



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 01:16 PM UTC

PDB ID : 3H0L / pdb_00003h0l
Title : Structure of trna-dependent amidotransferase gatcab from aquifex aeolicus
Authors : Wu, J.; Bu, W.; Sheppard, K.; Kitabatake, M.; Soll, D.; Smith, J.L.
Deposited on : 2009-04-09
Resolution : 2.30 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

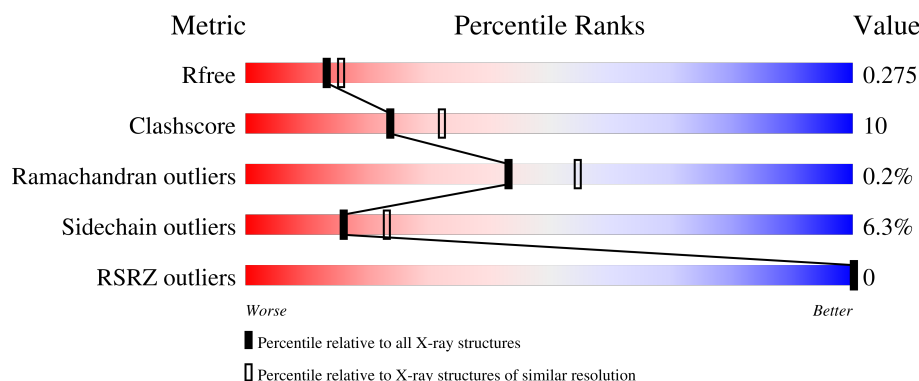
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



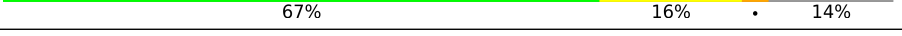
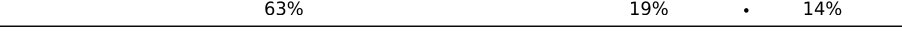
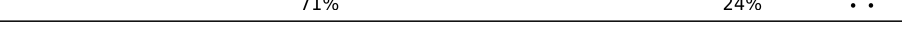
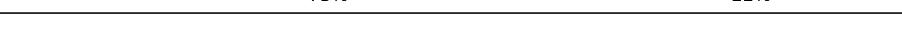
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	
1	D	478	
1	G	478	
1	J	478	
1	M	478	

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Mol	Chain	Length	Quality of chain
1	P	478	
1	S	478	
1	V	478	
2	B	478	
2	E	478	
2	H	478	
2	K	478	
2	N	478	
2	Q	478	
2	T	478	
2	W	478	
3	C	94	
3	F	94	
3	I	94	
3	L	94	
3	O	94	
3	R	94	
3	U	94	
3	X	94	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 63144 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	D	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	G	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	J	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	M	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	P	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	S	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			
1	V	478	Total	C	N	O	S	0	0	0
			3784	2450	615	712	7			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	E	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	H	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	K	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	N	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	Q	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

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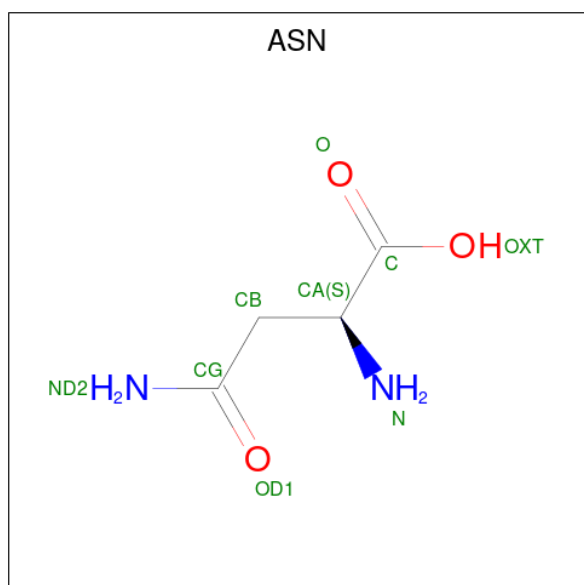
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			
2	W	410	Total	C	N	O	S	0	0	0
			3308	2104	567	622	15			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

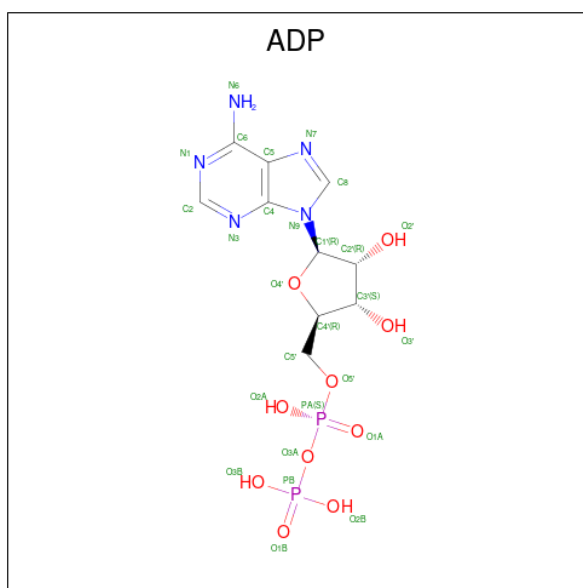
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	F	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	I	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	L	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	O	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	R	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	U	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			
3	X	91	Total	C	N	O	S	0	0	0
			764	487	125	150	2			

- Molecule 4 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	G	1	Total	C	N	O	0	0
			8	4	1	3		
4	J	1	Total	C	N	O	0	0
			8	4	1	3		
4	M	1	Total	C	N	O	0	0
			8	4	1	3		
4	P	1	Total	C	N	O	0	0
			8	4	1	3		
4	S	1	Total	C	N	O	0	0
			8	4	1	3		
4	V	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	W	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		
6	N	1	Total	Mg	0	0
			1	1		
6	Q	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	W	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		
7	E	1	Total	Zn	0	0
			1	1		
7	H	1	Total	Zn	0	0
			1	1		
7	K	1	Total	Zn	0	0
			1	1		
7	N	1	Total	Zn	0	0
			1	1		

