map value	-6.541	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.279	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.72	0/3425	1.19	3/4629 (0.1%)
1	B	0.71	0/3425	1.19	5/4629 (0.1%)
1	C	0.72	0/3425	1.21	3/4629 (0.1%)
1	D	0.72	0/3425	1.21	3/4629 (0.1%)
1	E	0.69	0/3425	1.13	4/4629 (0.1%)
1	F	0.72	1/3425 (0.0%)	1.20	7/4629 (0.2%)
1	G	0.70	0/3434	1.19	3/4640 (0.1%)
1	H	0.69	0/3442	1.18	5/4650 (0.1%)
All	All	0.71	1/27426 (0.0%)	1.19	33/37064 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	231	ARG	CZ-NH2	-5.49	1.26	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	CYS	CA-C-N	7.30	133.00	122.35
1	B	215	CYS	C-N-CA	7.30	133.00	122.35
1	E	503	VAL	N-CA-C	7.16	124.23	109.34
1	D	503	VAL	N-CA-C	7.11	124.12	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	315	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	315	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	315	ASP	CA-CB-CG	6.64	119.24	112.60
1	F	315	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	315	ASP	CA-CB-CG	6.54	119.14	112.60
1	G	315	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	315	ASP	CA-CB-CG	6.35	118.95	112.60
1	E	315	ASP	CA-CB-CG	6.28	118.88	112.60
1	F	502	GLY	CA-C-N	6.06	132.88	121.97
1	F	502	GLY	C-N-CA	6.06	132.88	121.97
1	H	502	GLY	CA-C-N	5.82	132.45	121.97
1	H	502	GLY	C-N-CA	5.82	132.45	121.97
1	B	215	CYS	O-C-N	-5.72	114.57	122.46
1	B	114	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	114	PHE	CA-CB-CG	5.50	119.30	113.80
1	C	502	GLY	CA-C-N	5.38	131.65	121.97
1	C	502	GLY	C-N-CA	5.38	131.65	121.97
1	E	114	PHE	CA-CB-CG	5.34	119.14	113.80
1	F	114	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	164	ASP	CA-CB-CG	5.32	117.92	112.60
1	F	454	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	G	114	PHE	CA-CB-CG	5.27	119.07	113.80
1	G	110	PHE	N-CA-C	5.25	116.81	111.14
1	H	114	PHE	CA-CB-CG	5.15	118.95	113.80
1	F	503	VAL	N-CA-C	5.12	120.00	109.34
1	H	110	PHE	N-CA-C	5.11	116.93	111.36
1	F	110	PHE	N-CA-C	5.07	116.61	111.14
1	A	110	PHE	N-CA-C	5.06	116.60	111.14
1	E	110	PHE	N-CA-C	5.01	116.55	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	282	TYR	Sidechain

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	3377	3446	3446	34	0
1	B	3377	3446	3446	47	0
1	C	3377	3446	3446	26	0
1	D	3377	3446	3446	27	0
1	E	3377	3446	3446	56	0
1	F	3377	3446	3446	45	0
1	G	3386	3459	3459	29	0
1	H	3394	3468	3468	37	0
2	A	62	24	24	0	0
2	B	62	24	24	0	0
2	C	62	24	24	0	0
2	D	62	24	24	0	0
2	E	62	24	24	0	0
2	F	62	24	24	0	0
2	G	62	24	24	0	0
2	H	62	24	24	0	0
All	All	27538	27795	27795	294	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 5.

All (294) 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:B:320:GLY:O	1:B:321:LEU:HG	1.77	0.85
1:D:320:GLY:O	1:D:321:LEU:HG	1.77	0.85
1:C:320:GLY:O	1:C:321:LEU:HG	1.77	0.84
1:B:120:VAL:HG11	1:B:145:THR:HG22	1.58	0.83
1:G:320:GLY:O	1:G:321:LEU:HG	1.78	0.83
1:A:320:GLY:O	1:A:321:LEU:HG	1.77	0.83
1:E:320:GLY:O	1:E:321:LEU:HG	1.78	0.82
1:F:29:GLY:HA3	1:F:342:PRO:HG2	1.63	0.80
1:A:29:GLY:HA3	1:A:342:PRO:HG2	1.62	0.79
1:C:370:VAL:O	1:C:374:VAL:HG23	1.85	0.77
1:D:370:VAL:O	1:D:374:VAL:HG23	1.85	0.77
1:E:370:VAL:O	1:E:374:VAL:HG23	1.85	0.77
1:F:370:VAL:O	1:F:374:VAL:HG23	1.85	0.76
1:B:146:GLU:N	1:B:146:GLU:OE1	2.19	0.76
1:G:293:LYS:HG2	1:G:294:TYR:CE1	2.22	0.74
1:C:293:LYS:HG2	1:C:294:TYR:CE1	2.23	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LYS:HG2	1:D:294:TYR:CE1	2.22	0.74
1:A:293:LYS:HG2	1:A:294:TYR:CE1	2.23	0.74
1:E:293:LYS:HG2	1:E:294:TYR:CE1	2.23	0.74
1:F:183:ILE:O	1:F:183:ILE:HG13	1.92	0.69
1:F:29:GLY:CA	1:F:342:PRO:HG2	2.24	0.68
1:A:29:GLY:CA	1:A:342:PRO:HG2	2.24	0.67
1:B:120:VAL:CG1	1:B:145:THR:HG22	2.23	0.67
1:B:146:GLU:HG2	1:B:147:THR:HG22	1.78	0.66
1:C:289:TYR:CE1	1:C:293:LYS:HE3	2.30	0.66
1:F:127:VAL:HG23	1:F:127:VAL:O	1.95	0.65
1:F:367:ILE:CD1	1:F:384:VAL:HG13	2.27	0.64
1:H:102:ASN:OD1	1:H:105:ARG:NH2	2.30	0.64
1:G:261:ASP:O	1:G:264:THR:HG22	1.97	0.64
1:F:123:PRO:HG3	1:F:155:VAL:HG21	1.79	0.64
1:E:261:ASP:O	1:E:264:THR:HG22	1.98	0.63
1:E:102:ASN:OD1	1:E:105:ARG:NH2	2.32	0.63
1:E:126:THR:HG23	1:E:174:LEU:O	1.99	0.63
1:E:386:MET:HE3	1:E:390:LEU:HD11	1.80	0.63
1:E:36:LEU:CD1	1:E:493:ARG:HD3	2.29	0.62
1:F:126:THR:HG23	1:F:174:LEU:O	1.98	0.62
1:G:120:VAL:HG22	1:G:143:PRO:HG2	1.81	0.62
1:B:386:MET:HE3	1:B:390:LEU:HD11	1.81	0.62
1:B:102:ASN:OD1	1:B:105:ARG:NH2	2.31	0.62
1:C:386:MET:HE3	1:C:390:LEU:HD11	1.82	0.61
1:F:131:LEU:HD12	1:F:131:LEU:O	2.00	0.60
1:H:386:MET:HE3	1:H:390:LEU:HD11	1.83	0.60
1:B:132:GLU:OE1	1:B:133:ALA:N	2.35	0.60
1:F:132:GLU:OE1	1:F:133:ALA:N	2.35	0.60
1:B:132:GLU:O	1:B:135:MET:N	2.35	0.60
1:A:386:MET:HE3	1:A:390:LEU:HD11	1.83	0.59
1:D:132:GLU:OE1	1:D:133:ALA:N	2.35	0.59
1:E:323:VAL:HG22	1:E:350:VAL:HG11	1.83	0.59
1:G:323:VAL:HG22	1:G:350:VAL:HG11	1.83	0.59
1:A:323:VAL:HG22	1:A:350:VAL:HG11	1.84	0.59
1:B:323:VAL:HG22	1:B:350:VAL:HG11	1.83	0.59
1:D:132:GLU:O	1:D:135:MET:N	2.35	0.59
1:H:132:GLU:OE1	1:H:133:ALA:N	2.35	0.59
1:B:96:THR:CG2	1:B:97:PRO:HD2	2.33	0.59
1:C:323:VAL:HG22	1:C:350:VAL:HG11	1.84	0.59
1:D:323:VAL:HG22	1:D:350:VAL:HG11	1.84	0.59
1:E:132:GLU:O	1:E:135:MET:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ALA:HB2	1:E:103:GLU:OE1	2.03	0.59
1:F:132:GLU:O	1:F:135:MET:N	2.36	0.59
1:B:76:ALA:HB2	1:B:103:GLU:OE1	2.03	0.58
1:E:132:GLU:OE1	1:E:133:ALA:N	2.35	0.58
1:F:367:ILE:HD13	1:F:384:VAL:HG13	1.84	0.58
1:G:132:GLU:OE1	1:G:133:ALA:N	2.36	0.58
1:E:96:THR:CG2	1:E:97:PRO:HD2	2.34	0.58
1:C:132:GLU:O	1:C:135:MET:N	2.36	0.58
1:C:132:GLU:OE1	1:C:133:ALA:N	2.36	0.58
1:H:96:THR:CG2	1:H:97:PRO:HD2	2.33	0.58
1:G:132:GLU:O	1:G:135:MET:N	2.36	0.58
1:H:76:ALA:HB2	1:H:103:GLU:OE1	2.03	0.57
1:D:386:MET:HE3	1:D:390:LEU:HD11	1.85	0.57
1:H:132:GLU:O	1:H:135:MET:N	2.38	0.57
1:E:36:LEU:HD12	1:E:493:ARG:HD3	1.87	0.56
1:E:100:GLN:OE1	1:E:259:ARG:NH1	2.39	0.56
1:B:145:THR:HG23	1:B:146:GLU:OE1	2.06	0.56
1:B:323:VAL:HG21	1:B:361:ILE:HD12	1.87	0.56
1:A:132:GLU:OE1	1:A:133:ALA:N	2.38	0.56
1:G:125:HIS:NE2	1:G:129:ASP:HB2	2.22	0.55
1:A:132:GLU:O	1:A:135:MET:N	2.38	0.55
1:E:323:VAL:HG21	1:E:361:ILE:HD12	1.87	0.55
1:A:323:VAL:HG21	1:A:361:ILE:HD12	1.88	0.55
1:H:100:GLN:OE1	1:H:259:ARG:NH1	2.38	0.55
1:F:183:ILE:O	1:F:183:ILE:CG1	2.54	0.55
1:B:95:CYS:HB2	1:B:99:PHE:HD2	1.72	0.54
1:D:323:VAL:HG21	1:D:361:ILE:HD12	1.87	0.54
1:B:100:GLN:OE1	1:B:259:ARG:NH1	2.38	0.54
1:F:166:LEU:N	1:F:166:LEU:HD23	2.23	0.54
1:G:323:VAL:HG21	1:G:361:ILE:HD12	1.88	0.54
1:C:323:VAL:HG21	1:C:361:ILE:HD12	1.88	0.54
1:F:125:HIS:NE2	1:F:129:ASP:HB2	2.23	0.54
1:E:95:CYS:HB2	1:E:99:PHE:HD2	1.73	0.54
1:B:146:GLU:CG	1:B:147:THR:H	2.20	0.54
1:E:125:HIS:NE2	1:E:129:ASP:HB2	2.23	0.54
1:H:126:THR:HA	1:H:176:SER:HA	1.89	0.54
1:B:146:GLU:HG2	1:B:147:THR:H	1.72	0.53
1:B:146:GLU:HG2	1:B:147:THR:N	2.24	0.53
1:H:95:CYS:HB2	1:H:99:PHE:HD2	1.73	0.53
1:A:37:ILE:CG2	1:A:488:LEU:HD11	2.39	0.53
1:D:323:VAL:CG2	1:D:361:ILE:HD12	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HD22	1:F:163:ILE:CG2	2.38	0.53
1:G:19:THR:HG22	1:G:22:GLN:NE2	2.24	0.52
1:G:126:THR:HA	1:G:176:SER:HA	1.90	0.52
1:G:363:ALA:HB2	1:G:381:ALA:HB2	1.92	0.52
1:E:323:VAL:CG2	1:E:361:ILE:HD12	2.40	0.52
1:A:323:VAL:CG2	1:A:361:ILE:HD12	2.40	0.52
1:B:323:VAL:CG2	1:B:361:ILE:HD12	2.39	0.52
1:E:37:ILE:CG2	1:E:488:LEU:HD11	2.40	0.52
1:F:121:LEU:HG	1:F:130:VAL:HG22	1.92	0.52
1:E:126:THR:HA	1:E:176:SER:HA	1.92	0.51
1:B:363:ALA:HB2	1:B:381:ALA:HB2	1.93	0.51
1:E:363:ALA:HB2	1:E:381:ALA:HB2	1.92	0.51
1:F:144:ILE:HG13	1:F:155:VAL:HG23	1.91	0.51
1:B:46:ALA:HB1	1:B:466:HIS:HD2	1.77	0.50
1:D:363:ALA:HB2	1:D:381:ALA:HB2	1.92	0.50
1:A:375:LYS:O	1:A:378:ALA:N	2.45	0.50
1:H:120:VAL:HG22	1:H:143:PRO:HG2	1.93	0.50
1:B:96:THR:HG23	1:B:97:PRO:HD2	1.93	0.50
1:F:363:ALA:HB2	1:F:381:ALA:HB2	1.94	0.50
1:G:289:TYR:CE1	1:G:293:LYS:HE3	2.47	0.50
1:C:323:VAL:CG2	1:C:361:ILE:HD12	2.40	0.50
1:H:46:ALA:HB1	1:H:466:HIS:HD2	1.77	0.49
1:A:289:TYR:CE1	1:A:293:LYS:HE3	2.47	0.49
1:F:126:THR:HA	1:F:176:SER:HA	1.93	0.49
1:H:125:HIS:NE2	1:H:129:ASP:HB2	2.27	0.49
1:G:323:VAL:CG2	1:G:361:ILE:HD12	2.41	0.49
1:D:37:ILE:CG2	1:D:488:LEU:HD11	2.42	0.49
1:A:363:ALA:HB2	1:A:381:ALA:HB2	1.93	0.49
1:E:289:TYR:CE1	1:E:293:LYS:HE3	2.48	0.49
1:E:375:LYS:O	1:E:378:ALA:N	2.46	0.49
1:D:323:VAL:HG11	1:D:347:VAL:HA	1.95	0.49
1:D:375:LYS:O	1:D:378:ALA:N	2.46	0.49
1:E:174:LEU:HD12	1:E:174:LEU:N	2.28	0.49
1:B:120:VAL:HG22	1:B:143:PRO:HG2	1.93	0.49
1:E:46:ALA:HB1	1:E:466:HIS:HD2	1.77	0.48
1:A:314:ILE:HD13	1:A:357:PHE:HD2	1.79	0.48
1:B:146:GLU:CG	1:B:147:THR:N	2.77	0.48
1:D:289:TYR:CE1	1:D:293:LYS:HE3	2.48	0.48
1:F:174:LEU:N	1:F:174:LEU:HD12	2.27	0.48
1:D:46:ALA:HB1	1:D:466:HIS:HD2	1.79	0.48
1:E:314:ILE:HD13	1:E:357:PHE:HD2	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:GLN:CD	1:H:263:LEU:HD11	2.39	0.48
1:H:363:ALA:HB2	1:H:381:ALA:HB2	1.94	0.48
1:E:132:GLU:O	1:E:135:MET:HB2	2.14	0.48
1:F:314:ILE:HD13	1:F:357:PHE:HD2	1.79	0.48
1:H:314:ILE:HD13	1:H:357:PHE:HD2	1.79	0.48
1:C:314:ILE:HD13	1:C:357:PHE:HD2	1.79	0.48
1:F:46:ALA:HB1	1:F:466:HIS:HD2	1.79	0.48
1:H:96:THR:HG23	1:H:97:PRO:HD2	1.95	0.48
1:C:132:GLU:O	1:C:135:MET:HB2	2.14	0.48
1:B:314:ILE:HD13	1:B:357:PHE:HD2	1.79	0.48
1:C:46:ALA:HB1	1:C:466:HIS:HD2	1.78	0.48
1:E:323:VAL:HG11	1:E:347:VAL:HA	1.96	0.47
1:C:314:ILE:HG21	1:C:357:PHE:CD2	2.49	0.47
1:A:46:ALA:HB1	1:A:466:HIS:HD2	1.78	0.47
1:A:323:VAL:HG11	1:A:347:VAL:HA	1.96	0.47
1:C:323:VAL:HG11	1:C:347:VAL:HA	1.96	0.47
1:E:265:GLN:OE1	1:E:265:GLN:HA	2.14	0.47
1:B:132:GLU:O	1:B:135:MET:HB2	2.14	0.47
1:E:96:THR:HG23	1:E:97:PRO:HD2	1.96	0.47
1:B:265:GLN:OE1	1:B:265:GLN:HA	2.13	0.47
1:H:124:SER:O	1:H:124:SER:OG	2.33	0.47
1:G:355:ARG:HD3	1:G:484:TYR:CE2	2.50	0.47
1:D:132:GLU:O	1:D:135:MET:HB2	2.14	0.47
1:G:125:HIS:NE2	1:G:129:ASP:CB	2.78	0.47
1:G:132:GLU:O	1:G:135:MET:HB2	2.15	0.47
1:A:323:VAL:O	1:A:323:VAL:HG12	2.15	0.46
1:C:323:VAL:O	1:C:323:VAL:HG12	2.15	0.46
1:E:314:ILE:HG21	1:E:357:PHE:CD2	2.49	0.46
1:E:323:VAL:O	1:E:323:VAL:HG12	2.15	0.46
1:G:323:VAL:O	1:G:323:VAL:HG12	2.15	0.46
1:G:323:VAL:HG11	1:G:347:VAL:HA	1.97	0.46
1:F:314:ILE:HG21	1:F:357:PHE:CD2	2.50	0.46
1:H:132:GLU:O	1:H:135:MET:HB2	2.15	0.46
1:H:314:ILE:HG21	1:H:357:PHE:CD2	2.50	0.46
1:F:125:HIS:NE2	1:F:129:ASP:CB	2.79	0.46
1:A:314:ILE:HG21	1:A:357:PHE:CD2	2.50	0.46
1:B:323:VAL:HG11	1:B:347:VAL:HA	1.97	0.46
1:F:132:GLU:O	1:F:135:MET:HB2	2.14	0.46
1:E:125:HIS:NE2	1:E:129:ASP:CB	2.78	0.46
1:B:370:VAL:O	1:B:374:VAL:HG23	2.16	0.46
1:D:323:VAL:HG12	1:D:323:VAL:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:O	1:F:158:VAL:HG13	2.15	0.46
1:F:460:LEU:HD23	1:F:460:LEU:HA	1.75	0.46
1:F:177:GLU:OE1	1:F:177:GLU:HA	2.15	0.46
1:F:363:ALA:O	1:F:367:ILE:HD11	2.16	0.46
1:H:96:THR:HG22	1:H:97:PRO:HD2	1.97	0.46
1:A:132:GLU:O	1:A:135:MET:HB2	2.17	0.45
1:E:96:THR:HG22	1:E:97:PRO:HD2	1.97	0.45
1:F:121:LEU:HG	1:F:130:VAL:CG2	2.45	0.45
1:H:370:VAL:O	1:H:374:VAL:HG23	2.17	0.45
1:B:314:ILE:HG21	1:B:357:PHE:CD2	2.51	0.45
1:C:363:ALA:HB2	1:C:381:ALA:HB2	1.99	0.45
1:H:119:VAL:HB	1:H:139:PHE:HZ	1.80	0.45
1:A:370:VAL:O	1:A:374:VAL:HG23	2.16	0.45
1:F:49:VAL:O	1:F:49:VAL:HG12	2.17	0.45
1:H:125:HIS:NE2	1:H:129:ASP:CB	2.79	0.45
1:C:257:LYS:HD3	1:C:289:TYR:CE1	2.52	0.45
1:F:456:PHE:CD1	1:F:456:PHE:C	2.94	0.45
1:G:137:HIS:HB2	1:G:139:PHE:CE2	2.52	0.45
1:H:96:THR:O	1:H:97:PRO:C	2.61	0.44
1:A:6:ILE:O	1:A:6:ILE:HG13	2.16	0.44
1:F:456:PHE:CD1	1:F:456:PHE:O	2.70	0.44
1:B:96:THR:HG22	1:B:97:PRO:HD2	1.98	0.44
1:B:323:VAL:O	1:B:323:VAL:HG12	2.16	0.44
1:B:145:THR:HG23	1:B:146:GLU:N	2.33	0.44
1:A:132:GLU:OE1	1:A:132:GLU:N	2.51	0.44
1:C:475:SER:O	1:C:476:LEU:C	2.61	0.44
1:G:475:SER:O	1:G:476:LEU:C	2.61	0.44
1:C:49:VAL:O	1:C:49:VAL:HG12	2.18	0.43
1:H:100:GLN:HE21	1:H:248:ALA:HB1	1.82	0.43
1:C:371:GLY:HA2	1:D:338:ALA:HB2	2.00	0.43
1:E:55:LEU:CD1	1:E:66:ILE:HD11	2.48	0.43
1:A:49:VAL:O	1:A:49:VAL:HG12	2.17	0.43
1:A:371:GLY:HA2	1:B:338:ALA:HB2	2.00	0.43
1:A:475:SER:O	1:A:476:LEU:C	2.61	0.43
1:G:500:GLU:C	1:G:500:GLU:CD	2.86	0.43
1:B:49:VAL:O	1:B:49:VAL:HG12	2.19	0.43
1:E:500:GLU:CD	1:E:500:GLU:C	2.85	0.43
1:B:132:GLU:OE1	1:B:132:GLU:N	2.52	0.43
1:E:475:SER:O	1:E:476:LEU:C	2.61	0.43
1:G:132:GLU:OE1	1:G:132:GLU:N	2.51	0.43
1:E:36:LEU:HD11	1:E:493:ARG:HD3	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:SER:O	1:F:125:HIS:HB2	2.19	0.43
1:H:475:SER:O	1:H:476:LEU:C	2.61	0.43
1:A:375:LYS:O	1:A:376:ALA:C	2.59	0.43
1:C:132:GLU:OE1	1:C:132:GLU:N	2.52	0.43
1:D:500:GLU:C	1:D:500:GLU:CD	2.86	0.43
1:E:49:VAL:O	1:E:49:VAL:HG12	2.18	0.43
1:E:96:THR:O	1:E:97:PRO:C	2.61	0.43
1:E:375:LYS:O	1:E:376:ALA:C	2.60	0.43
1:F:367:ILE:HD13	1:F:384:VAL:CG1	2.49	0.43
1:F:371:GLY:HA2	1:G:338:ALA:HB2	2.00	0.43
1:H:49:VAL:O	1:H:49:VAL:HG12	2.18	0.43
1:B:475:SER:O	1:B:476:LEU:C	2.61	0.42
1:D:375:LYS:O	1:D:376:ALA:C	2.60	0.42
1:D:475:SER:O	1:D:476:LEU:C	2.61	0.42
1:E:122:SER:O	1:E:125:HIS:HB2	2.19	0.42
1:E:132:GLU:OE1	1:E:132:GLU:N	2.52	0.42
1:H:119:VAL:HB	1:H:139:PHE:CZ	2.54	0.42
1:B:371:GLY:HA2	1:C:338:ALA:HB2	2.00	0.42
1:D:132:GLU:OE1	1:D:132:GLU:N	2.52	0.42
1:G:55:LEU:CD1	1:G:66:ILE:HD11	2.48	0.42
1:B:96:THR:O	1:B:97:PRO:C	2.60	0.42
1:F:132:GLU:OE1	1:F:132:GLU:N	2.51	0.42
1:H:71:ASP:HA	1:H:92:HIS:CD2	2.54	0.42
1:B:146:GLU:CD	1:B:147:THR:H	2.28	0.42
1:G:363:ALA:HB2	1:G:381:ALA:CB	2.49	0.42
1:H:97:PRO:CB	1:H:262:LEU:HD12	2.50	0.42
1:H:248:ALA:HB1	1:H:263:LEU:HD13	2.02	0.42
1:A:326:GLY:HA2	1:A:337:MET:SD	2.60	0.42
1:E:323:VAL:HG21	1:E:361:ILE:CD1	2.50	0.42
1:F:326:GLY:HA2	1:F:337:MET:SD	2.59	0.42
1:F:367:ILE:HD12	1:F:384:VAL:HG13	2.01	0.42
1:E:363:ALA:HB2	1:E:381:ALA:CB	2.49	0.42
1:G:323:VAL:CG2	1:G:350:VAL:HG11	2.50	0.42
1:C:323:VAL:CG2	1:C:350:VAL:HG11	2.50	0.42
1:F:475:SER:O	1:F:476:LEU:C	2.61	0.42
1:B:97:PRO:CB	1:B:262:LEU:HD12	2.50	0.41
1:E:326:GLY:HA2	1:E:337:MET:SD	2.60	0.41
1:G:475:SER:O	1:G:478:VAL:N	2.53	0.41
1:A:323:VAL:HG21	1:A:361:ILE:CD1	2.50	0.41
1:E:97:PRO:CB	1:E:262:LEU:HD12	2.50	0.41
1:E:337:MET:O	1:E:338:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:SER:O	1:G:125:HIS:HB2	2.20	0.41
1:H:454:GLN:CD	1:H:454:GLN:H	2.28	0.41
1:A:338:ALA:HB2	1:D:371:GLY:HA2	2.02	0.41
1:E:71:ASP:HA	1:E:92:HIS:CD2	2.55	0.41
1:E:371:GLY:HA2	1:F:338:ALA:HB2	2.02	0.41
1:F:337:MET:O	1:F:338:ALA:HB3	2.20	0.41
1:A:337:MET:O	1:A:338:ALA:HB3	2.20	0.41
1:B:46:ALA:CB	1:B:466:HIS:HD2	2.33	0.41
1:C:289:TYR:HE1	1:C:293:LYS:HE3	1.83	0.41
1:E:338:ALA:HB2	1:H:371:GLY:HA2	2.02	0.41
1:E:264:THR:HG23	1:E:265:GLN:NE2	2.35	0.41
1:B:475:SER:O	1:B:478:VAL:N	2.53	0.41
1:D:363:ALA:HB2	1:D:381:ALA:CB	2.49	0.41
1:H:132:GLU:OE1	1:H:132:GLU:N	2.53	0.41
1:A:46:ALA:CB	1:A:466:HIS:HD2	2.34	0.41
1:E:46:ALA:CB	1:E:466:HIS:HD2	2.34	0.41
1:A:32:TYR:OH	1:A:376:ALA:HB2	2.21	0.41
1:D:323:VAL:HG21	1:D:361:ILE:CD1	2.50	0.41
1:E:51:LEU:HB3	1:E:64:PRO:HD3	2.03	0.41
1:F:46:ALA:CB	1:F:466:HIS:HD2	2.34	0.41
1:C:46:ALA:CB	1:C:466:HIS:HD2	2.33	0.41
1:F:456:PHE:O	1:F:459:TYR:HB3	2.21	0.41
1:B:363:ALA:HB2	1:B:381:ALA:CB	2.50	0.40
1:D:46:ALA:CB	1:D:466:HIS:HD2	2.33	0.40
1:D:323:VAL:CG2	1:D:350:VAL:HG11	2.51	0.40
1:H:96:THR:O	1:H:99:PHE:N	2.54	0.40
1:A:363:ALA:HB2	1:A:381:ALA:CB	2.50	0.40
1:B:323:VAL:HG21	1:B:361:ILE:CD1	2.49	0.40
1:E:32:TYR:OH	1:E:376:ALA:HB2	2.22	0.40
1:B:51:LEU:HB3	1:B:64:PRO:HD3	2.04	0.40
1:H:46:ALA:CB	1:H:466:HIS:HD2	2.34	0.40
1:H:51:LEU:HB3	1:H:64:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	437/595 (73%)	393 (90%)	39 (9%)	5 (1%)	11	42
1	B	437/595 (73%)	394 (90%)	39 (9%)	4 (1%)	14	45
1	C	437/595 (73%)	396 (91%)	36 (8%)	5 (1%)	11	42
1	D	437/595 (73%)	399 (91%)	33 (8%)	5 (1%)	11	42
1	E	437/595 (73%)	389 (89%)	44 (10%)	4 (1%)	14	45
1	F	437/595 (73%)	396 (91%)	37 (8%)	4 (1%)	14	45
1	G	438/595 (74%)	394 (90%)	39 (9%)	5 (1%)	11	42
1	H	439/595 (74%)	394 (90%)	39 (9%)	6 (1%)	9	37
All	All	3499/4760 (74%)	3155 (90%)	306 (9%)	38 (1%)	14	42

