



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 01:49 PM EDT

PDB ID : 1CT9
Title : CRYSTAL STRUCTURE OF ASPARAGINE SYNTHETASE B FROM ES-
CHERICHIA COLI
Authors : Larsen, T.M.; Boehlein, S.K.; Schuster, S.M.; Richards, N.G.J.; Thoden, J.B.;
Holden, H.M.; Rayment, I.
Deposited on : 1999-08-20
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

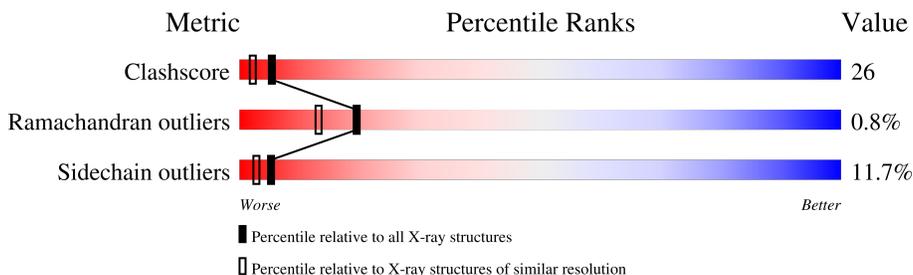
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	553	
1	B	553	
1	C	553	
1	D	553	

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
4	AMP	C	1114	-	-	X	-
4	AMP	D	1121	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 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.

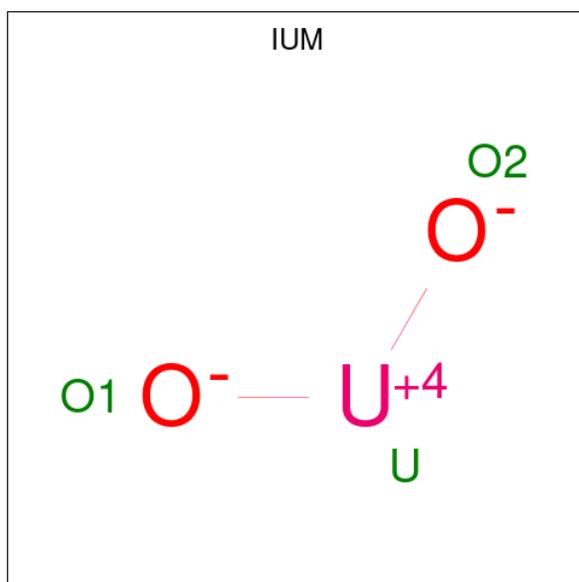
- Molecule 1 is a protein called ASPARAGINE SYNTHETASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3966	2530	671	745	20	0	0	0
1	B	495	3942	2518	665	739	20	0	0	0
1	C	495	3942	2518	665	739	20	0	0	0
1	D	495	3930	2507	664	739	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP P22106
B	1	ALA	CYS	engineered mutation	UNP P22106
C	1	ALA	CYS	engineered mutation	UNP P22106
D	1	ALA	CYS	engineered mutation	UNP P22106

- Molecule 2 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total U 1 1	0	0
2	A	1	Total O U 2 1 1	0	0
2	A	1	Total U 1 1	0	0
2	A	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	D	1	Total O U 2 1 1	0	0
2	D	1	Total U 1 1	0	0

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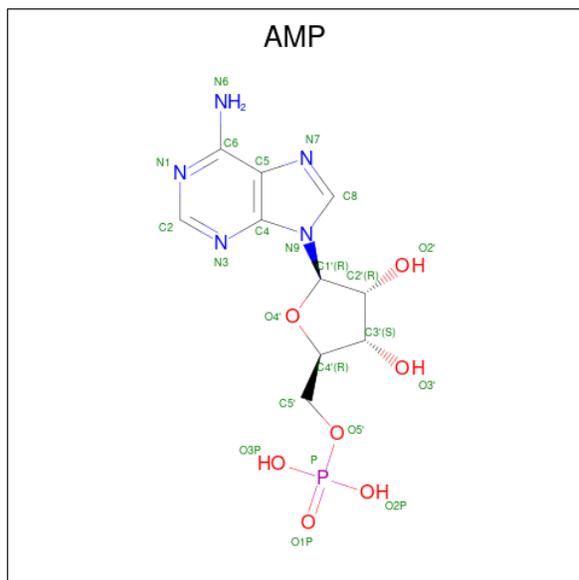
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total U 1 1	0	0
2	D	1	Total U 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