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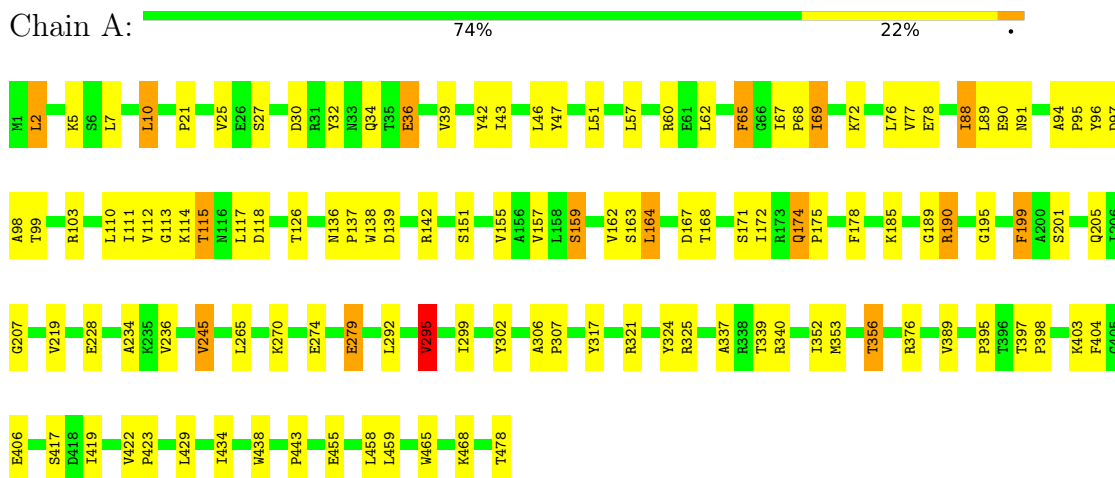
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Q	1	Total 1	Zn 1	0	0
7	T	1	Total 1	Zn 1	0	0
7	W	1	Total 1	Zn 1	0	0

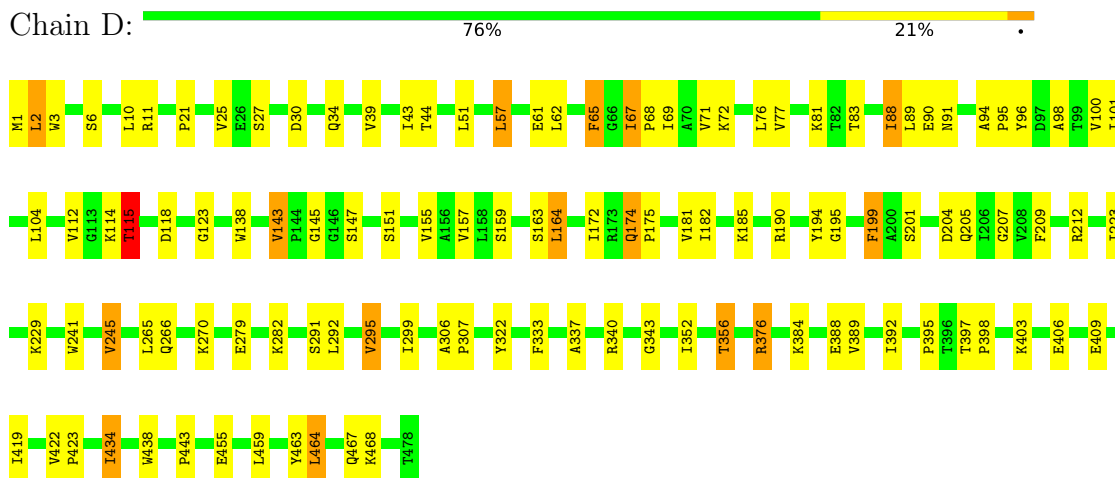
3 Residue-property plots [i](#)

