



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:04 AM UTC

PDB ID : 1CT9 / pdb_00001ct9
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.;
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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 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

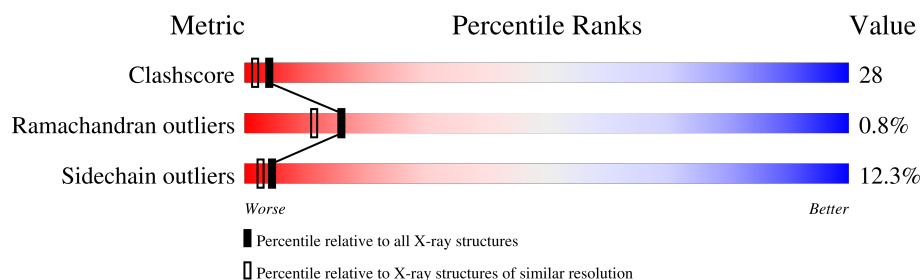
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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.

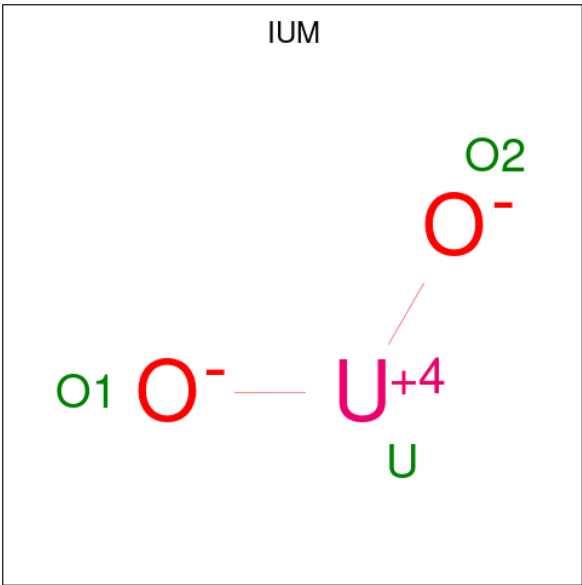
- Molecule 1 is a protein called ASPARAGINE SYNTHETASE B.

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

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 (CCD ID: 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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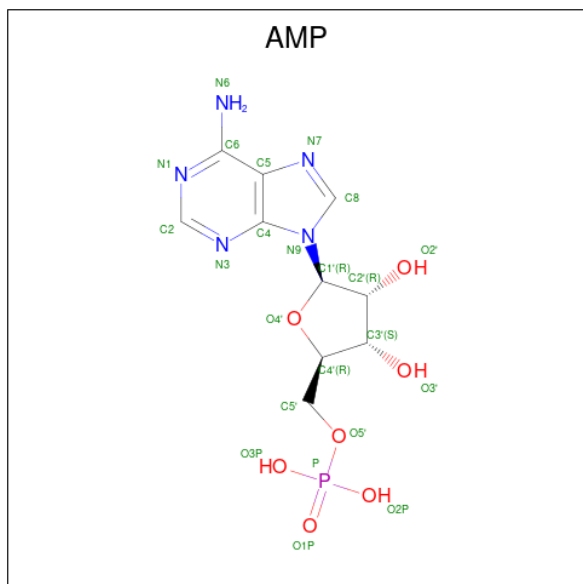
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	U	0	0
			1	1		
2	D	1	Total	U	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



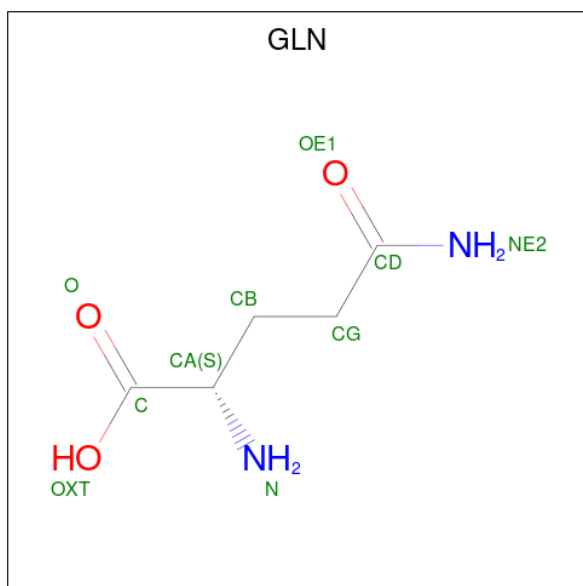
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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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 (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



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.