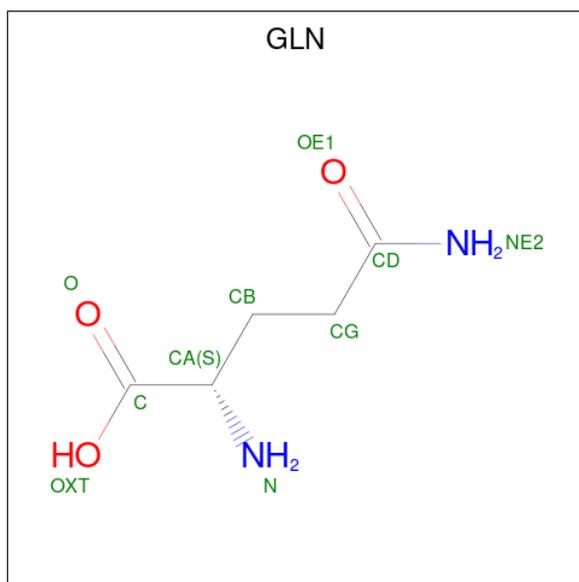
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 23 10 5 7 1	0	0
4	B	1	Total C N O P 23 10 5 7 1	0	0
4	C	1	Total C N O P 23 10 5 7 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

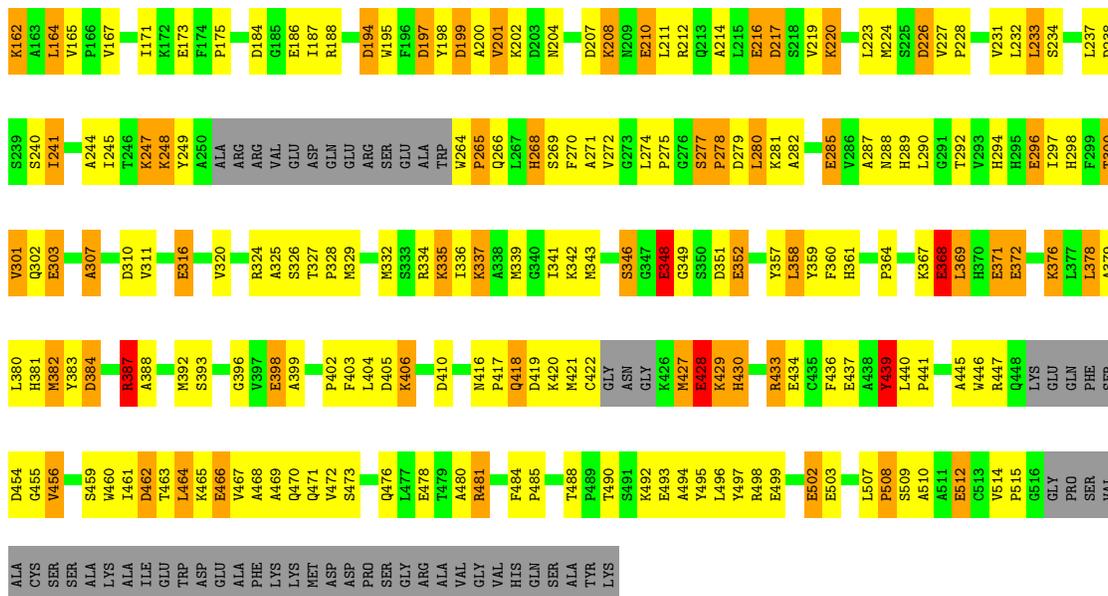
- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	235	Total	O	0	0
			235	235		
6	C	223	Total	O	0	0
			223	223		
6	D	296	Total	O	0	0
			296	296		