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

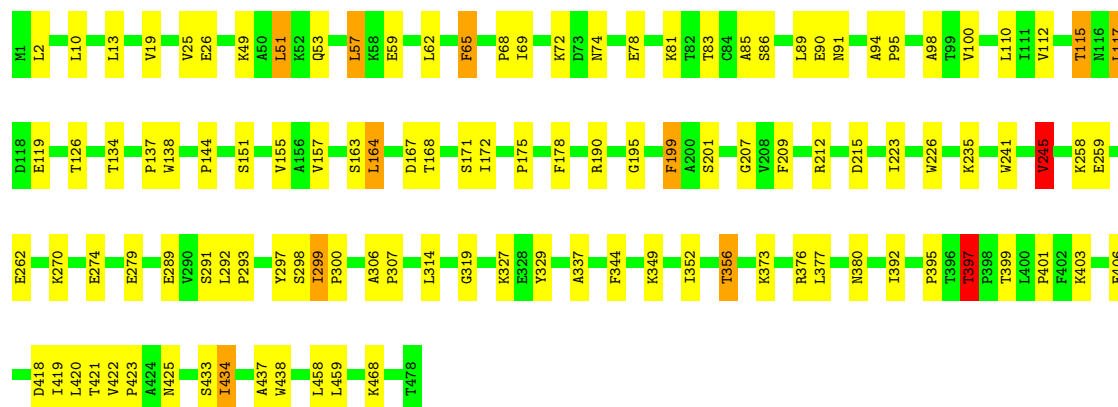


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

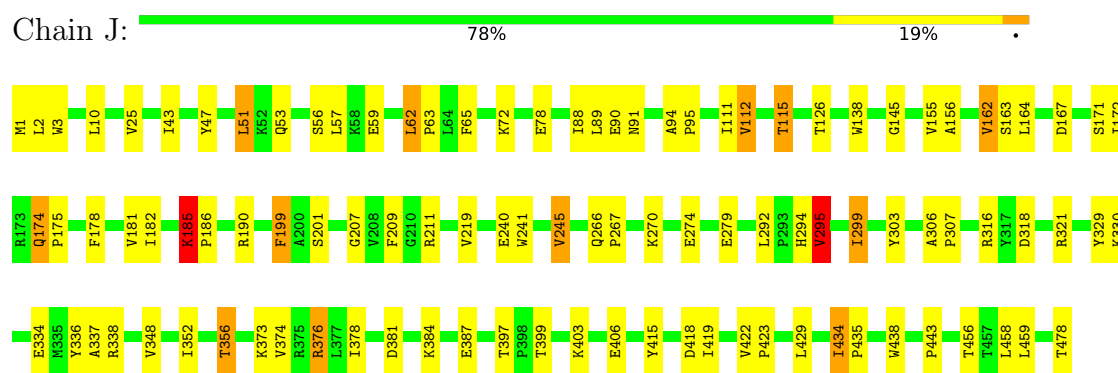


- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

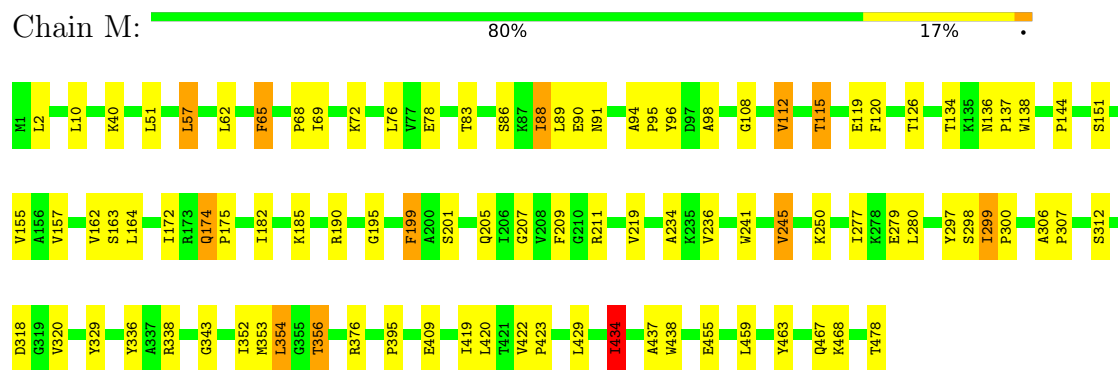




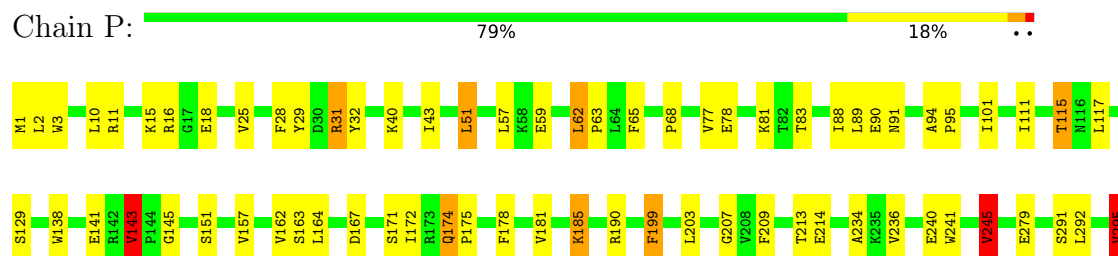
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



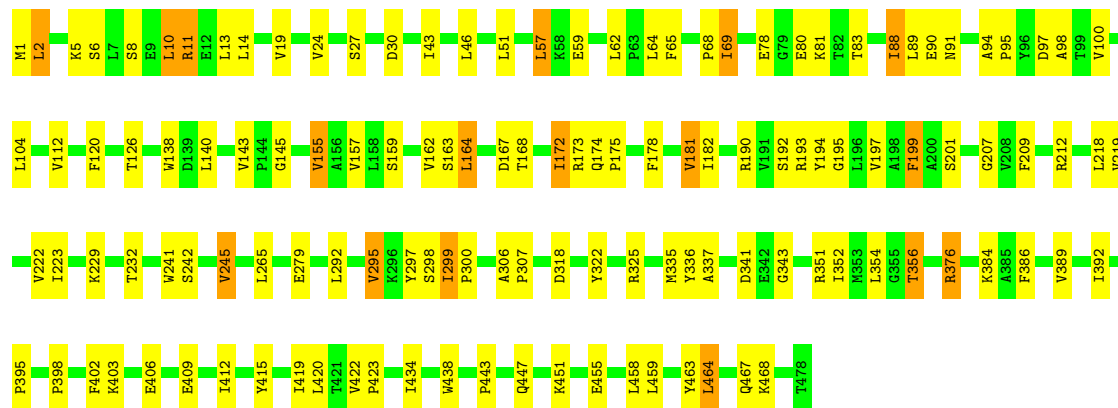
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A





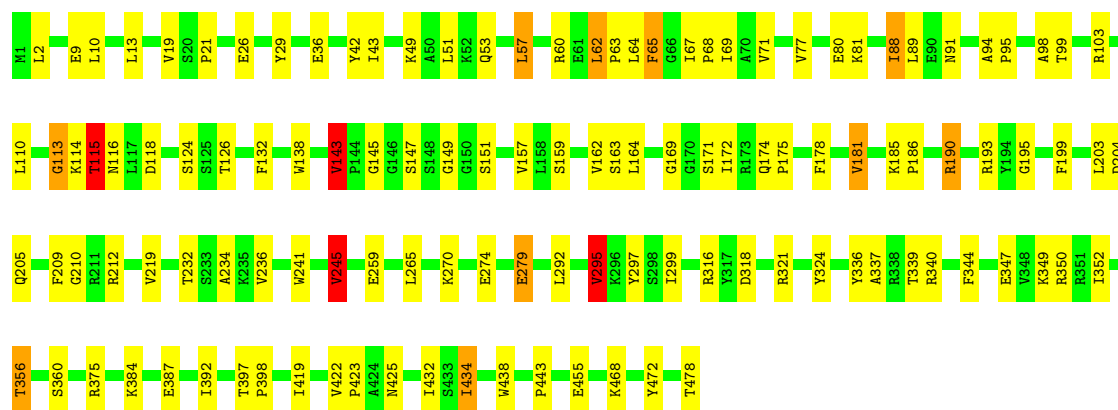
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain S: 73% 24% .