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	503	VAL
1	D	503	VAL
1	D	183	ILE
1	E	503	VAL
1	F	182	ARG
1	F	503	VAL
1	G	503	VAL
1	H	183	ILE
1	H	503	VAL
1	A	12	TYR
1	B	12	TYR
1	B	180	THR
1	C	12	TYR
1	D	12	TYR
1	E	12	TYR
1	F	12	TYR
1	G	12	TYR
1	H	12	TYR
1	H	355	ARG
1	A	205	LYS
1	C	183	ILE
1	C	205	LYS
1	D	205	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	183	ILE
1	E	205	LYS
1	F	205	LYS
1	G	183	ILE
1	G	205	LYS
1	H	156	GLY
1	H	205	LYS
1	C	127	VAL
1	G	156	GLY
1	B	113	GLY
1	A	180	THR
1	A	503	VAL
1	B	183	ILE
1	A	113	GLY
1	D	186	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 PDB entries followed by that with respect to all EM entries.

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	362/474 (76%)	352 (97%)	10 (3%)	38	58
1	B	362/474 (76%)	352 (97%)	10 (3%)	38	58
1	C	362/474 (76%)	354 (98%)	8 (2%)	45	63
1	D	362/474 (76%)	352 (97%)	10 (3%)	38	58
1	E	362/474 (76%)	353 (98%)	9 (2%)	42	61
1	F	362/474 (76%)	350 (97%)	12 (3%)	33	55
1	G	363/474 (77%)	354 (98%)	9 (2%)	42	61
1	H	364/474 (77%)	353 (97%)	11 (3%)	36	57
All	All	2899/3792 (76%)	2820 (97%)	79 (3%)	40	59

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	146	GLU
1	A	155	VAL
1	A	157	ILE
1	A	201	LEU
1	A	264	THR
1	A	283	GLN
1	A	455	LYS
1	A	496	SER
1	A	504	HIS
1	B	34	ASP
1	B	126	THR
1	B	157	ILE
1	B	175	LEU
1	B	180	THR
1	B	201	LEU
1	B	206	LYS
1	B	264	THR
1	B	277	GLN
1	B	342	PRO
1	C	7	SER
1	C	34	ASP
1	C	125	HIS
1	C	146	GLU
1	C	157	ILE
1	C	194	LEU
1	C	264	THR
1	C	455	LYS
1	D	34	ASP
1	D	146	GLU
1	D	157	ILE
1	D	194	LEU
1	D	201	LEU
1	D	206	LYS
1	D	264	THR
1	D	496	SER
1	D	503	VAL
1	D	504	HIS
1	E	34	ASP
1	E	130	VAL
1	E	146	GLU
1	E	157	ILE
1	E	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	194	LEU
1	E	211	ILE
1	E	503	VAL
1	E	504	HIS
1	F	34	ASP
1	F	146	GLU
1	F	157	ILE
1	F	179	MET
1	F	194	LEU
1	F	201	LEU
1	F	209	LEU
1	F	264	THR
1	F	277	GLN
1	F	455	LYS
1	F	503	VAL
1	F	504	HIS
1	G	34	ASP
1	G	146	GLU
1	G	155	VAL
1	G	157	ILE
1	G	227	LEU
1	G	277	GLN
1	G	496	SER
1	G	499	ILE
1	G	503	VAL
1	H	34	ASP
1	H	146	GLU
1	H	157	ILE
1	H	194	LEU
1	H	208	LYS
1	H	209	LEU
1	H	264	THR
1	H	306	THR
1	H	455	LYS
1	H	503	VAL
1	H	504	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	243	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	296	HIS
1	A	298	GLN
1	A	312	ASN
1	A	466	HIS
1	B	112	GLN
1	B	296	HIS
1	B	312	ASN
1	B	466	HIS
1	B	504	HIS
1	C	243	GLN
1	C	296	HIS
1	C	312	ASN
1	C	466	HIS
1	C	504	HIS
1	D	112	GLN
1	D	230	ASN
1	D	243	GLN
1	D	283	GLN
1	D	296	HIS
1	D	298	GLN
1	D	312	ASN
1	D	466	HIS
1	E	230	ASN
1	E	243	GLN
1	E	265	GLN
1	E	283	GLN
1	E	296	HIS
1	E	312	ASN
1	E	372	HIS
1	E	466	HIS
1	F	230	ASN
1	F	243	GLN
1	F	312	ASN
1	F	466	HIS
1	G	22	GLN
1	G	112	GLN
1	G	230	ASN
1	G	243	GLN
1	G	296	HIS
1	G	312	ASN
1	G	498	GLN
1	H	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	230	ASN
1	H	283	GLN
1	H	372	HIS
1	H	466	HIS

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](#)