GLY	E512	GLY	C347	Q266	S189	A1
PRO	R433	E348	E349	L267	Y190	F4
SER	E434	R627	S350	H268	Y191	D8
VAL	E437	E428	D351	S269	H192	Q118
ALA	E437	K429	E352	F270	R193	I9
CYS	V444	H430	V353	A271	D194	K10
SER	V444	R433	F354	V272	D197	K11
SER	V444	E357	Y357	G273	Y198	D12
ALA	Q448	L358	Y359	L274	D199	T11
ALA	LYS	P278	P278	S277	A200	M12
LYS	GLU	D279	D279	S277	V201	V14
ALA	ALA	L280	L280	P278	K202	E15
ILE	GLN	K281	K281	D279	D203	E22
GLU	PHE	E285	E285	M204	M205	R25
TRP	SER	V293	V293	V205	T206	R28
ASP	ASP	H294	H294	D207	D207	D33
GLU	GLU	H295	H295	E210	E210	W34
ALA	ALA	E296	E296	E216	E216	D41
PHE	PHE	I297	I297	D217	D217	D41
LYS	LYS	H298	H298	S218	S218	A46
MET	MET	F299	F299	V219	V219	H47
ASP	ASP	T300	T300	K220	K220	E48
ALA	ALA	E303	E303	S221	S221	R49
ASP	ASP	H381	H381	H222	H222	L50
PRO	PRO	M382	M382	Y149	Y149	S51
SER	SER	Y383	Y383	L223	L223	I52
GLY	GLY	D384	D384	M224	M224	M64
ARG	ARG	R387	R387	S225	S225	Q65
ALA	ALA	A388	A388	D226	D226	Q66
VAL	VAL	W395	W395	V227	V227	K67
HIS	HIS	E398	E398	P228	P228	T68
SER	SER	A399	A399	Y229	Y229	H69
ALA	ALA	R400	R400	G230	G230	Y78
TYR	TYR	V401	V401	V231	V231	N79
LYS	LYS	P402	P402	L232	L232	H80
		D405	D405	L233	L233	Q81
		K406	K406	S234	S234	R84
		A494	A494	G235	G235	A85
		Y495	Y495	D238	D238	E86
		L496	L496	S239	S239	D89
		Y497	Y497	A251	A251	R90
		R498	R498	ARG	ARG	Y91
		E499	E499	ARG	ARG	Q92
		E502	E502	VAL	VAL	D89
		E503	E503	GLU	GLU	R90
		P506	P506	GLN	GLN	Y91
		L507	L507	GLU	GLU	Q92
		P508	P508	GLU	GLU	D89
		S509	S509	ARG	ARG	R90
				SER	SER	Y91
				GLU	GLU	Q92
				ALA	ALA	D89
				TRP	TRP	R90
				ALA	ALA	Y91
				TRP	TRP	Q92
				PRD	PRD	D89
						R90
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.93Å 127.10Å 204.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (30.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.197 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: IUM, CL, AMP

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	1.02	24/4060 (0.6%)	1.48	66/5493 (1.2%)
1	B	1.04	32/4037 (0.8%)	1.50	67/5466 (1.2%)
1	C	1.01	33/4037 (0.8%)	1.44	63/5466 (1.2%)
1	D	1.06	30/4022 (0.7%)	1.49	67/5443 (1.2%)
All	All	1.03	119/16156 (0.7%)	1.48	263/21868 (1.2%)

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	9.23	1.35	1.25
1	D	398	GLU	CD-OE2	8.52	1.35	1.25
1	B	466	GLU	CD-OE2	7.96	1.34	1.25
1	D	48	GLU	CD-OE2	7.61	1.34	1.25
1	B	296	GLU	CD-OE2	7.58	1.33	1.25

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CB-CG-OD2	-14.12	105.59	118.30
1	A	150	ASP	CB-CG-OD2	-13.62	106.05	118.30
1	C	150	ASP	CB-CG-OD2	-10.79	108.59	118.30
1	D	194	ASP	CB-CG-OD1	10.22	127.50	118.30
1	B	238	ASP	CB-CG-OD2	-10.11	109.20	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3966	0	3862	192	0
1	B	3942	0	3828	247	0
1	C	3942	0	3827	204	0
1	D	3930	0	3818	186	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	5	0
4	B	23	0	12	3	0
4	C	23	0	11	7	0
4	D	23	0	12	8	0
5	A	10	0	7	2	0
5	B	10	0	7	4	0
5	C	10	0	7	1	0
5	D	10	0	7	2	0
6	A	292	0	0	8	0
6	B	235	0	0	13	0
6	C	223	0	0	7	0
6	D	296	0	0	19	0
All	All	16980	0	15409	822	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 26.