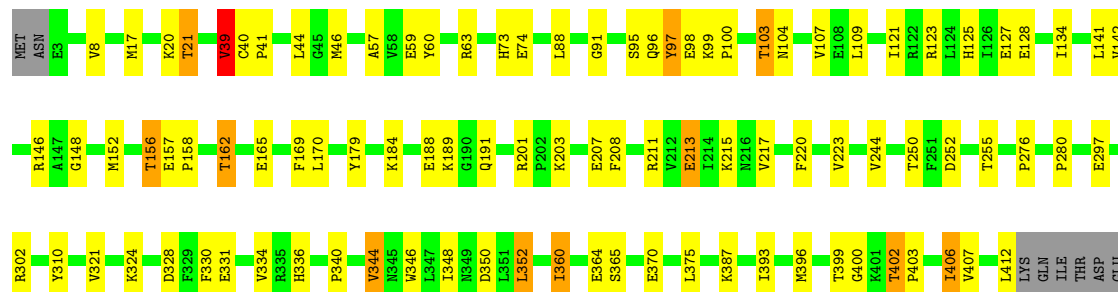
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain V: 74% 23% ..



• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B: 65% 18% 14%



ASN	GLN	ILE	LYS	GLU	VAL	LYS	LYS	ILE	PHE	GLU	LYS	HIS	PRO	LYS	GLU	VAL	GLU	ARG	LEU	GLN	GLY	GLU	GLU	LYS	LEU	ILE	GLY	PHE	PHE	VAL	GLY	GLN	VAL	VAL	MET	ARG	GLU	THR	ARG	GLY	LYS	ALA	ASN	PRO	GLN	VAL	VAL	ASN	LYS	VAL	ILE	ARG	GLU	LEU	VAL	LYS	GLU	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain E:  65% 18% 14%

LEU	VAL	LYS	ILE	PHE	GLU	LYS	HIS	PRO	LYS	GLU	VAL	GLU	ARG	LEU	LYS	GLN	GLY	GLY	PHE	PHE	VAL	GLY	GLN	VAL	MET	ARG	GLU	THR	ARG	GLY	LYS	ALA	ASN	PRO	GLN	VAL	VAL	ASN	LYS	VAL	ILE	ARG	GLU	LEU	VAL	LYS	GLU	VAL
D277	L278	V279	P280	V283	L306	Y310	G311	L312	H323	V334	P340	K341	V344	L352	S361	I362	E363	E364	E374	L375	K387	K390	I393	M396	V397	T402	P403	S404	Q405	I406	V407	L412	LYS	GLN	ILE	THR	ASP	GLU	ASN	GLN	ILE	LYS	GLU	VAL				
K118	V119	R123	L124	H125	L126	E127	E128	I134	K139	T140	R146	A147	G148	M152	T156	E157	P158	T162	P163	E164	F169	L170	R201	S205	F220	R221	F222	V223	Q224	K225	E232	V244	D252	P253	Q254	T255	G256	K257	T258	Y259	R262	D275	P276					
MET	ASN	E3	V8	M17	T21	K22	C27	V39	C40	P41	L44	G45	M46	P47	A57	Y60	H73	E74	V77	R80	Y85	P86	D87	L88	P89	K90	G91	S95	Q96	E98	K99	P100	T103	N104	G105	W106	L109	N110	N113	G114	E115							

• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain H:  65% 18% 14%

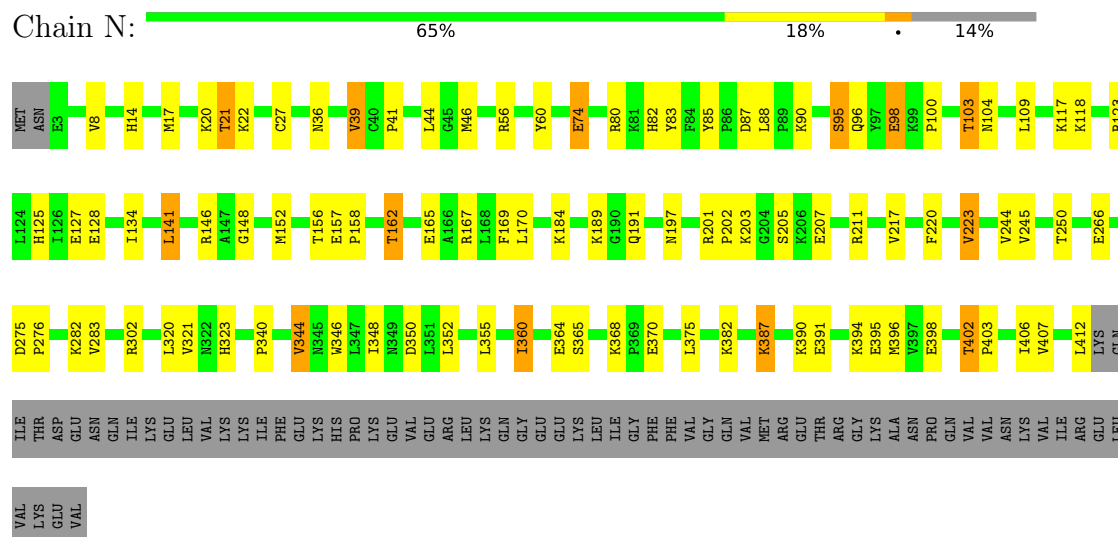
ILE	LYS	D252	GLU	T255	VAL	LYS	LYS	E266	PHE	GLU	D275	P276	K282	PRO	HIS	LYS	K132	N133	L144	N145	R146	L320	ARG	LEU	LYS	GLN	GLY	GLU	GLU	GLU	LYS	V344	N345	W346	D350	L351	L352	GLY	GLN	VAL	VAL	MET	ARG	GLU	THR	ARG	GLY	LYS	ALA	E395	PRO	PRO	GLM	VAL	VAL	ASN	VAL	VAL	ILE	ARG	GLU	LEU	VAL	LYS	GLU	GLU	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