16 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	ATP	A	602	-	32,33,33	1.14	1 (3%)	48,52,52	1.29	5 (10%)
2	ATP	A	601	-	32,33,33	1.15	3 (9%)	48,52,52	1.25	6 (12%)
2	ATP	D	601	-	32,33,33	1.26	3 (9%)	48,52,52	1.17	5 (10%)
2	ATP	B	601	-	32,33,33	1.26	3 (9%)	48,52,52	1.22	3 (6%)
2	ATP	D	602	-	32,33,33	1.15	2 (6%)	48,52,52	1.15	5 (10%)
2	ATP	E	602	-	32,33,33	1.26	4 (12%)	48,52,52	1.21	4 (8%)
2	ATP	G	602	-	32,33,33	1.19	3 (9%)	48,52,52	1.24	6 (12%)
2	ATP	E	601	-	32,33,33	1.19	3 (9%)	48,52,52	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	H	602	-	32,33,33	1.21	3 (9%)	48,52,52	1.22	7 (14%)
2	ATP	C	602	-	32,33,33	1.17	2 (6%)	48,52,52	1.32	5 (10%)
2	ATP	F	601	-	32,33,33	1.26	3 (9%)	48,52,52	1.20	6 (12%)
2	ATP	C	601	-	32,33,33	1.20	3 (9%)	48,52,52	1.15	4 (8%)
2	ATP	H	601	-	32,33,33	1.38	4 (12%)	48,52,52	1.20	5 (10%)
2	ATP	G	601	-	32,33,33	1.20	3 (9%)	48,52,52	1.23	6 (12%)
2	ATP	F	602	-	32,33,33	1.22	3 (9%)	48,52,52	1.26	6 (12%)
2	ATP	B	602	-	32,33,33	1.14	2 (6%)	48,52,52	1.23	6 (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
2	ATP	A	602	-	-	6/22/38/38	0/3/3/3
2	ATP	A	601	-	-	6/22/38/38	0/3/3/3
2	ATP	D	601	-	-	5/22/38/38	0/3/3/3
2	ATP	B	601	-	-	5/22/38/38	0/3/3/3
2	ATP	D	602	-	-	2/22/38/38	0/3/3/3
2	ATP	E	602	-	-	2/22/38/38	0/3/3/3
2	ATP	G	602	-	-	3/22/38/38	0/3/3/3
2	ATP	E	601	-	-	3/22/38/38	0/3/3/3
2	ATP	H	602	-	-	3/22/38/38	0/3/3/3
2	ATP	C	602	-	-	6/22/38/38	0/3/3/3
2	ATP	F	601	-	-	3/22/38/38	0/3/3/3
2	ATP	C	601	-	-	3/22/38/38	0/3/3/3
2	ATP	H	601	-	-	3/22/38/38	0/3/3/3
2	ATP	G	601	-	-	5/22/38/38	0/3/3/3
2	ATP	F	602	-	-	0/22/38/38	0/3/3/3
2	ATP	B	602	-	-	0/22/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	602	ATP	PA-O3A	-3.45	1.55	1.59
2	B	601	ATP	PA-O3A	-3.33	1.55	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	ATP	PA-O3A	-3.28	1.56	1.59
2	F	601	ATP	PA-O3A	-3.24	1.56	1.59
2	H	601	ATP	PB-O3B	-3.20	1.56	1.59
2	H	602	ATP	PA-O3A	-3.19	1.56	1.59
2	D	601	ATP	PB-O3A	-3.07	1.56	1.59
2	C	601	ATP	PA-O3A	-3.01	1.56	1.59
2	H	601	ATP	PB-O3A	-2.98	1.56	1.59
2	F	602	ATP	PA-O3A	-2.95	1.56	1.59
2	E	601	ATP	PA-O3A	-2.90	1.56	1.59
2	G	601	ATP	PA-O3A	-2.90	1.56	1.59
2	D	601	ATP	PA-O3A	-2.86	1.56	1.59
2	B	602	ATP	PA-O3A	-2.74	1.56	1.59
2	D	602	ATP	PA-O3A	-2.65	1.56	1.59
2	B	601	ATP	PB-O3A	-2.53	1.56	1.59
2	G	602	ATP	PA-O3A	-2.52	1.56	1.59
2	H	602	ATP	PB-O3B	-2.47	1.56	1.59
2	F	602	ATP	PB-O3B	-2.42	1.56	1.59
2	A	601	ATP	PA-O3A	-2.38	1.56	1.59
2	C	602	ATP	PA-O3A	-2.38	1.56	1.59
2	G	602	ATP	PB-O3B	-2.32	1.57	1.59
2	E	602	ATP	PB-O3A	-2.31	1.57	1.59
2	A	601	ATP	PB-O3B	-2.22	1.57	1.59
2	A	602	ATP	PA-O3A	-2.21	1.57	1.59
2	E	602	ATP	PB-O3B	-2.21	1.57	1.59
2	G	601	ATP	PB-O3B	-2.20	1.57	1.59
2	H	601	ATP	C5-C4	-2.17	1.35	1.39
2	A	601	ATP	C5-C4	-2.13	1.35	1.39
2	C	601	ATP	C5-C4	-2.12	1.35	1.39
2	D	602	ATP	C5-C4	-2.11	1.35	1.39
2	F	602	ATP	C5-C4	-2.10	1.35	1.39
2	C	601	ATP	PB-O3B	-2.10	1.57	1.59
2	E	602	ATP	C5-C4	-2.10	1.35	1.39
2	B	602	ATP	C5-C4	-2.08	1.35	1.39
2	C	602	ATP	PB-O3B	-2.08	1.57	1.59
2	E	601	ATP	C5-C4	-2.08	1.35	1.39
2	D	601	ATP	C5-C4	-2.08	1.35	1.39
2	E	601	ATP	PB-O3B	-2.06	1.57	1.59
2	G	601	ATP	C5-C4	-2.05	1.35	1.39
2	F	601	ATP	C5-C4	-2.05	1.35	1.39
2	F	601	ATP	PB-O3A	-2.05	1.57	1.59
2	B	601	ATP	C5-C4	-2.03	1.35	1.39
2	H	602	ATP	C5-C4	-2.02	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	602	ATP	C5-C4	-2.02	1.35	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	ATP	O2A-PA-O3A	3.32	116.23	107.27
2	C	602	ATP	O2A-PA-O3A	3.31	116.22	107.27
2	C	602	ATP	O2B-PB-O3B	3.25	116.05	107.27
2	A	602	ATP	O2B-PB-O3B	3.14	115.75	107.27
2	D	602	ATP	C4-C5-N7	3.10	114.12	110.58
2	B	602	ATP	O2B-PB-O3B	3.05	115.51	107.27
2	A	601	ATP	O2A-PA-O3A	3.04	115.48	107.27
2	G	602	ATP	O2B-PB-O3B	2.99	115.35	107.27
2	H	601	ATP	O3G-PG-O3B	2.96	114.58	104.64
2	F	602	ATP	O2B-PB-O3B	2.94	115.21	107.27
2	C	601	ATP	C4-C5-N7	2.93	113.93	110.58
2	F	602	ATP	C4-C5-N7	2.93	113.93	110.58
2	G	602	ATP	C4-C5-N7	2.90	113.90	110.58
2	G	602	ATP	O2A-PA-O3A	2.89	115.09	107.27
2	B	602	ATP	C4-C5-N7	2.89	113.88	110.58
2	C	602	ATP	C4-C5-N7	2.88	113.87	110.58
2	G	601	ATP	O2B-PB-O3A	2.85	114.97	107.27
2	D	601	ATP	O2G-PG-O3B	2.84	114.18	104.64
2	F	602	ATP	O2A-PA-O3A	2.84	114.96	107.27
2	B	601	ATP	C4-C5-N7	2.81	113.80	110.58
2	E	602	ATP	C4-C5-N7	2.80	113.78	110.58
2	F	601	ATP	C4-C5-N7	2.80	113.78	110.58
2	H	602	ATP	C4-C5-N7	2.79	113.78	110.58
2	G	601	ATP	C4-C5-N7	2.78	113.76	110.58
2	A	602	ATP	C4-C5-N7	2.78	113.76	110.58
2	B	602	ATP	O2A-PA-O3A	2.77	114.75	107.27
2	A	601	ATP	C4-C5-N7	2.75	113.73	110.58
2	E	601	ATP	C4-C5-N7	2.74	113.71	110.58
2	B	601	ATP	C5-C4-N3	-2.72	122.97	126.72
2	H	601	ATP	C4-C5-N7	2.72	113.69	110.58
2	E	602	ATP	O2B-PB-O3B	2.68	114.51	107.27
2	D	601	ATP	C4-C5-N7	2.66	113.62	110.58
2	C	601	ATP	O2B-PB-O3A	2.64	114.41	107.27
2	H	601	ATP	C5-C4-N3	-2.64	123.09	126.72
2	A	601	ATP	C5-C4-N3	-2.62	123.11	126.72
2	E	601	ATP	C5-C4-N3	-2.60	123.14	126.72
2	E	602	ATP	C5-C4-N3	-2.57	123.17	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	602	ATP	C5-C4-N3	-2.54	123.22	126.72
2	A	601	ATP	O2G-PG-O3B	2.53	113.12	104.64
2	F	601	ATP	O3G-PG-O3B	2.52	113.09	104.64
2	B	602	ATP	C5-C4-N3	-2.51	123.26	126.72
2	C	602	ATP	C5-C4-N3	-2.50	123.28	126.72
2	D	601	ATP	C5-C4-N3	-2.49	123.28	126.72
2	G	601	ATP	C5-C4-N3	-2.46	123.32	126.72
2	H	601	ATP	O2A-PA-O3A	2.45	113.90	107.27
2	H	602	ATP	O2B-PB-O3A	2.44	113.88	107.27
2	D	602	ATP	C5-C4-N3	-2.44	123.36	126.72
2	F	601	ATP	O2B-PB-O3A	2.43	113.84	107.27
2	F	602	ATP	C5-C4-N3	-2.41	123.39	126.72
2	D	602	ATP	O2B-PB-O3B	2.40	113.75	107.27
2	A	602	ATP	C5-C4-N3	-2.39	123.42	126.72
2	F	602	ATP	O3G-PG-O3B	2.38	112.60	104.64
2	C	601	ATP	O3G-PG-O3B	2.36	112.56	104.64
2	G	601	ATP	O2G-PG-O3B	2.35	112.52	104.64
2	C	602	ATP	O2G-PG-O3B	2.34	112.49	104.64
2	C	601	ATP	C5-C4-N3	-2.32	123.52	126.72
2	E	601	ATP	O2B-PB-O3A	2.31	113.51	107.27
2	A	602	ATP	O2G-PG-O3B	2.31	112.37	104.64
2	D	601	ATP	O2A-PA-O3A	2.29	113.46	107.27
2	G	602	ATP	C5-C4-N3	-2.29	123.56	126.72
2	F	601	ATP	C5-C4-N3	-2.28	123.57	126.72
2	A	601	ATP	O3G-PG-O3B	2.26	112.21	104.64
2	H	602	ATP	O3G-PG-O3B	2.26	112.20	104.64
2	B	601	ATP	O2B-PB-O3A	2.24	113.34	107.27
2	D	602	ATP	O2G-PG-O3B	2.18	111.96	104.64
2	F	601	ATP	O2G-PG-O3B	2.16	111.87	104.64
2	G	601	ATP	N6-C6-N1	-2.15	113.59	118.38
2	D	602	ATP	O2A-PA-O3A	2.14	113.06	107.27
2	G	601	ATP	O3G-PG-O3B	2.14	111.81	104.64
2	A	601	ATP	C2-N1-C6	-2.11	115.26	118.73
2	D	601	ATP	N6-C6-N1	-2.11	113.67	118.38
2	B	602	ATP	O2G-PG-O3B	2.10	111.68	104.64
2	E	601	ATP	N6-C6-N1	-2.10	113.70	118.38
2	H	601	ATP	C2-N1-C6	-2.09	115.29	118.73
2	G	602	ATP	O3G-PG-O3B	2.09	111.65	104.64
2	F	601	ATP	N6-C6-N1	-2.09	113.73	118.38
2	H	602	ATP	C2-N1-C6	-2.08	115.31	118.73
2	E	602	ATP	C2-N1-C6	-2.05	115.36	118.73
2	H	602	ATP	N6-C6-N1	-2.05	113.81	118.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	ATP	N6-C6-N1	-2.03	113.86	118.38
2	G	602	ATP	N6-C6-N1	-2.01	113.90	118.38
2	F	602	ATP	O2B-PB-O3A	2.01	112.69	107.27
2	H	602	ATP	C5-C6-N1	2.00	122.60	117.51

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ATP	C5'-O5'-PA-O1A
2	A	601	ATP	C5'-O5'-PA-O2A
2	A	601	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O2A
2	A	602	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	O4'-C4'-C5'-O5'
2	B	601	ATP	C2'-C1'-N9-C8
2	C	602	ATP	C5'-O5'-PA-O1A
2	C	602	ATP	C5'-O5'-PA-O2A
2	C	602	ATP	C5'-O5'-PA-O3A
2	C	602	ATP	O4'-C4'-C5'-O5'
2	E	602	ATP	C5'-O5'-PA-O3A
2	G	602	ATP	C5'-O5'-PA-O1A
2	G	602	ATP	C5'-O5'-PA-O3A
2	H	602	ATP	C5'-O5'-PA-O1A
2	H	602	ATP	C5'-O5'-PA-O2A
2	H	602	ATP	C5'-O5'-PA-O3A
2	A	602	ATP	C3'-C4'-C5'-O5'
2	C	602	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	O4'-C4'-C5'-O5'
2	A	602	ATP	C4'-C5'-O5'-PA
2	C	602	ATP	C4'-C5'-O5'-PA
2	B	601	ATP	C2'-C1'-N9-C4
2	A	601	ATP	C2'-C1'-N9-C8
2	D	601	ATP	C2'-C1'-N9-C8
2	E	601	ATP	C2'-C1'-N9-C8
2	F	601	ATP	C2'-C1'-N9-C8
2	G	601	ATP	C2'-C1'-N9-C8
2	H	601	ATP	C2'-C1'-N9-C8
2	D	601	ATP	PG-O3B-PB-O1B
2	B	601	ATP	C3'-C4'-C5'-O5'
2	B	601	ATP	C5'-O5'-PA-O1A

Continued on next page...

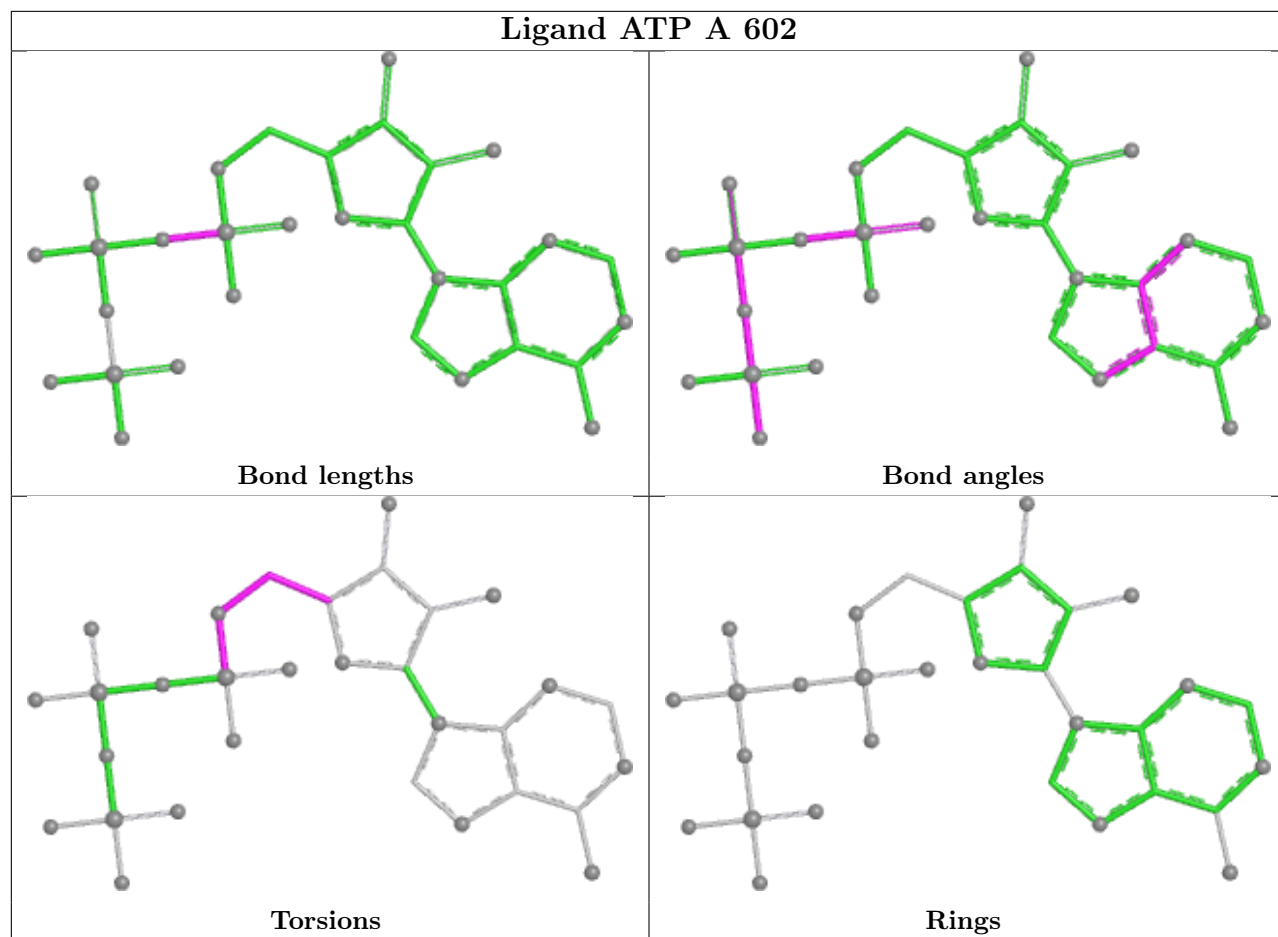
Continued from previous page...