The worst 5 of 822 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:C:364:PRO:HG2	1:C:368:GLU:HG2	1.26	1.17
1:D:472:VAL:HB	1:D:492:LYS:HG2	1.22	1.12
1:D:364:PRO:HG2	1:D:368:GLU:HG2	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:HG22	1:B:303:GLU:H	1.29	0.96
1:D:64:ASN:HB3	1:D:67:LYS:N	1.80	0.95

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	491/553 (89%)	465 (95%)	24 (5%)	2 (0%)	34 30
1	B	487/553 (88%)	449 (92%)	31 (6%)	7 (1%)	11 5
1	C	487/553 (88%)	450 (92%)	33 (7%)	4 (1%)	19 13
1	D	487/553 (88%)	467 (96%)	18 (4%)	2 (0%)	34 30
All	All	1952/2212 (88%)	1831 (94%)	106 (5%)	15 (1%)	19 13

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLU
1	C	266	GLN
1	A	138	ASP
1	B	265	PRO
1	B	460	TRP

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	418/462 (90%)	371 (89%)	47 (11%)	6	3
1	B	414/462 (90%)	358 (86%)	56 (14%)	4	2
1	C	414/462 (90%)	364 (88%)	50 (12%)	5	2
1	D	412/462 (89%)	371 (90%)	41 (10%)	7	4
All	All	1658/1848 (90%)	1464 (88%)	194 (12%)	5	3

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	150	ASP
1	C	420	LYS
1	C	171	ILE
1	C	337	LYS
1	C	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	183	GLN
1	D	81	GLN
1	C	288	ASN
1	C	471	GLN
1	D	192	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are modelled with single atom and 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	B	1107	2	22,25,25	1.19	3 (13%)	25,38,38	1.49	4 (16%)
2	IUM	A	1102	-	0,1,2	-	-	-	-	-
5	GLN	C	1120	-	5,9,9	2.28	1 (20%)	5,11,11	1.29	1 (20%)
2	IUM	D	1122	4	0,1,2	-	-	-	-	-
5	GLN	A	1106	-	5,9,9	2.86	1 (20%)	5,11,11	0.86	0
4	AMP	D	1121	2	22,25,25	1.00	2 (9%)	25,38,38	2.44	6 (24%)
5	GLN	B	1113	-	5,9,9	2.25	1 (20%)	5,11,11	0.46	0
4	AMP	A	1100	-	22,25,25	1.20	3 (13%)	25,38,38	1.87	4 (16%)
4	AMP	C	1114	-	22,25,25	1.19	3 (13%)	25,38,38	2.12	7 (28%)
5	GLN	D	1127	-	5,9,9	2.21	1 (20%)	5,11,11	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	B	1107	2	-	0/6/26/26	0/3/3/3
5	GLN	C	1120	-	-	0/5/9/9	-
5	GLN	A	1106	-	-	0/5/9/9	-
4	AMP	D	1121	2	-	6/6/26/26	0/3/3/3
5	GLN	B	1113	-	-	0/5/9/9	-
4	AMP	A	1100	-	-	0/6/26/26	0/3/3/3
4	AMP	C	1114	-	-	0/6/26/26	0/3/3/3
5	GLN	D	1127	-	-	0/5/9/9	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	GLN	CA-N	-6.31	1.33	1.47
5	B	1113	GLN	CA-N	-5.00	1.35	1.47
5	C	1120	GLN	CA-N	-4.99	1.35	1.47
5	D	1127	GLN	CA-N	-4.77	1.36	1.47
4	C	1114	AMP	O2'-C2'	3.19	1.50	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	C5-C6-N6	6.53	130.28	120.35
4	D	1121	AMP	O2P-P-O5'	-5.78	91.36	106.73
4	C	1114	AMP	C2'-C3'-C4'	-5.57	91.82	102.64
4	A	1100	AMP	O3'-C3'-C2'	5.12	128.39	111.82
4	D	1121	AMP	C2'-C3'-C4'	-4.50	93.90	102.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1121	AMP	C5'-O5'-P-O1P
4	D	1121	AMP	C5'-O5'-P-O2P
4	D	1121	AMP	C5'-O5'-P-O3P
4	D	1121	AMP	O4'-C4'-C5'-O5'
4	D	1121	AMP	C3'-C4'-C5'-O5'