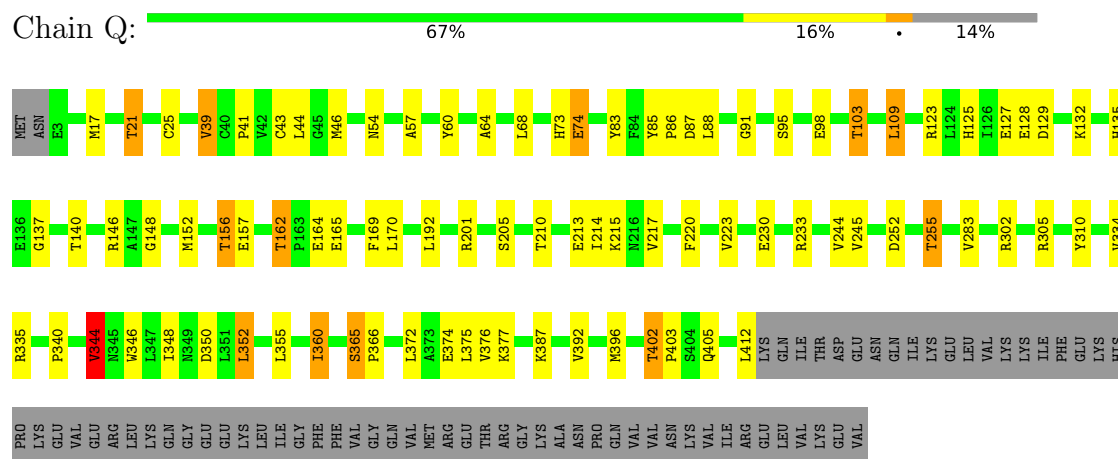
Chain K:  69% 15% 14%

LYS	LEU	ILE	GLY	PHE	PHE	VAL	GLY	GLN	VAL	MET	ARG	ARG	GLU	THR	ARG	GLY	LYS	ALA	ASN	PRO	GLN	VAL	VAL	ASN	LYS	VAL	ILE	ARG	GLU	LEU	VAL	LYS	LYS	GLU	GLU	VAL			
L355	L355	L360	E363	E364	S365	P366	L372	A373	E374	L375	V376	K377	L378	L379	I384	V392	M396	Q405	L412	LYS	GLN	ILE	THR	ASP	GLU	ASN	GLN	ILE	LYS	GLU	LEU	VAL	LYS	LYS	GLU	GLU	VAL		
R146	A147	G148	M152	T156	E157	P158	T162	P163	E164	E165	A166	L167	L168	F169	L170	L192	R201	S205	N218	S219	F220	V223	V244	V245	D252	T255	Y259	E266	V283	Y310	F330	E331	V334	K338	E339	P340	K341	V344	L352
MET	ASN	E3	V8	M17	T21	E30	V39	C40	P41	L44	G45	M46	Y60	H73	E74	Y85	P86	D87	K90	G91	S95	E98	K99	P100	T103	N104	L109	M113	G114	E115	R123	E127	E128	K132	N133	I134	T140	L141	V142

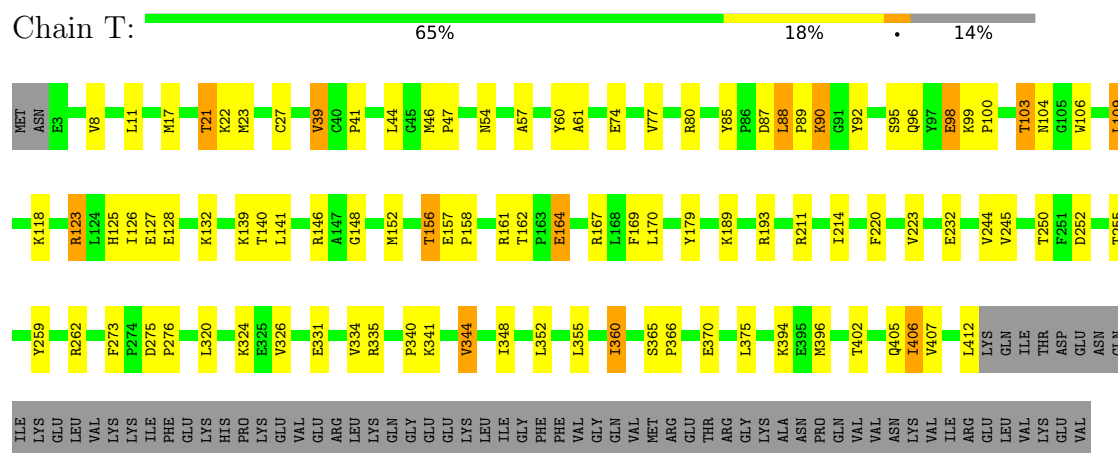
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



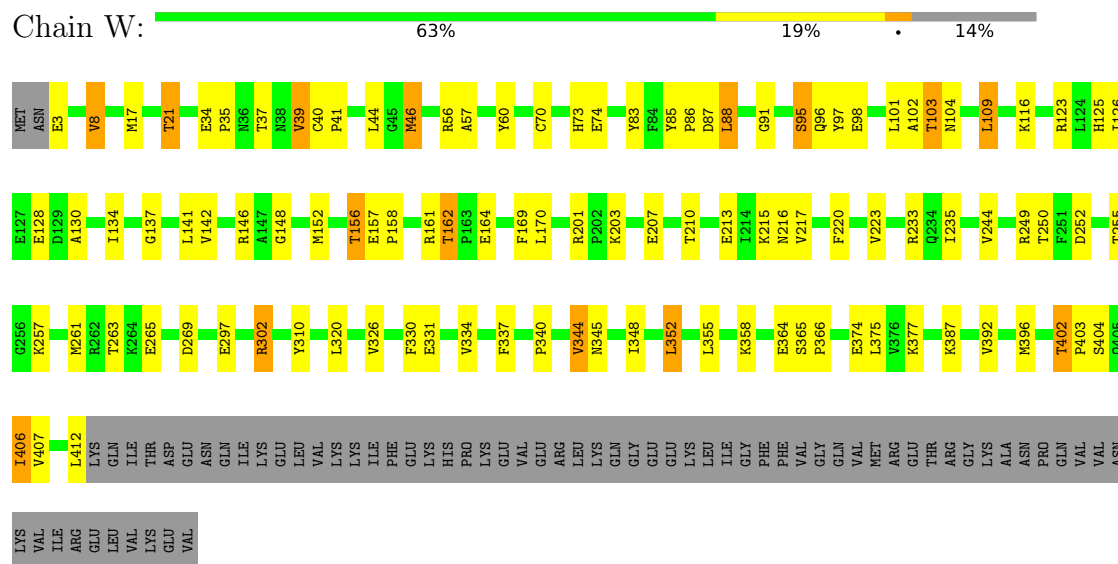
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