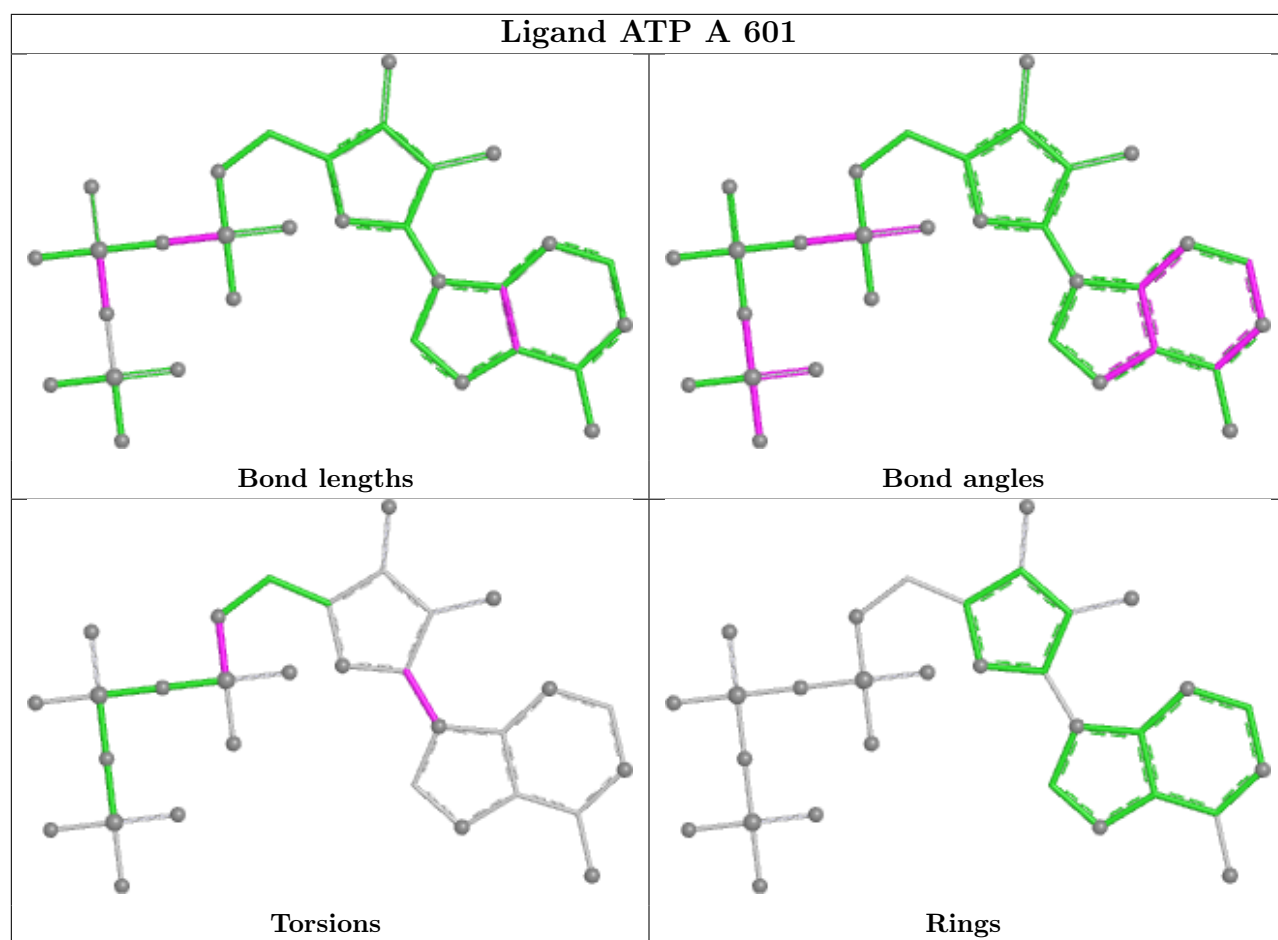
Mol	Chain	Res	Type	Atoms
2	E	602	ATP	C5'-O5'-PA-O1A
2	G	602	ATP	C5'-O5'-PA-O2A
2	C	601	ATP	C2'-C1'-N9-C4
2	E	601	ATP	C2'-C1'-N9-C4
2	G	601	ATP	C2'-C1'-N9-C4
2	H	601	ATP	C2'-C1'-N9-C4
2	C	601	ATP	C2'-C1'-N9-C8
2	D	601	ATP	C2'-C1'-N9-C4
2	E	601	ATP	O4'-C1'-N9-C8
2	F	601	ATP	O4'-C1'-N9-C8
2	F	601	ATP	C2'-C1'-N9-C4
2	D	601	ATP	O4'-C1'-N9-C8
2	G	601	ATP	O4'-C1'-N9-C8
2	A	601	ATP	O4'-C1'-N9-C8
2	D	602	ATP	PG-O3B-PB-O1B
2	D	602	ATP	PG-O3B-PB-O2B
2	H	601	ATP	O4'-C1'-N9-C8
2	A	601	ATP	C2'-C1'-N9-C4
2	C	601	ATP	PG-O3B-PB-O2B
2	D	601	ATP	PG-O3B-PB-O2B
2	G	601	ATP	PA-O3A-PB-O1B
2	G	601	ATP	PA-O3A-PB-O2B

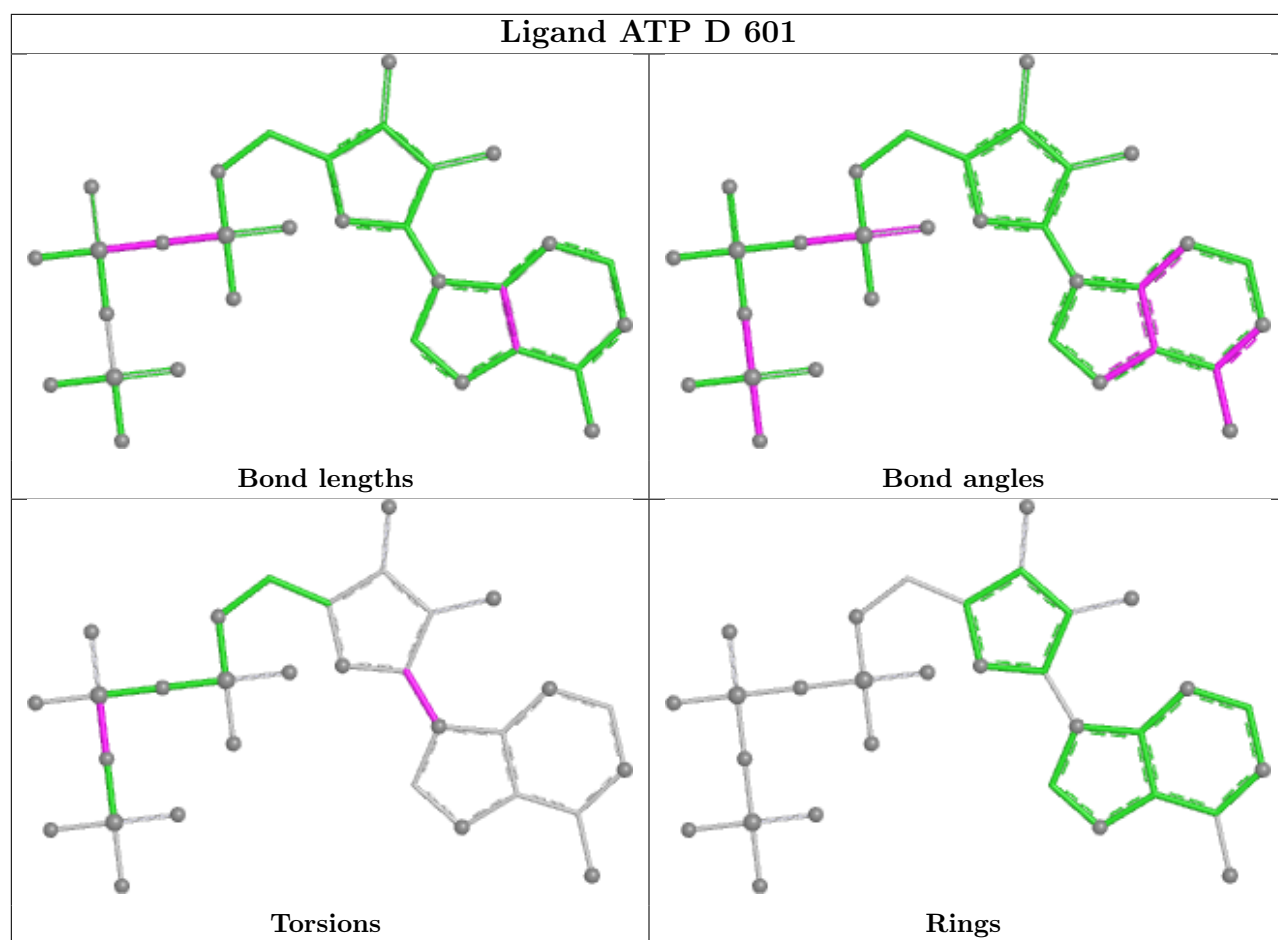
There are no ring outliers.

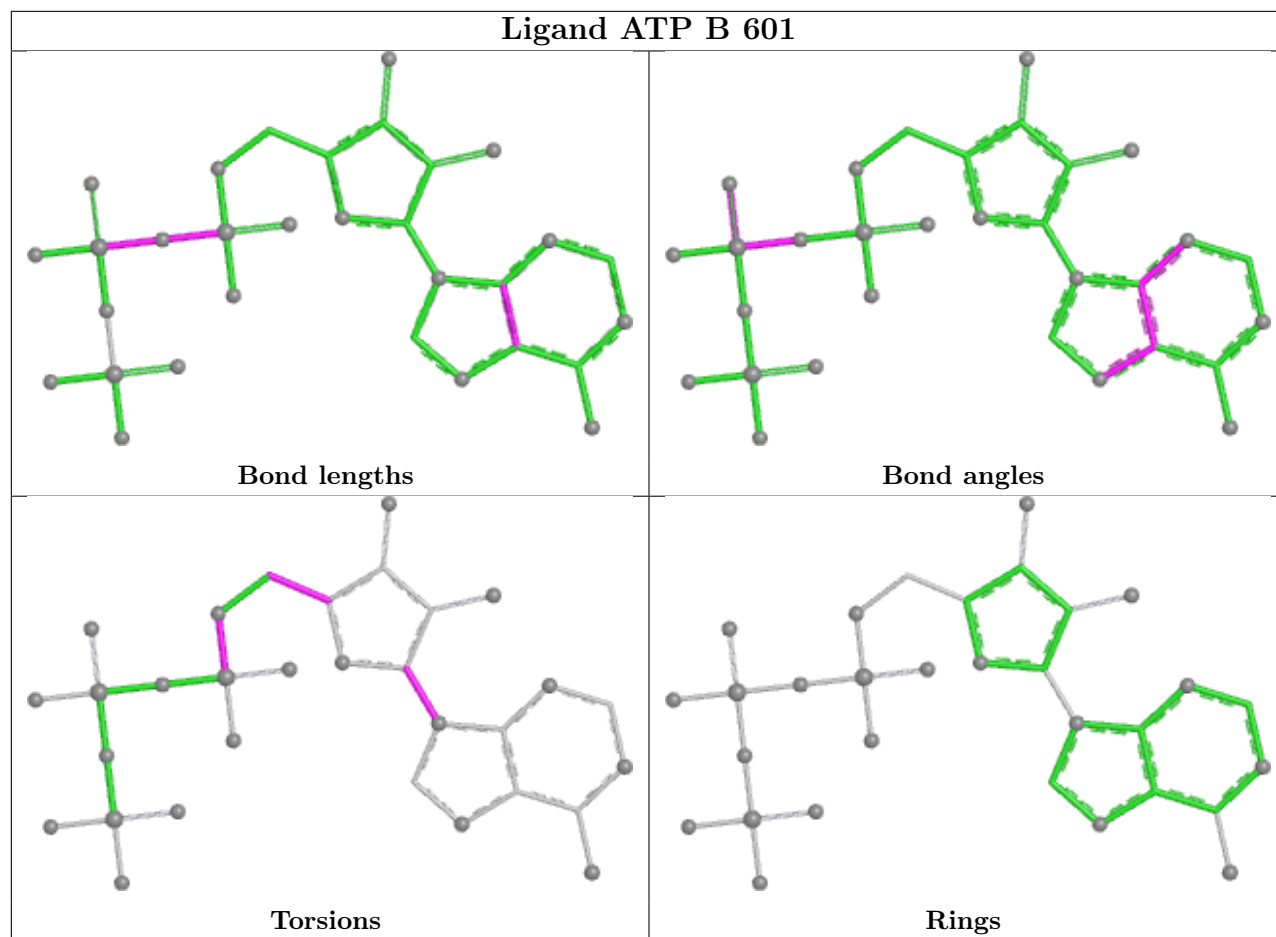
No monomer is involved in short contacts.

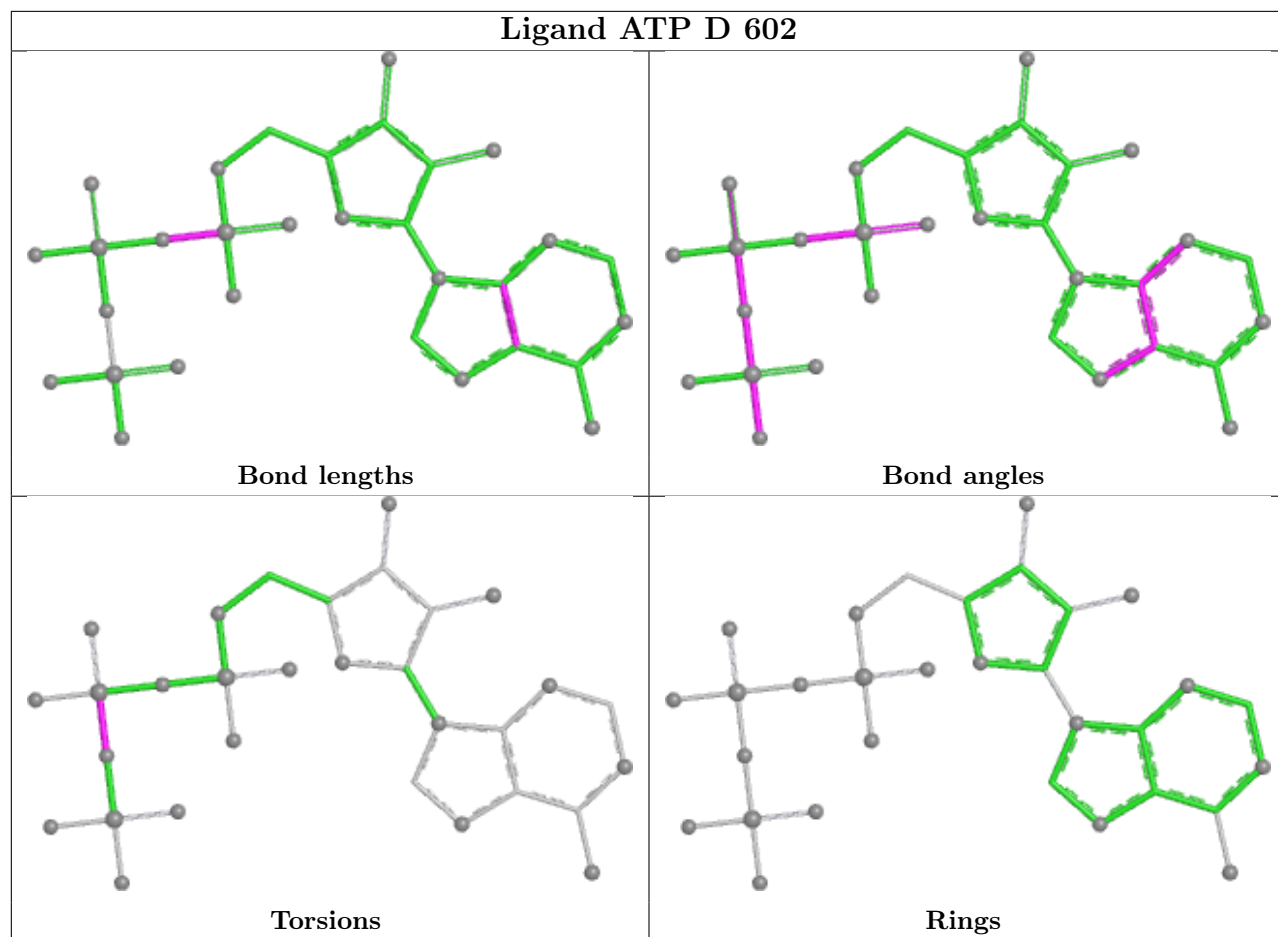
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