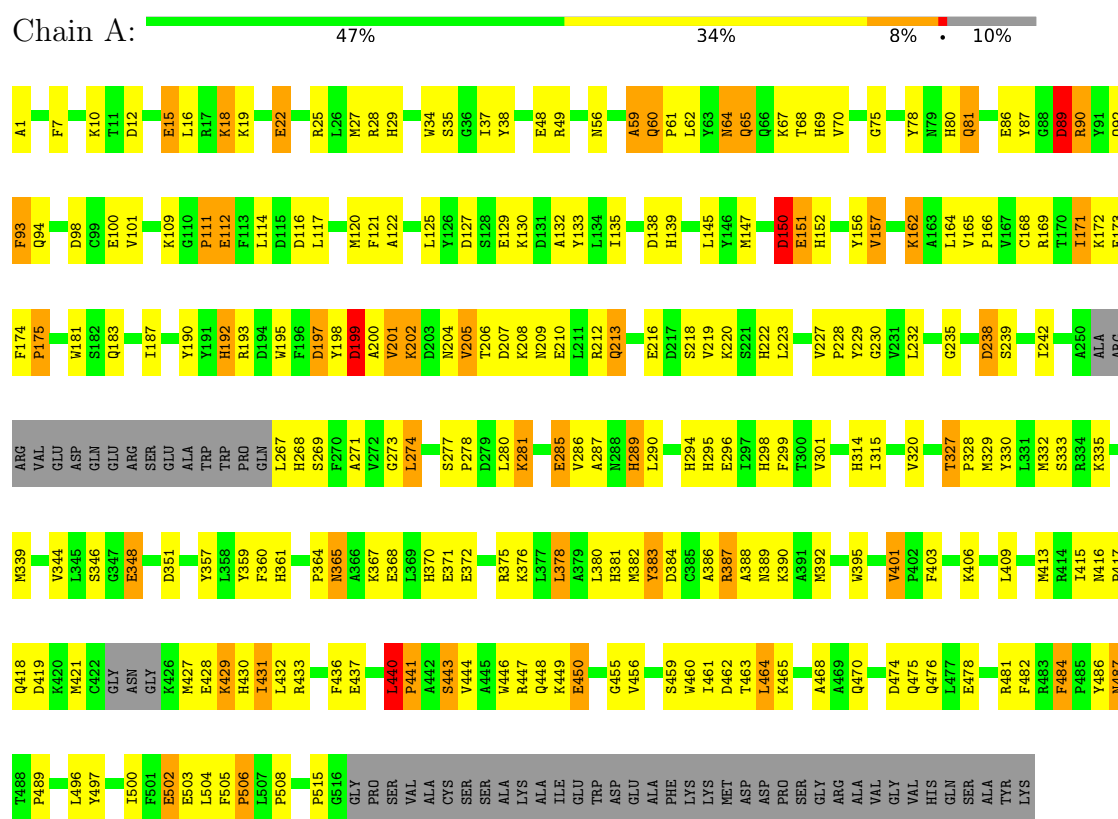
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	235	Total	O	0	0
			235	235		
6	C	223	Total	O	0	0
			223	223		
6	D	296	Total	O	0	0
			296	296		