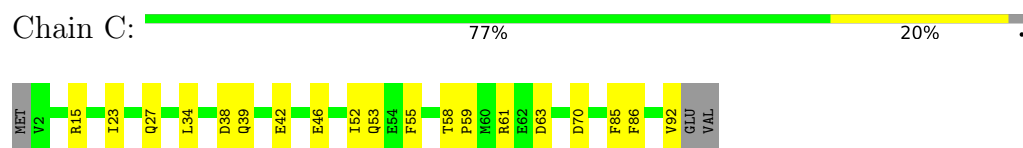
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B



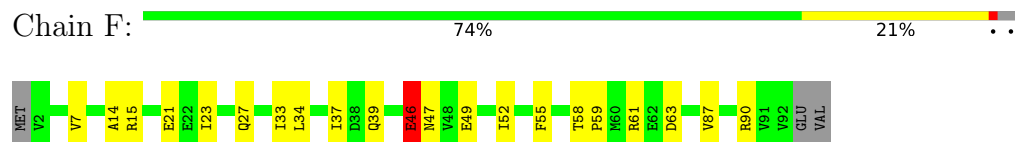
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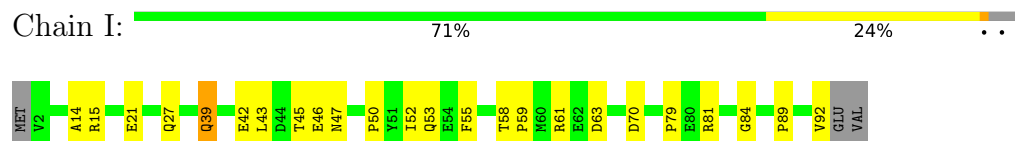
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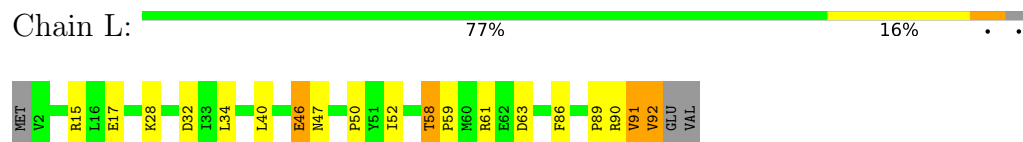
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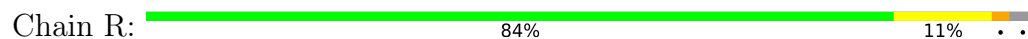


- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

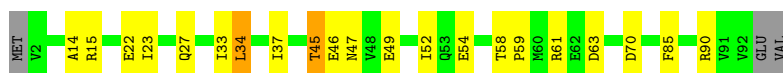




- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



- Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.48Å 131.01Å 154.67Å 90.02° 90.00° 89.91°	Depositor
Resolution (Å)	40.50 – 2.30 40.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.7 (40.50-2.30) 91.4 (40.50-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.273 0.251 , 0.275	Depositor DCC
R_{free} test set	20322 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	1.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.146 for h,-k,-l 0.459 for -h,k,-l 0.146 for -h,-k,l 0.000 for -k,-h,-l 0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	63144	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2482e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, MG

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	0/3874	0.98	4/5244 (0.1%)
1	D	0.72	0/3874	0.97	4/5244 (0.1%)
1	G	0.72	2/3874 (0.1%)	0.96	5/5244 (0.1%)
1	J	0.75	2/3874 (0.1%)	0.97	4/5244 (0.1%)
1	M	0.70	0/3874	0.96	1/5244 (0.0%)
1	P	0.73	1/3874 (0.0%)	0.97	4/5244 (0.1%)
1	S	0.72	1/3874 (0.0%)	0.98	1/5244 (0.0%)
1	V	0.74	0/3874	0.99	8/5244 (0.2%)
2	B	0.64	0/3371	0.93	3/4541 (0.1%)
2	E	0.71	2/3371 (0.1%)	0.94	6/4541 (0.1%)
2	H	0.68	0/3371	0.94	3/4541 (0.1%)
2	K	0.68	0/3371	0.94	3/4541 (0.1%)
2	N	0.69	1/3371 (0.0%)	0.94	3/4541 (0.1%)
2	Q	0.69	1/3371 (0.0%)	0.96	5/4541 (0.1%)
2	T	0.69	0/3371	0.94	3/4541 (0.1%)
2	W	0.69	2/3371 (0.1%)	0.92	4/4541 (0.1%)
3	C	0.72	2/778 (0.3%)	1.00	0/1050
3	F	0.65	0/778	0.97	1/1050 (0.1%)
3	I	0.73	3/778 (0.4%)	0.93	0/1050
3	L	0.67	0/778	1.01	5/1050 (0.5%)
3	O	0.66	0/778	0.95	2/1050 (0.2%)
3	R	0.68	0/778	1.02	1/1050 (0.1%)
3	U	0.63	0/778	0.92	0/1050
3	X	0.66	0/778	0.98	1/1050 (0.1%)
All	All	0.70	17/64184 (0.0%)	0.96	71/86680 (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
2	B	0	2
3	I	0	1
3	O	0	1
3	U	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	299	ILE	CA-CB	9.16	1.59	1.54
1	J	299	ILE	CA-CB	9.11	1.59	1.54
1	G	299	ILE	CA-CB	7.26	1.58	1.54
2	E	110	ASN	CG-OD1	6.16	1.35	1.23
3	I	27	GLN	CD-OE1	5.73	1.34	1.23

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	VAL	CB-CA-C	-7.74	101.90	112.04
2	W	98	GLU	N-CA-C	-6.98	101.31	110.53
2	B	88	LEU	CA-C-N	6.68	126.47	119.05
2	B	88	LEU	C-N-CA	6.68	126.47	119.05
2	E	323	HIS	CB-CG-CD2	-6.68	122.52	131.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	VAL	Peptide
2	B	97	TYR	Peptide
3	I	45	THR	Peptide
3	O	45	THR	Peptide
3	U	45	THR	Peptide