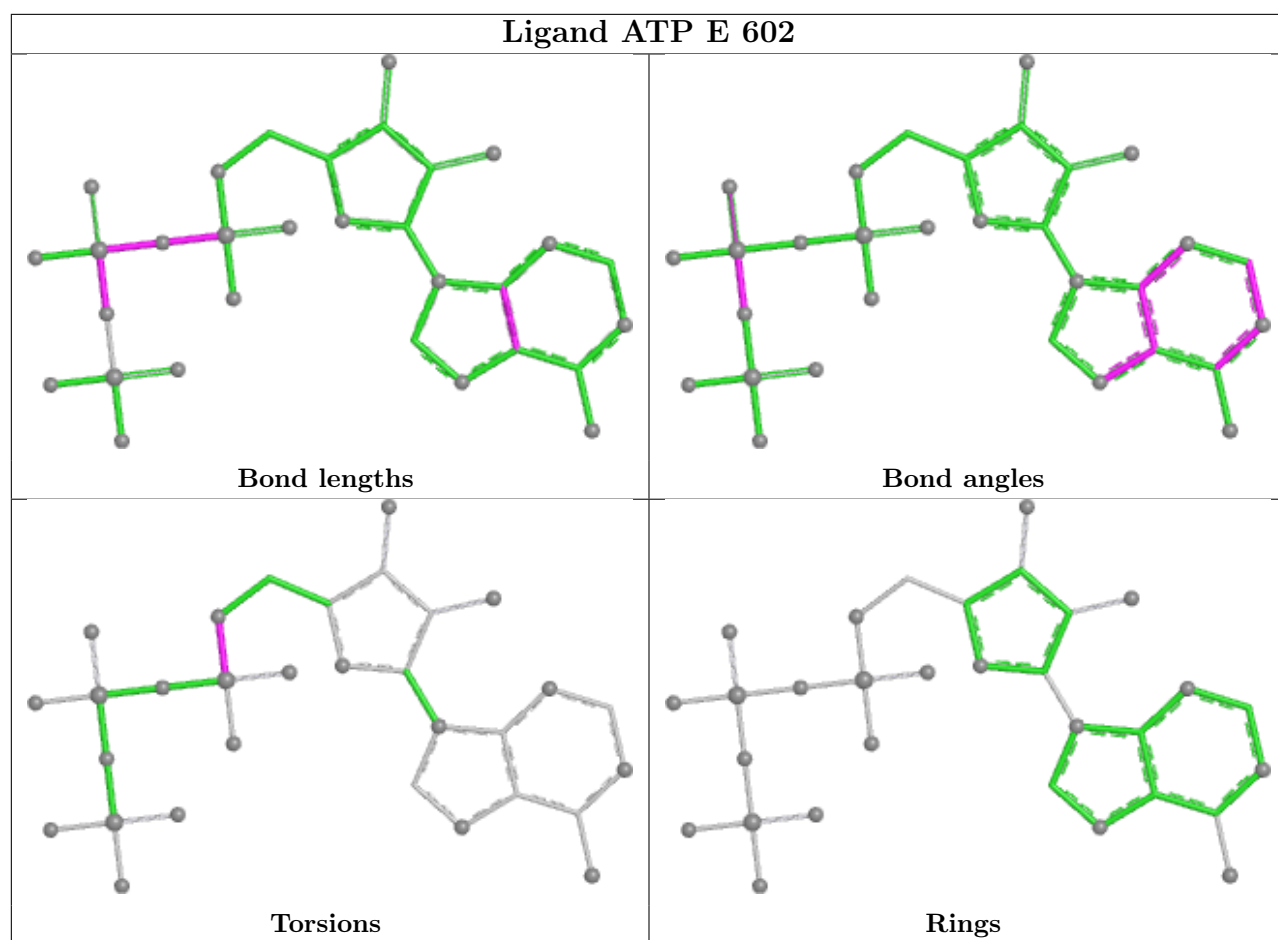


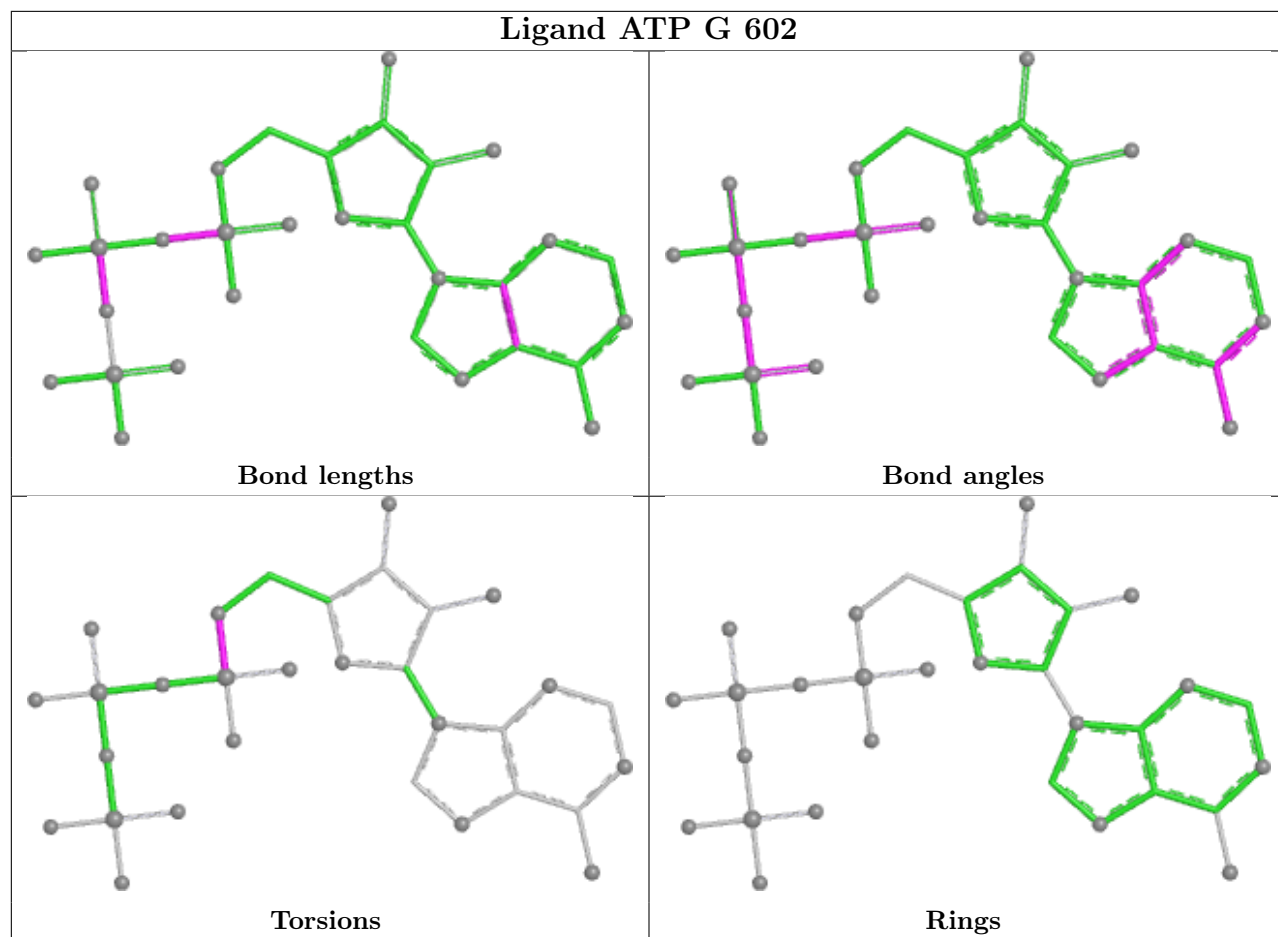


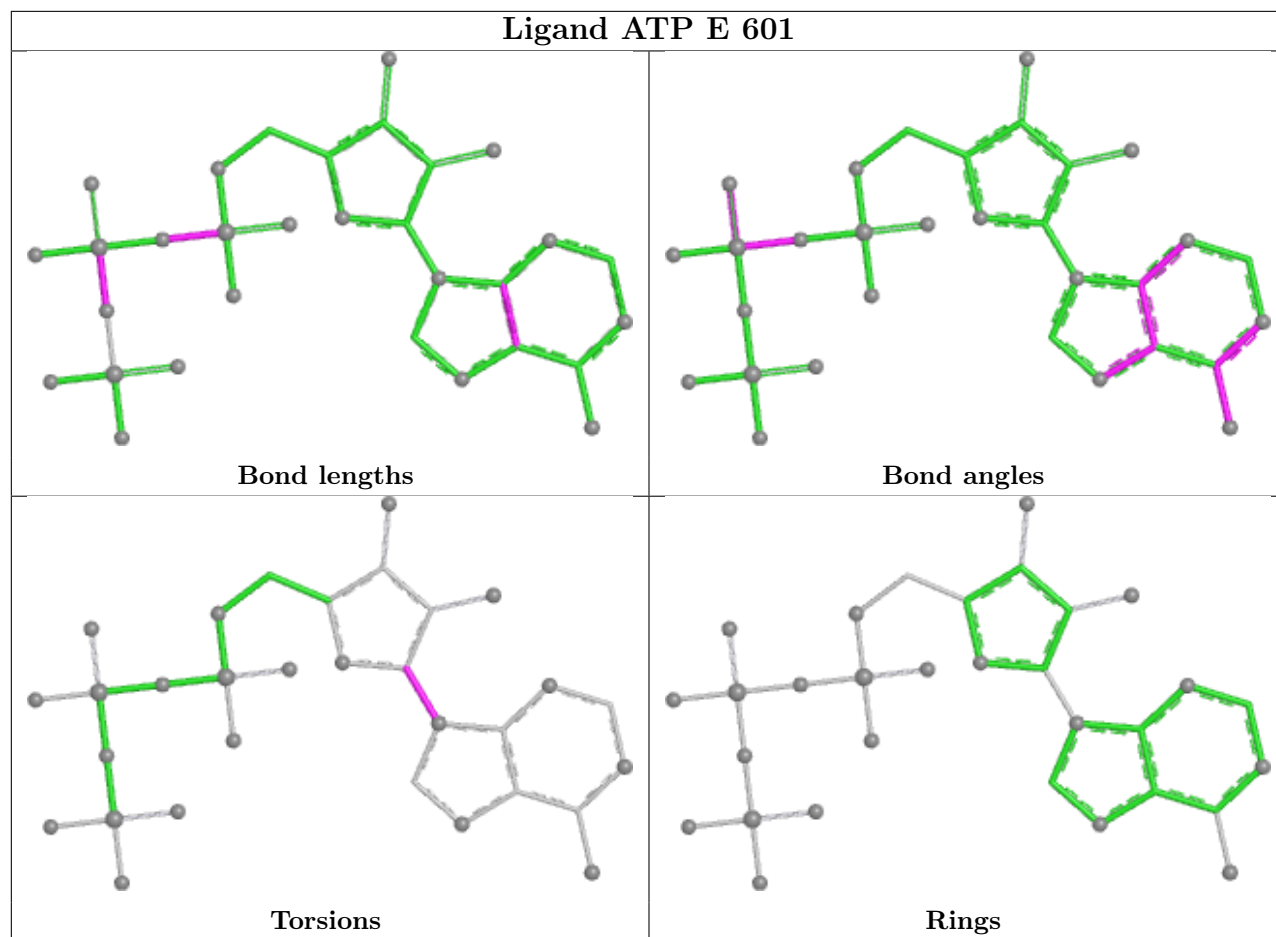


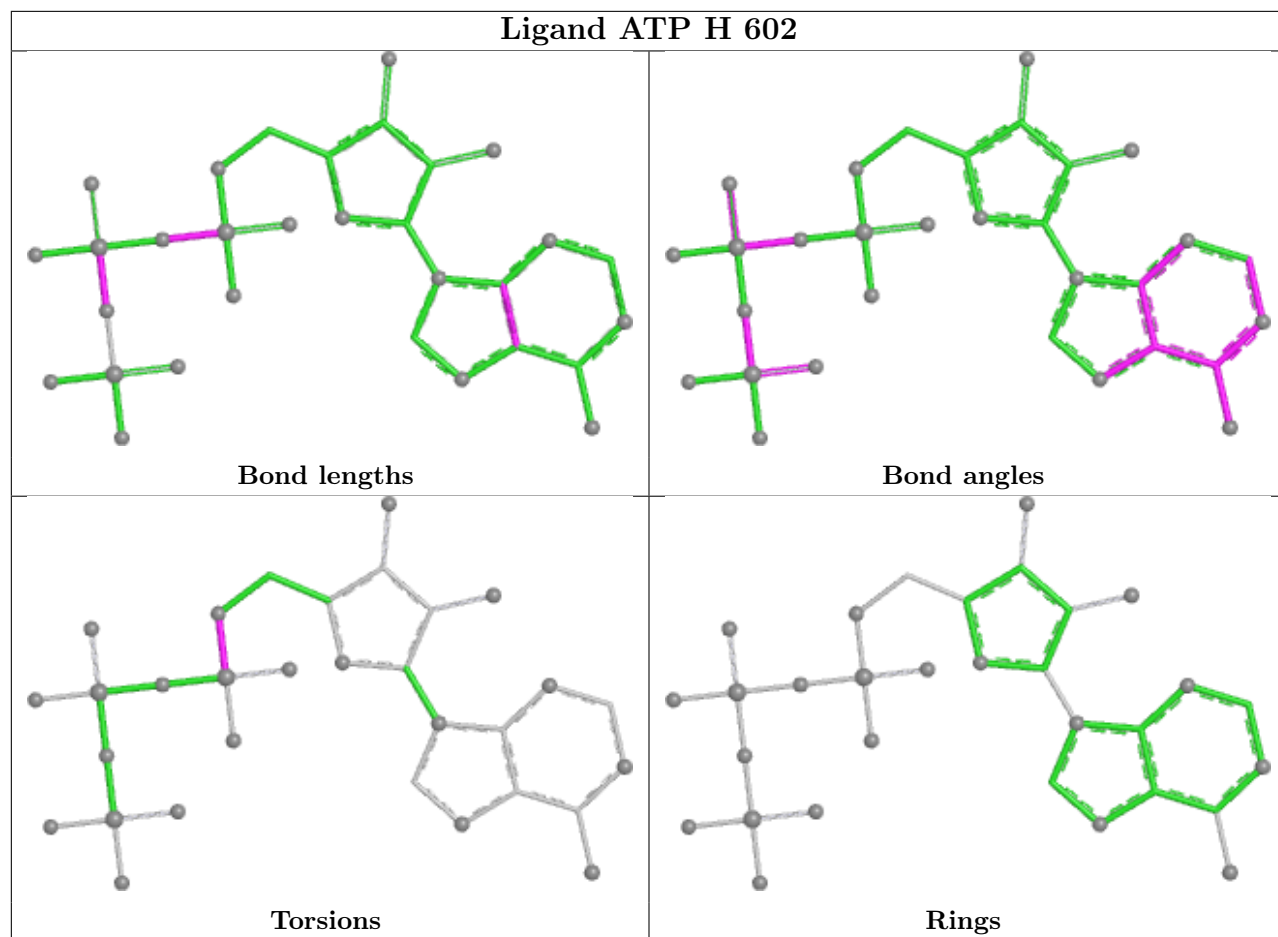


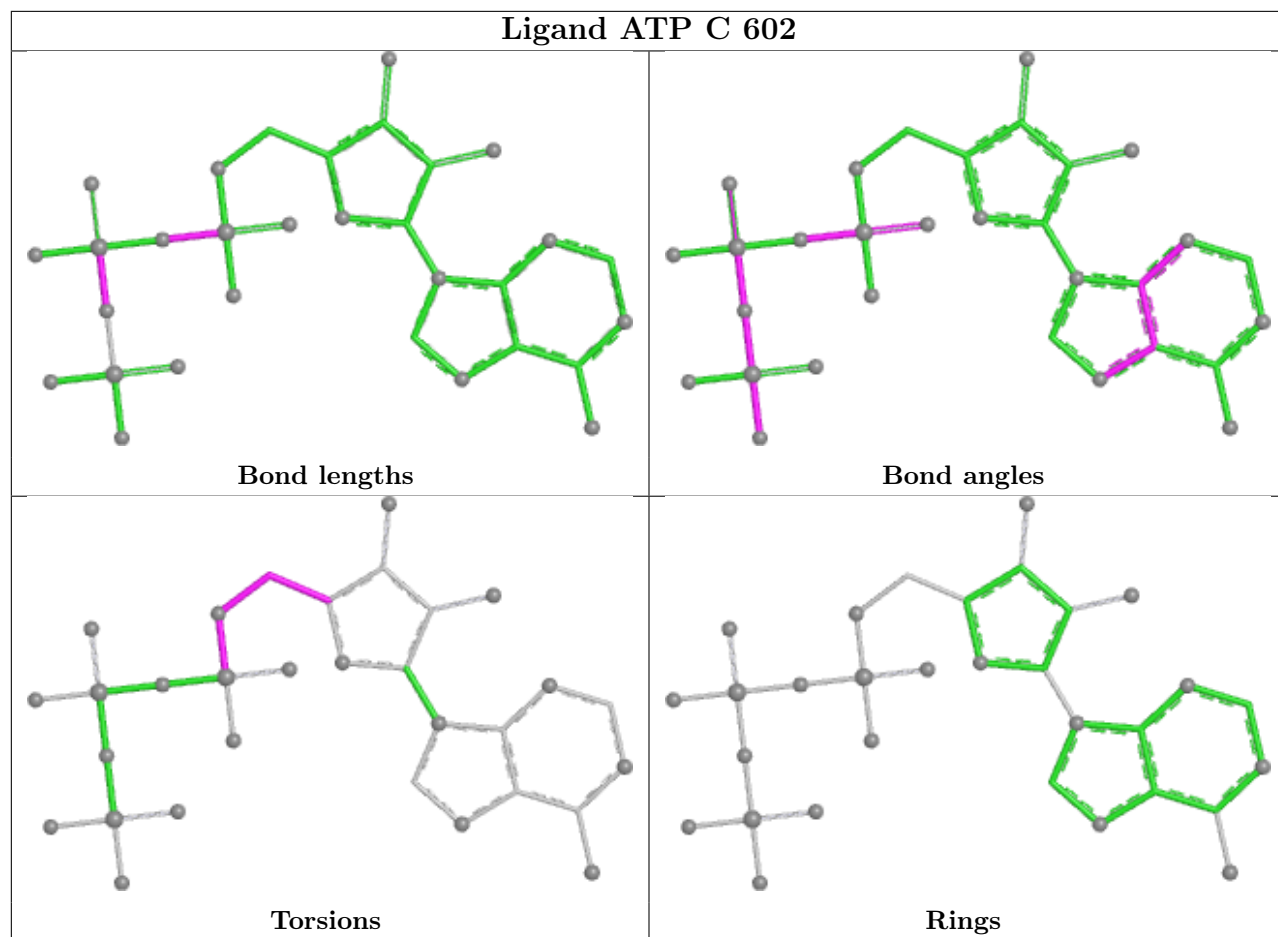


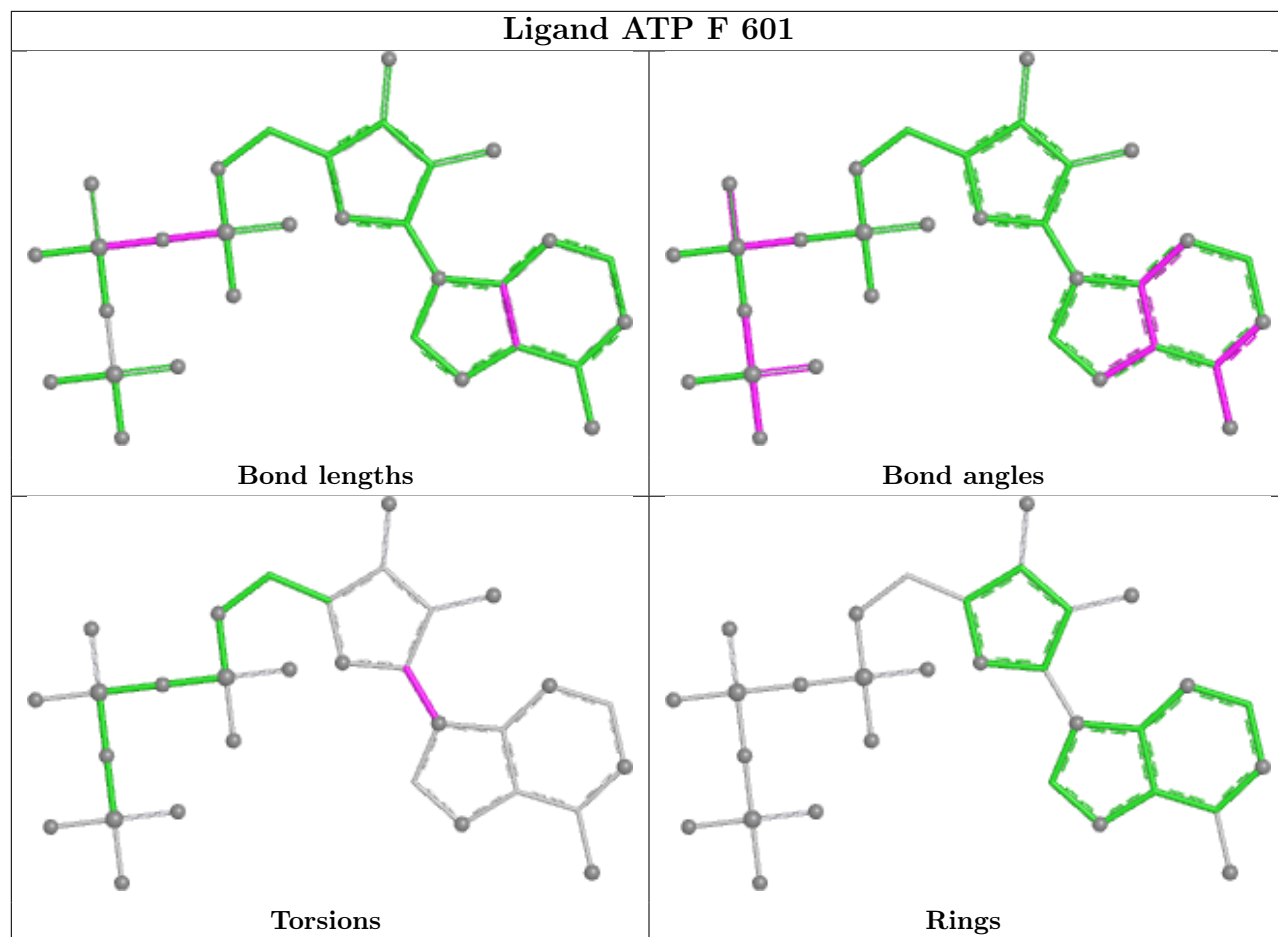


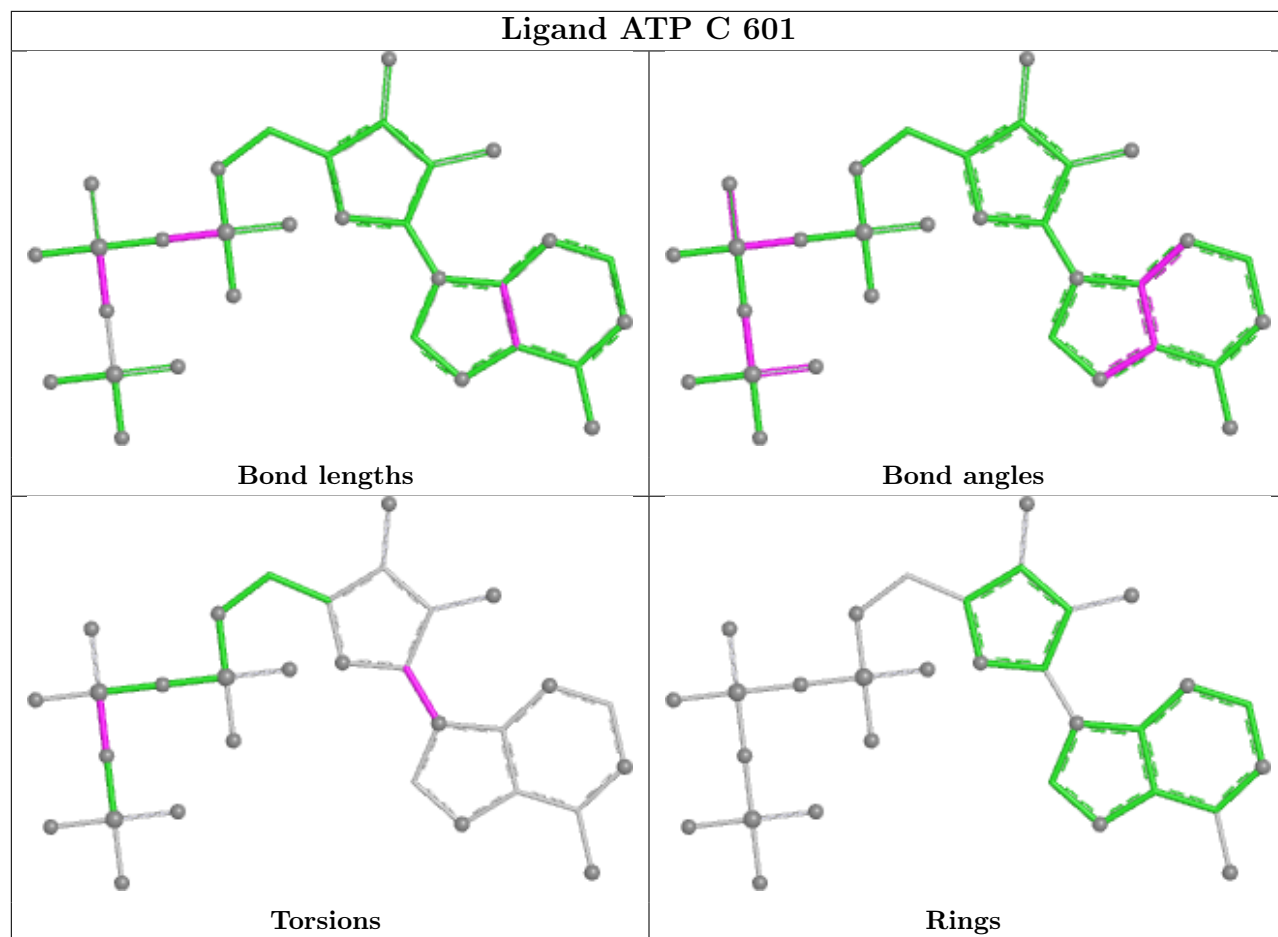


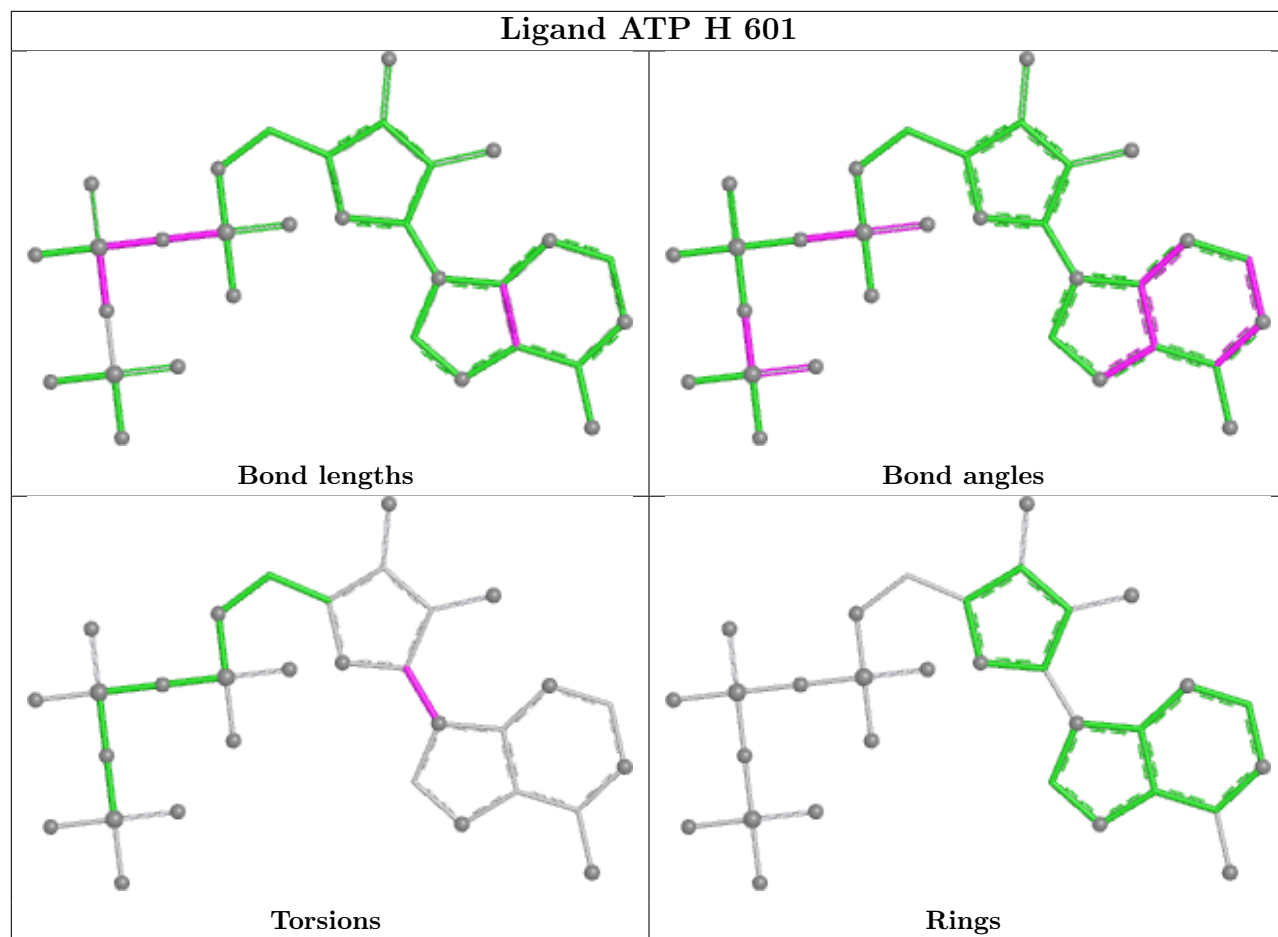


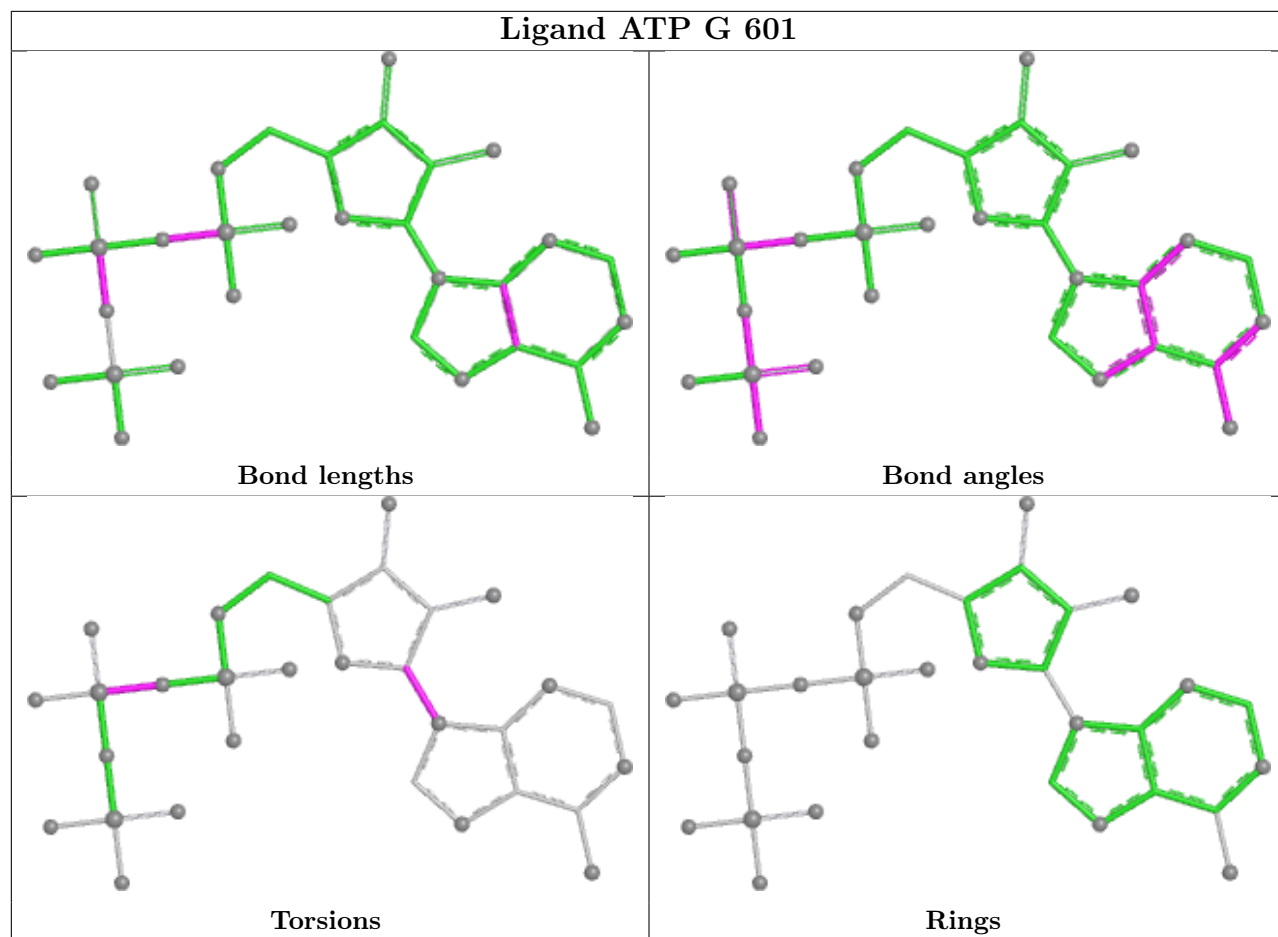


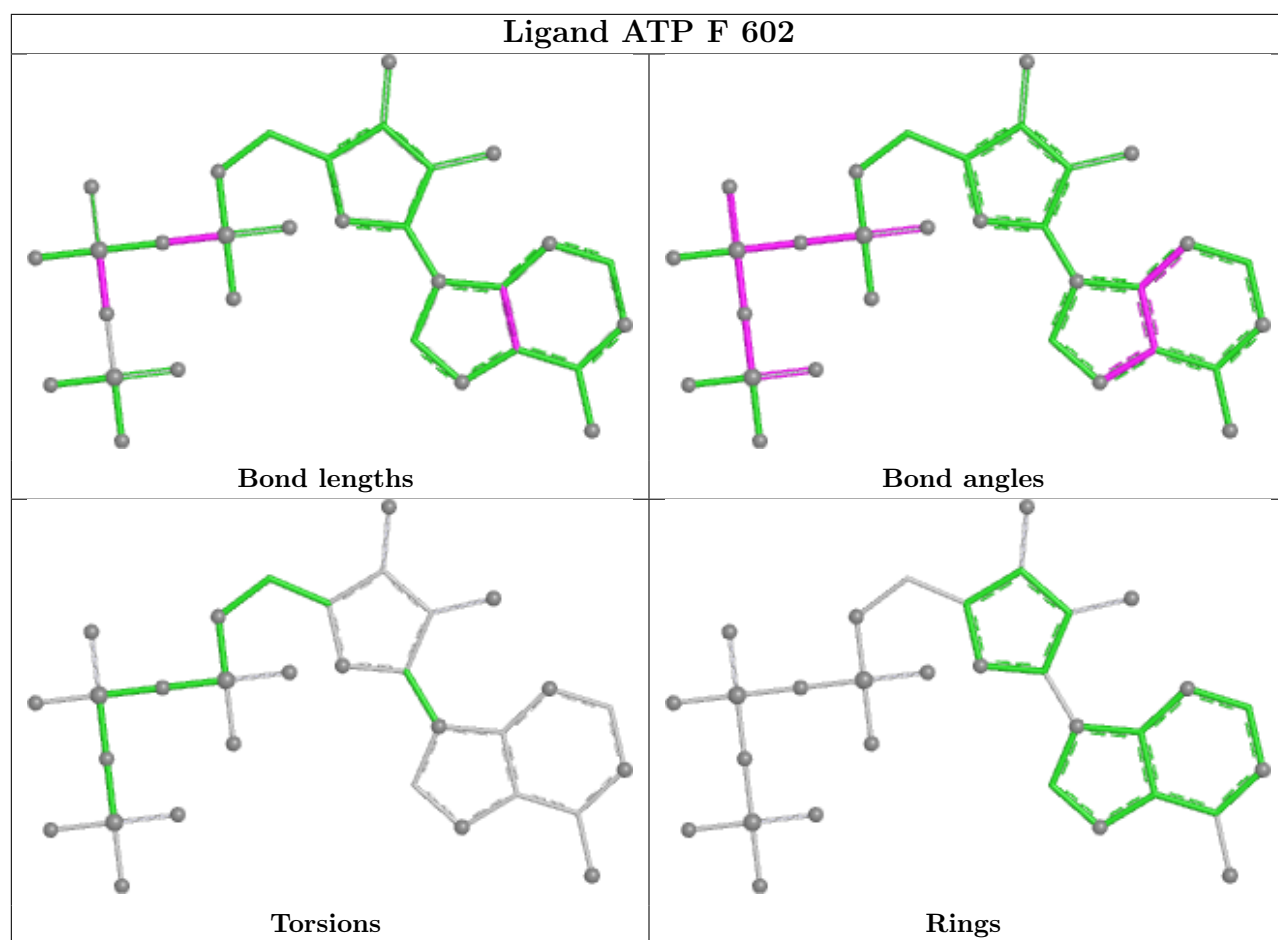


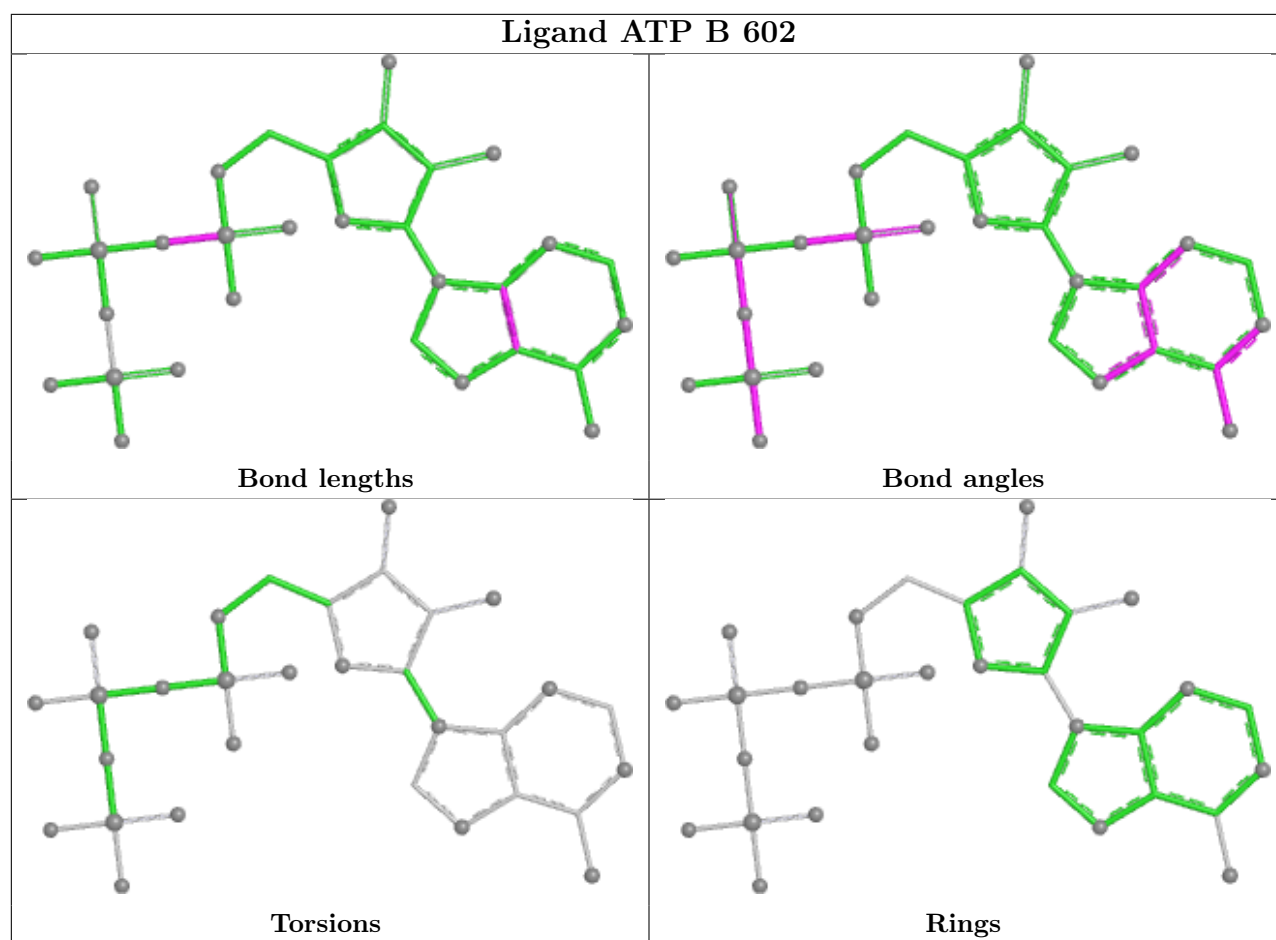