3 Residue-property plots

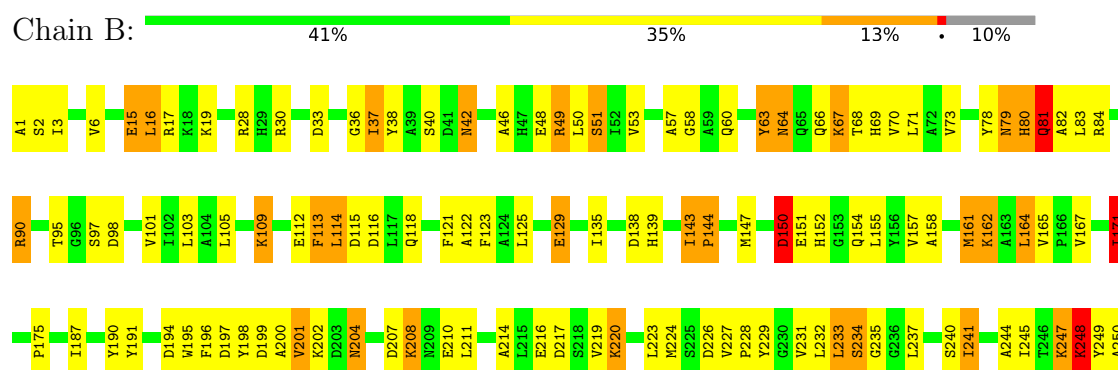
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARAGINE SYNTHETASE B





VAL	E428	D351	PRO	G185	K109
ALA	K429	E352	Q266	E186	G110
CYS	H430	V353	L267	I187	P111
SER		F354	H268	R188	E112
SER	R433		S269	S189	F113
ALA		Y357	F270	Y190	L114
LYS	V444	L358	A271	L115	D115
ALA		Y359	V272	Y191	D116
ILE	Q448	F360	G273	H192	L117
GLU	LYS	H361	L274	R193	Q118
TRP	GLU	K362		G119	G119
ASP	GLN	A363	S277	D197	M120
GLU	PHE	P364	P278	Y198	
ALA	SER		D279	D199	L125
PHE	D454	K367	L280	A200	Y126
LYS	G455	E368	K281	V201	
LYS	V456		K202	D203	E129
MET	G457	E371	V293	N204	A132
ASP	Y458	E372	H294	D205	
ASP	S459		H295	I206	R137
PRO	W460	R375	I297	D207	D138
SER		L380	H298		H139
GLY	L464	H381	F299	E210	L140
ARG	K465	M382	T300		
ALA	E466	Y383		V219	I143
VAL		D384	D310	K220	P144
GLY	Q470				L145
VAL	Q471	R387	H314	L223	Y146
HIS	V472	A388	I315	M224	M147
GLN	S473	D474	E316	S225	G148
SER		Q475	T317	D226	Y149
ALA	Q476	W395	Y318	V227	D150
ALA	L477	E398	D319	P228	E151
LYS	E478	A399	V320	Y229	H152
		R400	I323	G230	G153
	N487	V401		V231	Q154
		P402	T327	L232	L155
	K492	D405	P328	L233	Y156
E493	A494	K406		S234	V157
Y495	L496	K407	M332	G235	
L497	Y497	D410	S333	S239	E160
			R334		M161
	F501	R414	K335	K247	K162
E502		I415	K337		
	P506	N416	A338	A251	V165
L507	P508	P417	M339	ARG	P166
S509		Q418	G340	ARG	C168
		D419	I341	VAL	R169
C513	V514	K420	K342	GLU	T170
	P515	M421	M343	ASP	
G516		C422	V344	GLN	E173
GLY		P515	L345	GLU	F174
PRO		G423	S346	ARG	P175
SER		ASN	G347	SER	
		GLY	E348	GLU	W181
		K426	G349	ALA	S182
		M427	S350	TRP	Q183
				TRP	D184

4 Data and refinement statistics

Xtriage (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.	Xtriage
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, AMP, CL

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	1.20	0/4060	1.71	50/5493 (0.9%)
1	B	1.18	1/4037 (0.0%)	1.74	64/5466 (1.2%)
1	C	1.14	1/4037 (0.0%)	1.66	51/5466 (0.9%)
1	D	1.22	6/4022 (0.1%)	1.72	58/5443 (1.1%)
All	All	1.18	8/16156 (0.0%)	1.71	223/21868 (1.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	5.50	1.35	1.25
1	D	150	ASP	CA-CB	5.36	1.61	1.53
1	D	87	TYR	CA-C	-5.31	1.45	1.52
1	B	33	ASP	CG-OD2	5.30	1.35	1.25
1	C	231	VAL	C-O	5.24	1.29	1.24