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	3784	0	3816	96	0
1	D	3784	0	3816	80	0
1	G	3784	0	3816	93	0
1	J	3784	0	3816	74	0
1	M	3784	0	3816	73	0
1	P	3784	0	3816	77	0
1	S	3784	0	3816	92	0
1	V	3784	0	3816	101	0
2	B	3308	0	3354	85	0
2	E	3308	0	3353	77	0
2	H	3308	0	3353	77	0
2	K	3308	0	3353	67	0
2	N	3308	0	3353	68	0
2	Q	3308	0	3353	66	0
2	T	3308	0	3353	77	0
2	W	3308	0	3353	77	0
3	C	764	0	755	11	0
3	F	764	0	755	17	0
3	I	764	0	755	18	0
3	L	764	0	755	22	0
3	O	764	0	755	16	0
3	R	764	0	755	15	0
3	U	764	0	755	15	0
3	X	764	0	755	17	0
4	A	8	0	3	1	0
4	D	8	0	3	1	0
4	G	8	0	3	0	0
4	J	8	0	3	0	0
4	M	8	0	3	0	0
4	P	8	0	3	1	0
4	S	8	0	3	1	0
4	V	8	0	3	0	0
5	B	27	0	12	1	0
5	E	27	0	12	0	0
5	H	27	0	12	0	0
5	K	27	0	12	0	0
5	N	27	0	12	0	0
5	Q	27	0	12	0	0
5	T	27	0	12	1	0
5	W	27	0	12	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	1	0	0	0	0
6	N	1	0	0	0	0
6	Q	1	0	0	0	0
6	T	1	0	0	0	0
6	W	1	0	0	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
7	Q	1	0	0	0	0
7	T	1	0	0	0	0
7	W	1	0	0	0	0
All	All	63144	0	63513	1283	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 10.

The worst 5 of 1283 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:V:77:VAL:CG2	1:V:114:LYS:HZ2	1.57	1.16
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.05	1.16
1:V:77:VAL:HG21	1:V:114:LYS:NZ	1.61	1.13
1:V:77:VAL:HG21	1:V:114:LYS:HZ2	0.94	1.08
1:A:47:TYR:O	1:A:51:LEU:HD13	1.54	1.07

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 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	476/478 (100%)	455 (96%)	19 (4%)	2 (0%)	30	38
1	D	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	30	38
1	G	476/478 (100%)	453 (95%)	21 (4%)	2 (0%)	30	38
1	J	476/478 (100%)	457 (96%)	17 (4%)	2 (0%)	30	38
1	M	476/478 (100%)	456 (96%)	18 (4%)	2 (0%)	30	38
1	P	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	30	38
1	S	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	30	38
1	V	476/478 (100%)	454 (95%)	20 (4%)	2 (0%)	30	38
2	B	408/478 (85%)	393 (96%)	15 (4%)	0	100	100
2	E	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	H	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	K	408/478 (85%)	393 (96%)	14 (3%)	1 (0%)	43	55
2	N	408/478 (85%)	394 (97%)	14 (3%)	0	100	100
2	Q	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
2	T	408/478 (85%)	396 (97%)	12 (3%)	0	100	100
2	W	408/478 (85%)	395 (97%)	13 (3%)	0	100	100
3	C	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
3	F	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	I	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	L	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	O	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
3	R	89/94 (95%)	89 (100%)	0	0	100	100
3	U	89/94 (95%)	86 (97%)	3 (3%)	0	100	100
3	X	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
All	All	7784/8400 (93%)	7490 (96%)	277 (4%)	17 (0%)	43	55

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	LEU
1	S	2	LEU
1	S	409	GLU
1	G	2	LEU
1	G	65	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/406 (100%)	385 (95%)	21 (5%)	21	31
1	D	406/406 (100%)	377 (93%)	29 (7%)	13	19
1	G	406/406 (100%)	386 (95%)	20 (5%)	22	34
1	J	406/406 (100%)	379 (93%)	27 (7%)	15	21
1	M	406/406 (100%)	384 (95%)	22 (5%)	20	29
1	P	406/406 (100%)	376 (93%)	30 (7%)	13	17
1	S	406/406 (100%)	380 (94%)	26 (6%)	16	23
1	V	406/406 (100%)	387 (95%)	19 (5%)	23	35
2	B	364/427 (85%)	341 (94%)	23 (6%)	16	23
2	E	364/427 (85%)	340 (93%)	24 (7%)	15	21
2	H	364/427 (85%)	338 (93%)	26 (7%)	13	19
2	K	364/427 (85%)	342 (94%)	22 (6%)	17	25
2	N	364/427 (85%)	337 (93%)	27 (7%)	13	17
2	Q	364/427 (85%)	341 (94%)	23 (6%)	16	23
2	T	364/427 (85%)	338 (93%)	26 (7%)	13	19
2	W	364/427 (85%)	337 (93%)	27 (7%)	13	17
3	C	86/89 (97%)	80 (93%)	6 (7%)	14	19
3	F	86/89 (97%)	82 (95%)	4 (5%)	23	35
3	I	86/89 (97%)	80 (93%)	6 (7%)	14	19
3	L	86/89 (97%)	82 (95%)	4 (5%)	23	35
3	O	86/89 (97%)	81 (94%)	5 (6%)	18	26
3	R	86/89 (97%)	82 (95%)	4 (5%)	23	35
3	U	86/89 (97%)	81 (94%)	5 (6%)	18	26
3	X	86/89 (97%)	81 (94%)	5 (6%)	18	26
All	All	6848/7376 (93%)	6417 (94%)	431 (6%)	16	23

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	409	GLU
1	P	245	VAL
2	W	8	VAL
2	N	98	GLU
2	N	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	294	ASN
2	W	301	GLN
2	N	218	ASN
1	V	53	GLN
1	M	275	ASN