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

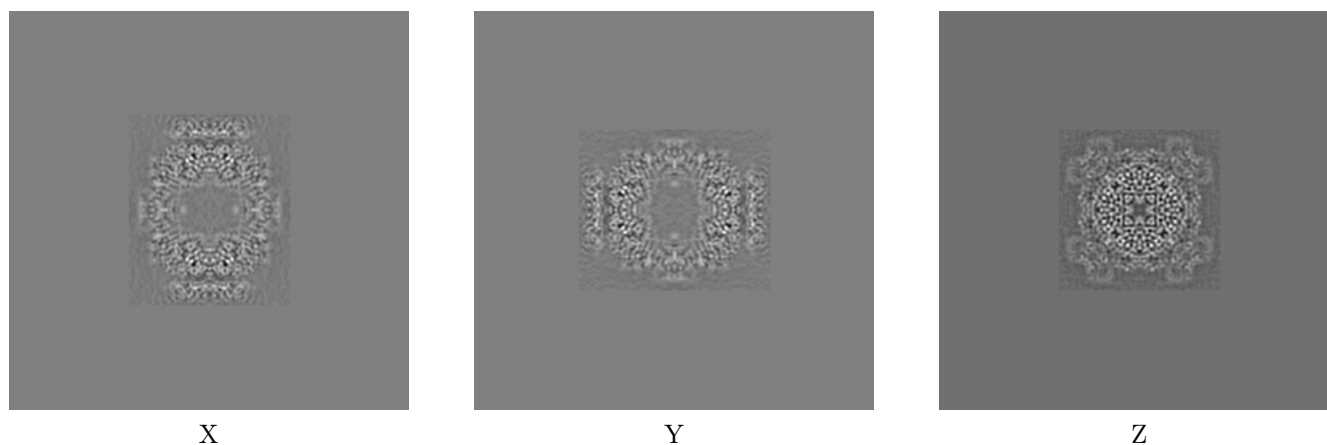
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24442. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

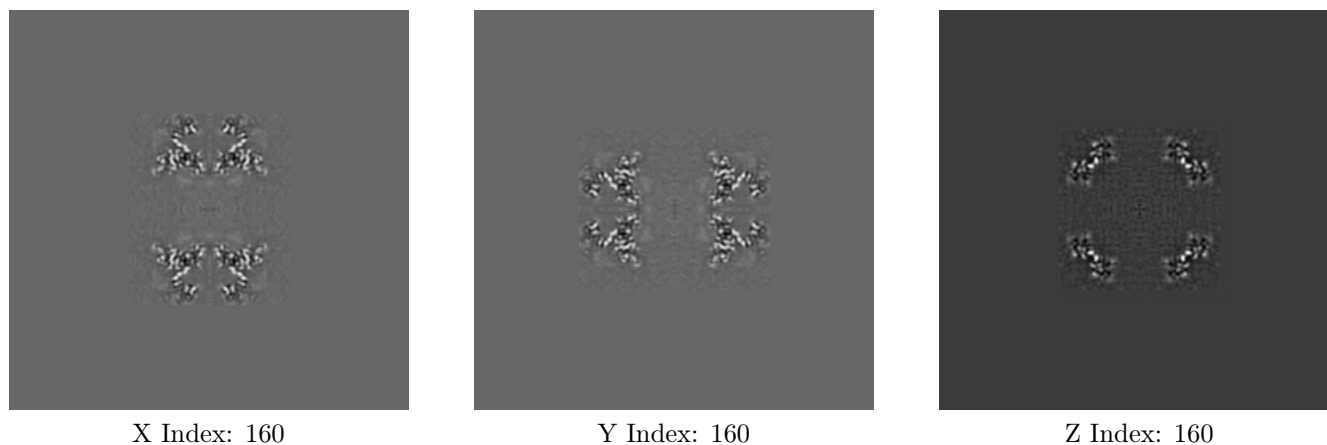
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

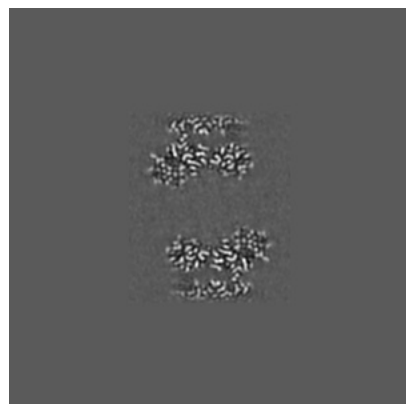
6.2.1 Primary map



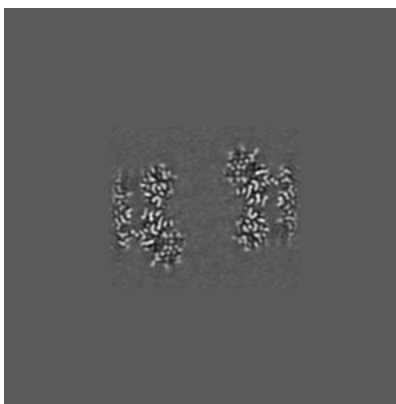
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

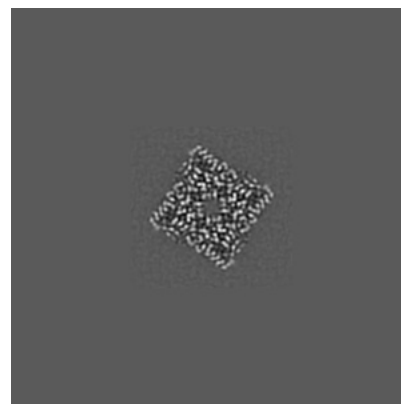