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CA-CB-CG	-12.34	100.26	112.60
1	A	150	ASP	CA-CB-CG	-12.23	100.37	112.60
1	D	64	ASN	CA-CB-CG	-12.21	100.39	112.60
1	A	482	PHE	CA-CB-CG	-11.83	101.97	113.80
1	B	430	HIS	CA-CB-CG	-11.27	102.53	113.80

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	206	0
1	B	3942	0	3828	258	0
1	C	3942	0	3827	212	0
1	D	3930	0	3818	195	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	6	0
4	B	23	0	12	3	0
4	C	23	0	11	8	0
4	D	23	0	12	9	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	9	0
6	B	235	0	0	14	0
6	C	223	0	0	7	0
6	D	296	0	0	19	0
All	All	16980	0	15409	864	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 28.

The worst 5 of 864 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%)	30	27
1	B	487/553 (88%)	449 (92%)	31 (6%)	7 (1%)	9	4
1	C	487/553 (88%)	450 (92%)	33 (7%)	4 (1%)	16	11
1	D	487/553 (88%)	467 (96%)	18 (4%)	2 (0%)	30	27
All	All	1952/2212 (88%)	1831 (94%)	106 (5%)	15 (1%)	16	11

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%)	351 (85%)	63 (15%)	3	1
1	C	414/462 (90%)	361 (87%)	53 (13%)	4	2
1	D	412/462 (89%)	370 (90%)	42 (10%)	7	4
All	All	1658/1848 (90%)	1453 (88%)	205 (12%)	4	2

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	GLN
1	C	341	ILE
1	D	456	VAL
1	C	81	GLN
1	C	201	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	94	GLN
1	C	470	GLN
1	C	183	GLN
1	C	302	GLN
1	D	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	D	1121	2	25,25,25	1.19	3 (12%)	37,38,38	1.84	7 (18%)
5	GLN	B	1113	-	8,9,9	1.26	1 (12%)	8,11,11	0.92	1 (12%)
5	GLN	C	1120	-	8,9,9	1.32	2 (25%)	8,11,11	1.49	2 (25%)
5	GLN	D	1127	-	8,9,9	1.35	1 (12%)	8,11,11	0.87	0
2	IUM	A	1102	-	0,1,2	-	-	-	-	-
4	AMP	B	1107	2	25,25,25	1.20	3 (12%)	37,38,38	1.05	3 (8%)
5	GLN	A	1106	-	8,9,9	1.33	1 (12%)	8,11,11	0.95	0
4	AMP	A	1100	-	25,25,25	1.28	3 (12%)	37,38,38	1.60	5 (13%)
2	IUM	D	1122	4	0,1,2	-	-	-	-	-
4	AMP	C	1114	-	25,25,25	1.28	3 (12%)	37,38,38	1.69	6 (16%)

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	D	1121	2	-	6/10/26/26	0/3/3/3
5	GLN	B	1113	-	-	0/9/9/9	-
5	GLN	C	1120	-	-	0/9/9/9	-
5	GLN	D	1127	-	-	0/9/9/9	-
4	AMP	B	1107	2	-	0/10/26/26	0/3/3/3
5	GLN	A	1106	-	-	0/9/9/9	-
4	AMP	A	1100	-	-	0/10/26/26	0/3/3/3
4	AMP	C	1114	-	-	0/10/26/26	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	GLN	CA-N	-3.08	1.33	1.48
4	C	1114	AMP	O2'-C2'	3.05	1.50	1.43
4	C	1114	AMP	O3'-C3'	3.03	1.50	1.43
4	A	1100	AMP	O2'-C2'	2.93	1.50	1.43
4	A	1100	AMP	O3'-C3'	2.91	1.50	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	O2P-P-O5'	-5.87	91.36	106.67
4	C	1114	AMP	C2'-C3'-C4'	-5.59	91.82	102.61
4	A	1100	AMP	O3'-C3'-C2'	5.17	128.39	111.82
4	D	1121	AMP	C2'-C3'-C4'	-4.51	93.90	102.61
4	C	1114	AMP	O3'-C3'-C2'	4.37	125.83	111.82