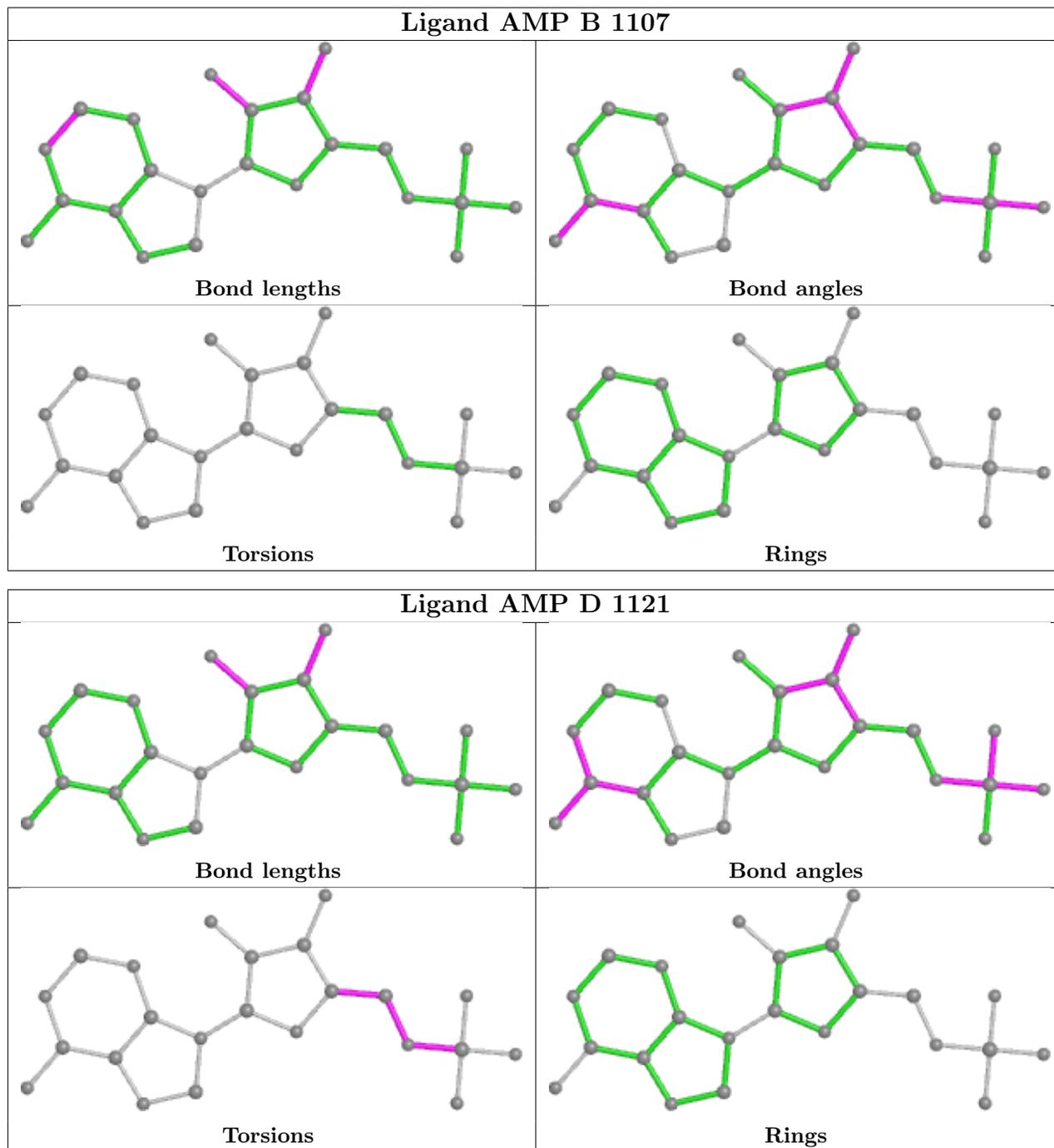
There are no ring outliers.