6.3.1 Primary map



X Index: 175



Y Index: 175

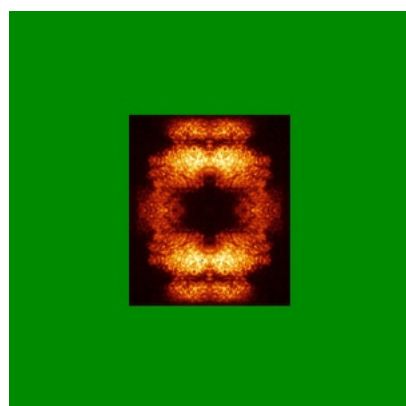


Z Index: 200

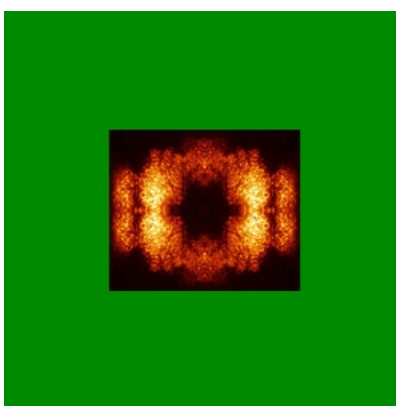
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

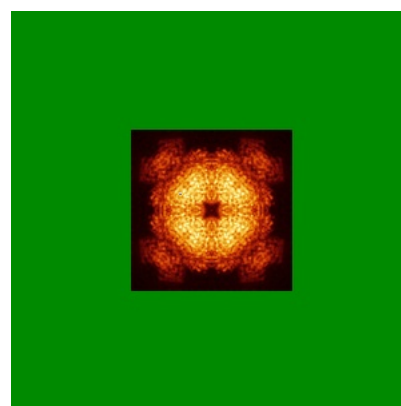
6.4.1 Primary map



X



Y

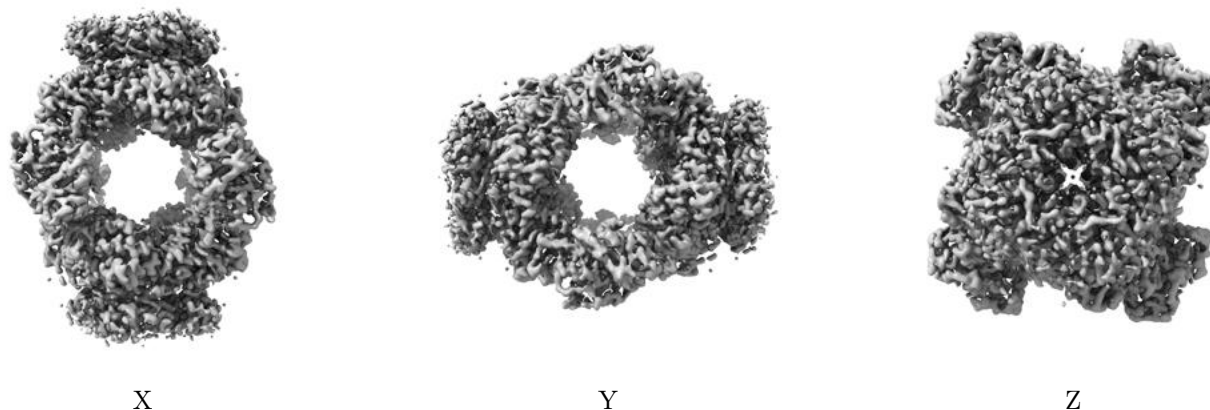


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

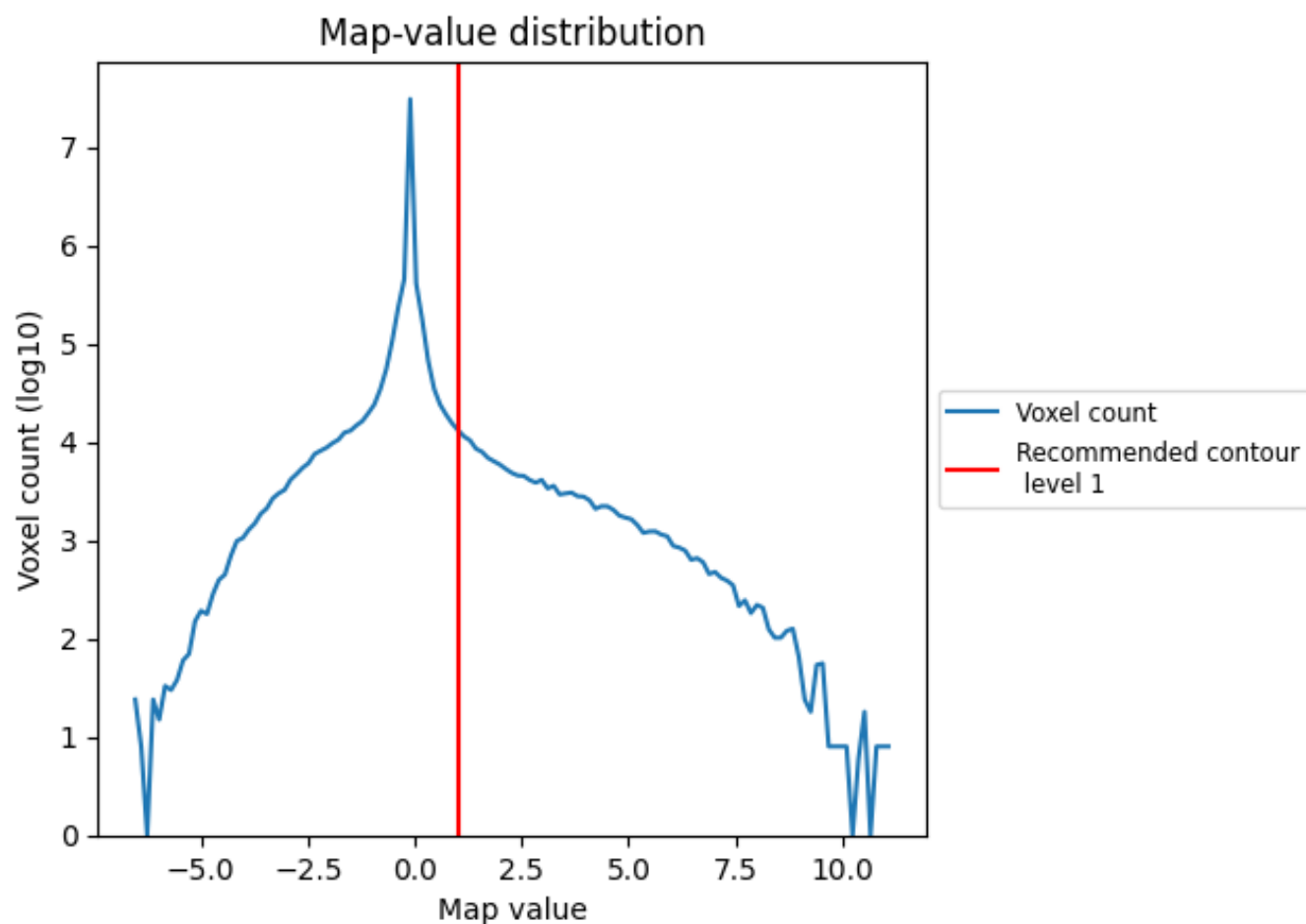
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