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'

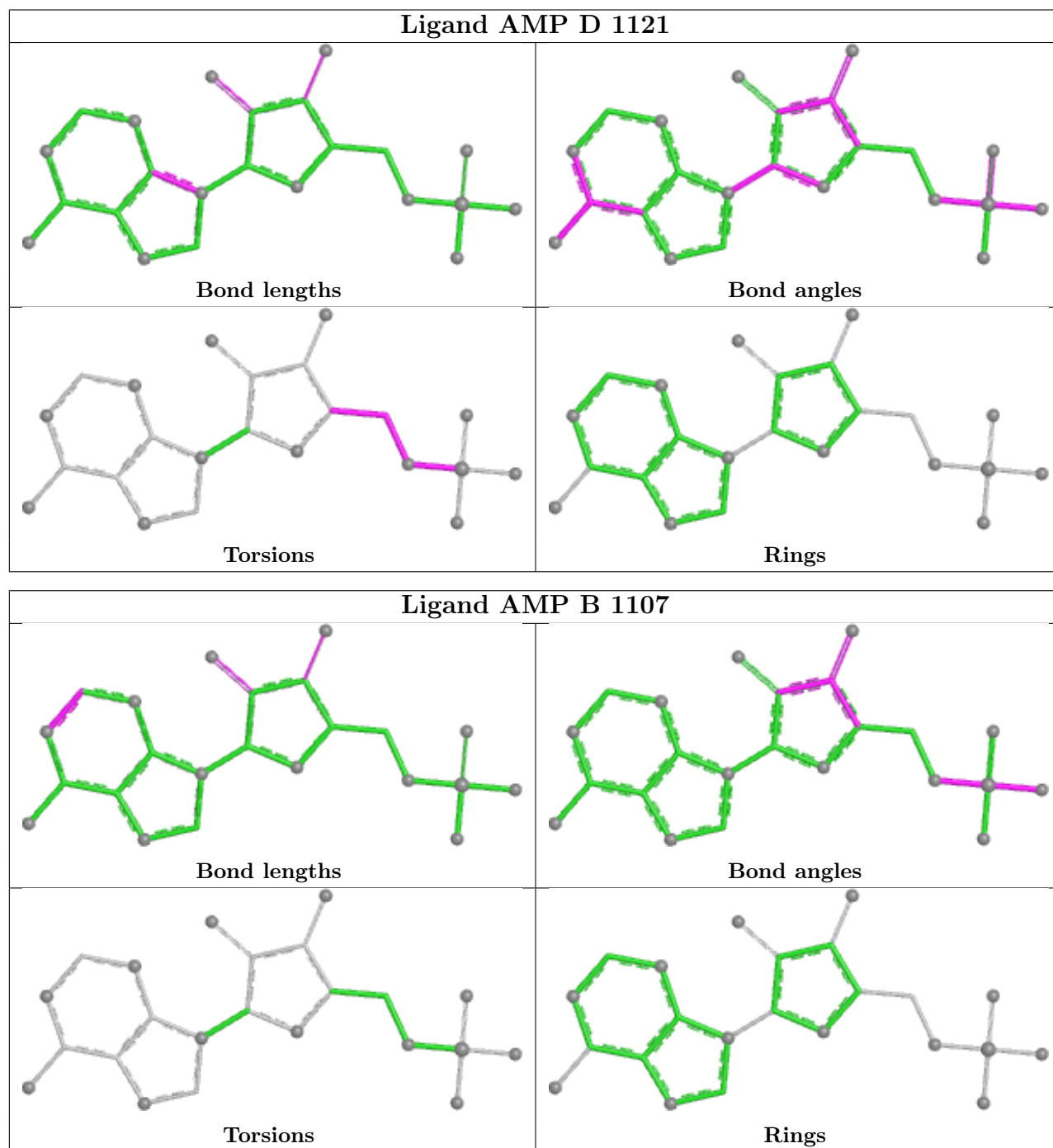
There are no ring outliers.