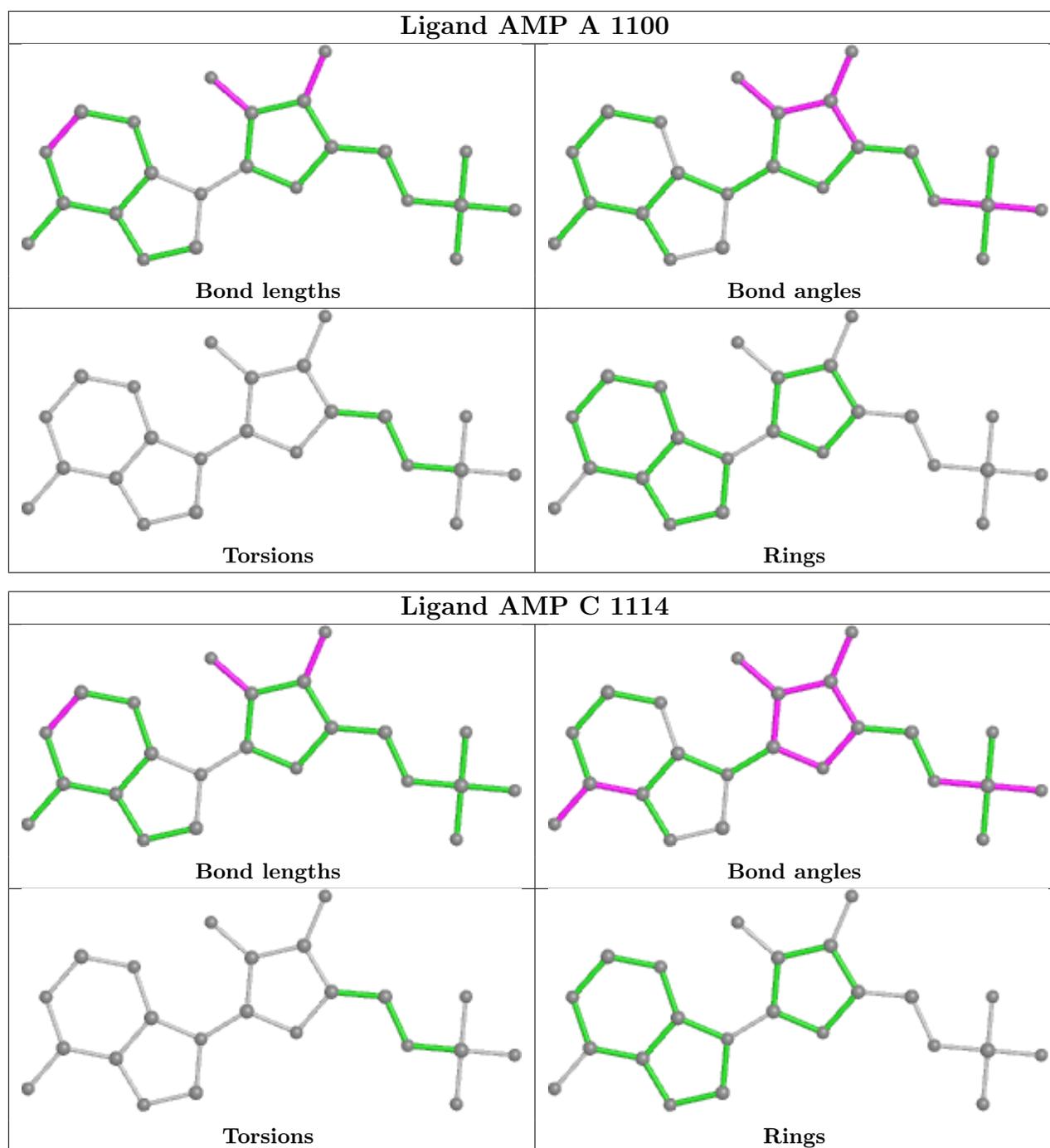
8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1107	AMP	3	0
5	C	1120	GLN	1	0
5	A	1106	GLN	2	0
4	D	1121	AMP	8	0
5	B	1113	GLN	4	0
4	A	1100	AMP	5	0
4	C	1114	AMP	7	0
5	D	1127	GLN	2	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 [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.