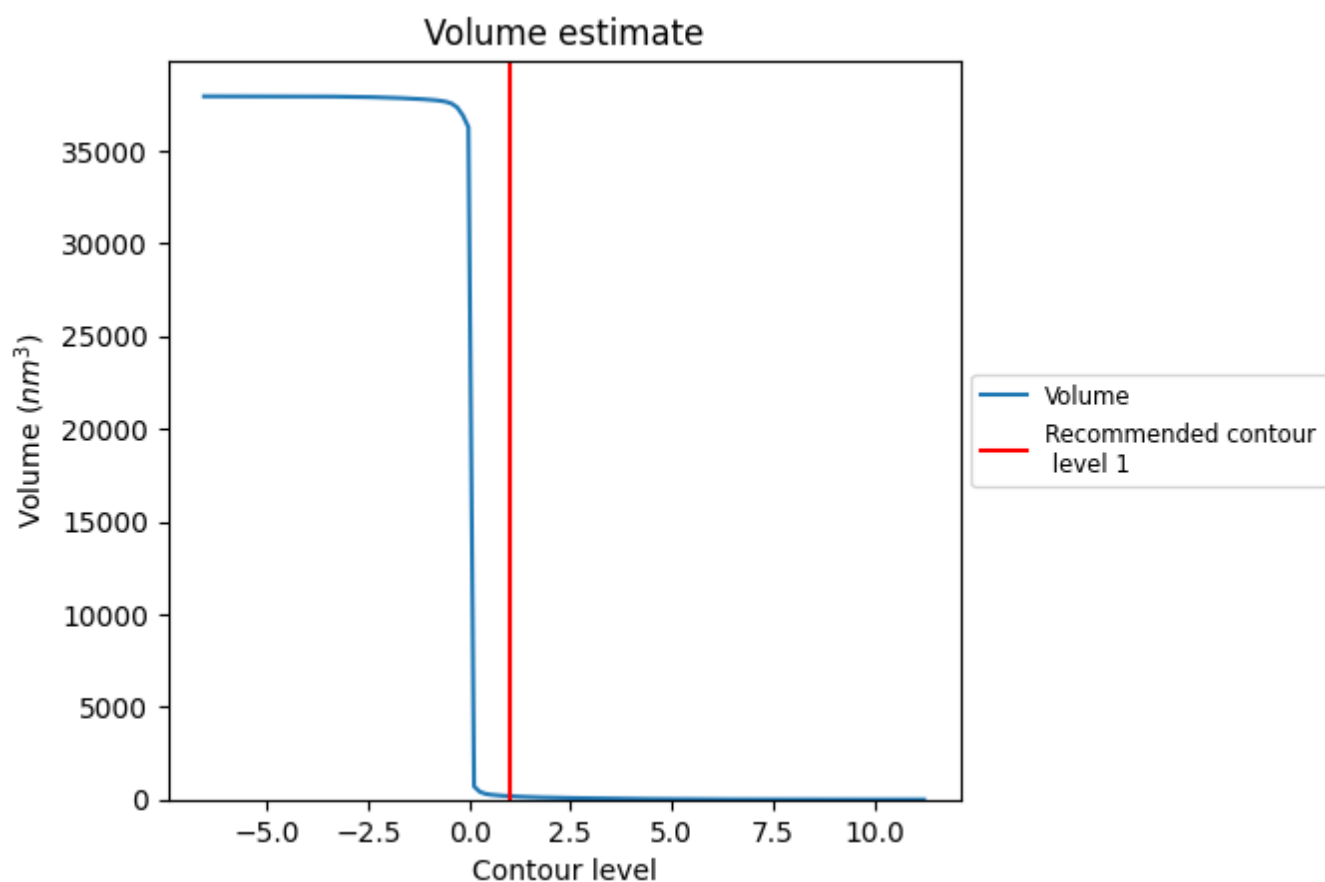
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

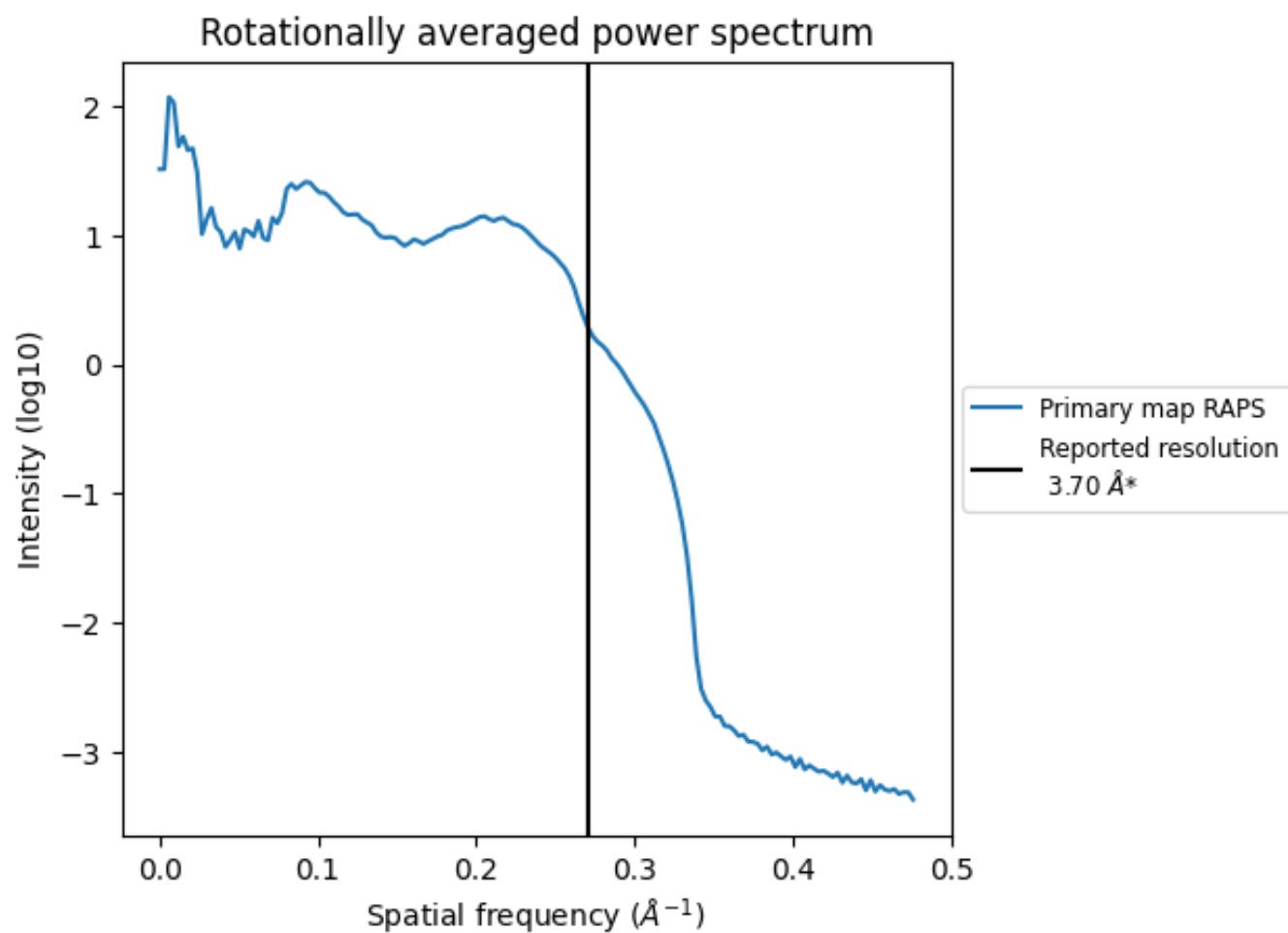
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm³; this corresponds to an approximate mass of 164 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

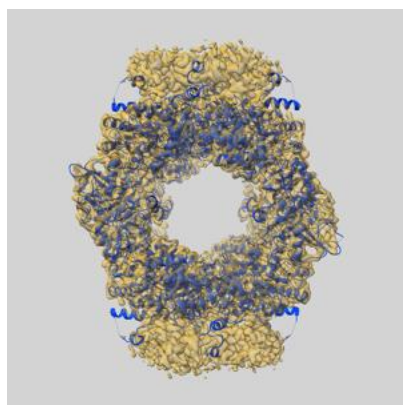
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

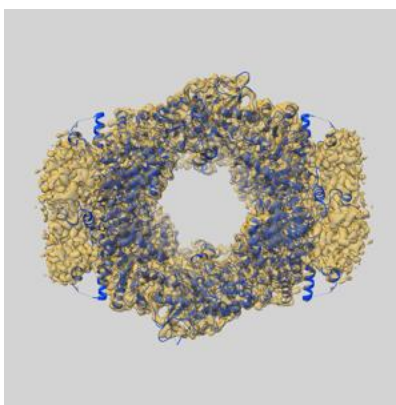
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24442 and PDB model 7RFH. Per-residue inclusion information can be found in section 3 on page 19.

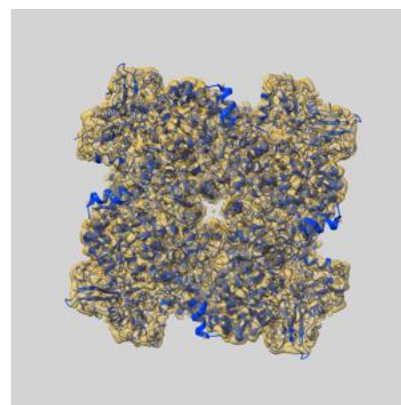
9.1 Map-model overlay [i](#)



X



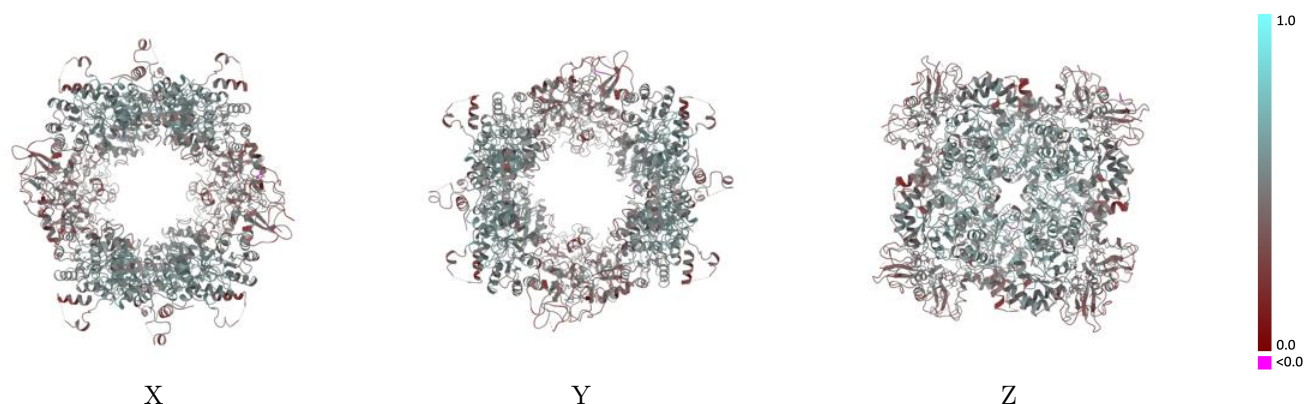
Y



Z

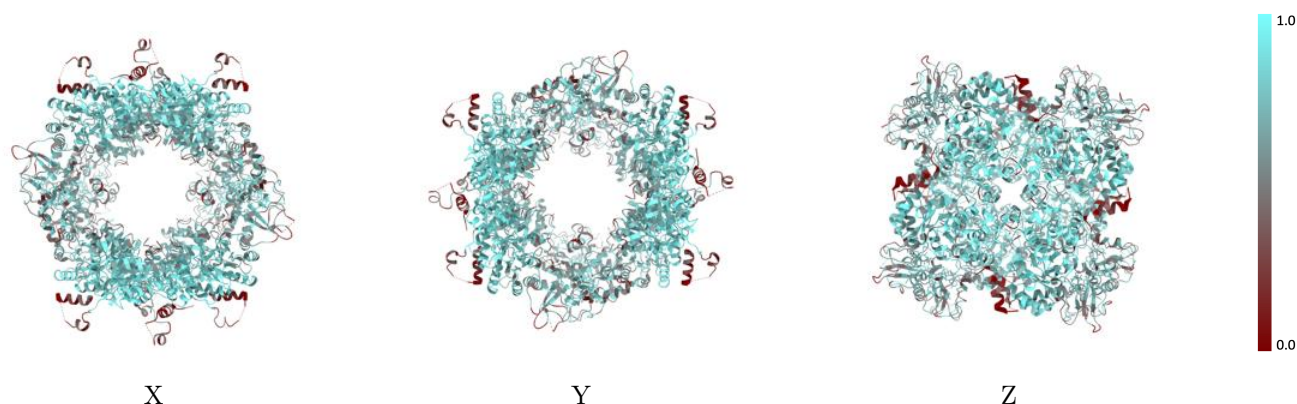
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



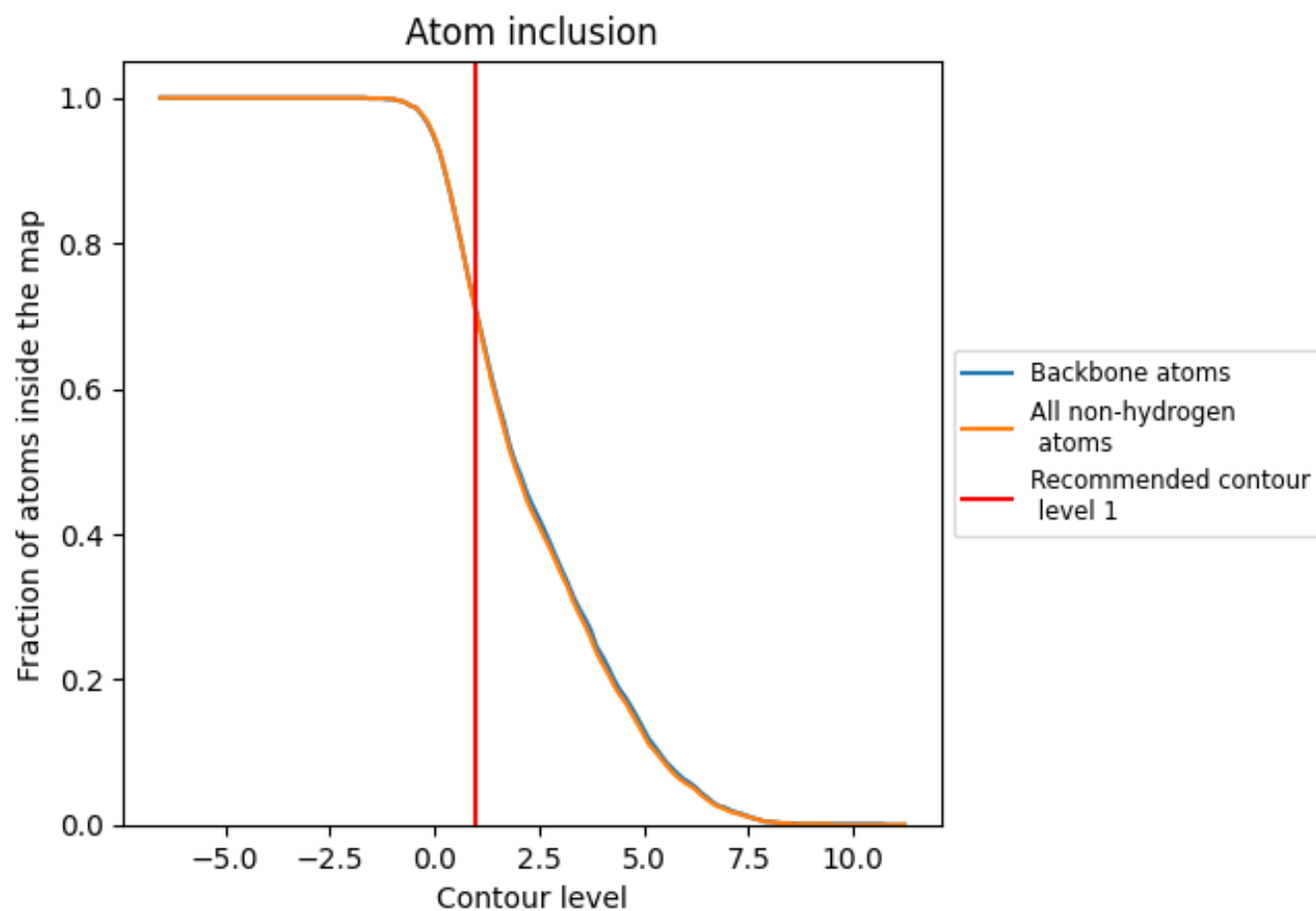
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7030	0.4750
A	0.7020	0.4720
B	0.7060	0.4740
C	0.7050	0.4760
D	0.7080	0.4750
E	0.7110	0.4800
F	0.7080	0.4760
G	0.7030	0.4750
H	0.7050	0.4760

1.0

0.0

<0.0