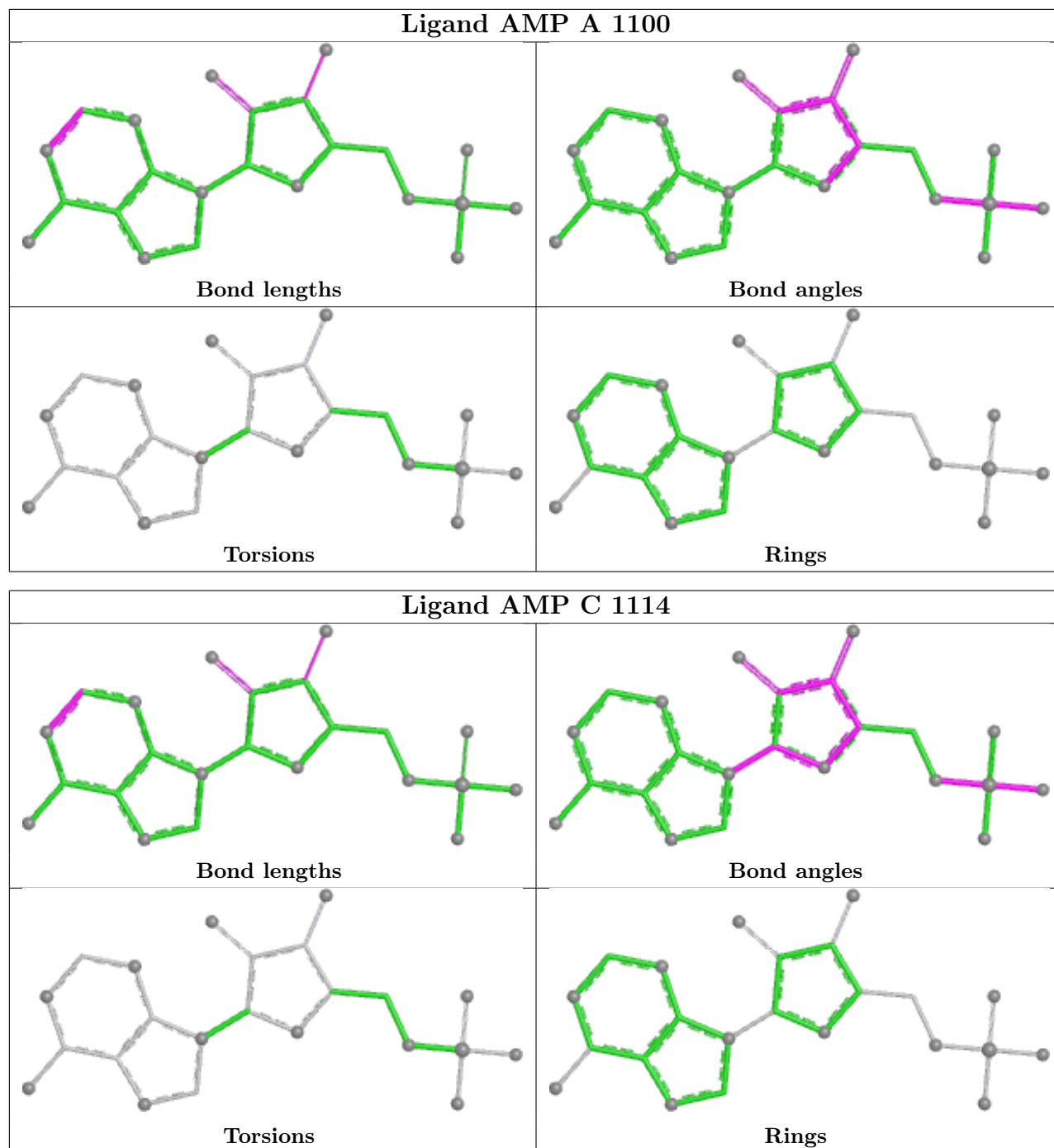
8 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1121	AMP	9	0
5	B	1113	GLN	4	0
5	C	1120	GLN	1	0
5	D	1127	GLN	2	0
4	B	1107	AMP	3	0
5	A	1106	GLN	2	0
4	A	1100	AMP	6	0
4	C	1114	AMP	8	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.