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](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	ASN	P	906	1	6,7,8	1.10	0	3,8,10	1.49	0
5	ADP	W	708	-	28,29,29	1.47	5 (17%)	43,45,45	1.80	8 (18%)
4	ASN	G	903	1	6,7,8	1.20	1 (16%)	3,8,10	2.38	1 (33%)
4	ASN	D	902	1	6,7,8	1.12	1 (16%)	3,8,10	1.51	1 (33%)
4	ASN	S	907	1	6,7,8	1.52	2 (33%)	3,8,10	2.23	1 (33%)
5	ADP	N	705	-	28,29,29	1.61	6 (21%)	43,45,45	1.68	8 (18%)
4	ASN	M	905	1	6,7,8	1.24	1 (16%)	3,8,10	1.82	1 (33%)
4	ASN	A	901	1	6,7,8	1.18	1 (16%)	3,8,10	1.25	0
5	ADP	K	704	-	28,29,29	1.50	5 (17%)	43,45,45	1.78	6 (13%)
5	ADP	Q	706	-	28,29,29	1.51	4 (14%)	43,45,45	1.79	9 (20%)
4	ASN	V	908	1	6,7,8	1.39	1 (16%)	3,8,10	1.58	1 (33%)
5	ADP	E	702	-	28,29,29	1.43	6 (21%)	43,45,45	1.75	11 (25%)
5	ADP	H	703	-	28,29,29	1.66	6 (21%)	43,45,45	1.64	6 (13%)
5	ADP	T	707	-	28,29,29	1.44	6 (21%)	43,45,45	1.75	10 (23%)
4	ASN	J	904	1	6,7,8	1.24	1 (16%)	3,8,10	1.76	1 (33%)
5	ADP	B	701	-	28,29,29	1.59	4 (14%)	43,45,45	1.78	9 (20%)

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	ASN	P	906	1	-	1/7/7/8	-
5	ADP	W	708	-	-	4/16/32/32	0/3/3/3
4	ASN	G	903	1	-	2/7/7/8	-
4	ASN	D	902	1	-	2/7/7/8	-
4	ASN	S	907	1	-	2/7/7/8	-
5	ADP	N	705	-	-	4/16/32/32	0/3/3/3
4	ASN	M	905	1	-	2/7/7/8	-
4	ASN	A	901	1	-	1/7/7/8	-
5	ADP	K	704	-	-	4/16/32/32	0/3/3/3
5	ADP	Q	706	-	-	6/16/32/32	0/3/3/3
4	ASN	V	908	1	-	0/7/7/8	-
5	ADP	E	702	-	-	3/16/32/32	0/3/3/3
5	ADP	H	703	-	-	5/16/32/32	0/3/3/3
5	ADP	T	707	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ASN	J	904	1	-	2/7/7/8	-
5	ADP	B	701	-	-	4/16/32/32	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	701	ADP	C5-C4	5.23	1.48	1.39
5	N	705	ADP	C5-C4	4.99	1.48	1.39
5	H	703	ADP	C5-C4	4.90	1.47	1.39
5	W	708	ADP	C5-C4	4.88	1.47	1.39
5	Q	706	ADP	C5-C4	4.84	1.47	1.39

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	708	ADP	C5-C4-N3	-6.03	118.42	126.72
5	Q	706	ADP	C5-C4-N3	-5.99	118.47	126.72
5	B	701	ADP	C5-C4-N3	-5.89	118.60	126.72
5	T	707	ADP	C5-C4-N3	-5.66	118.92	126.72
5	K	704	ADP	C5-C4-N3	-5.47	119.18	126.72

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

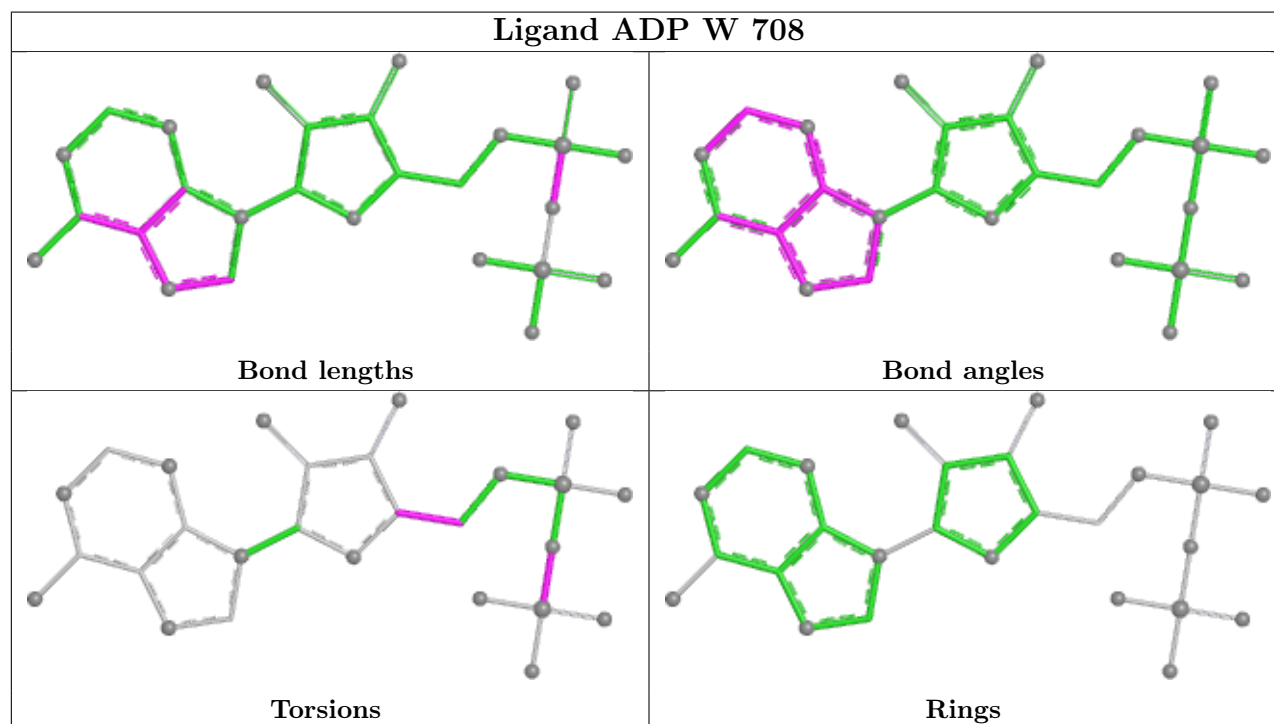
Mol	Chain	Res	Type	Atoms
5	B	701	ADP	PA-O3A-PB-O2B
5	B	701	ADP	O4'-C4'-C5'-O5'
5	E	702	ADP	C5'-O5'-PA-O1A
5	K	704	ADP	PA-O3A-PB-O3B
5	K	704	ADP	O4'-C4'-C5'-O5'

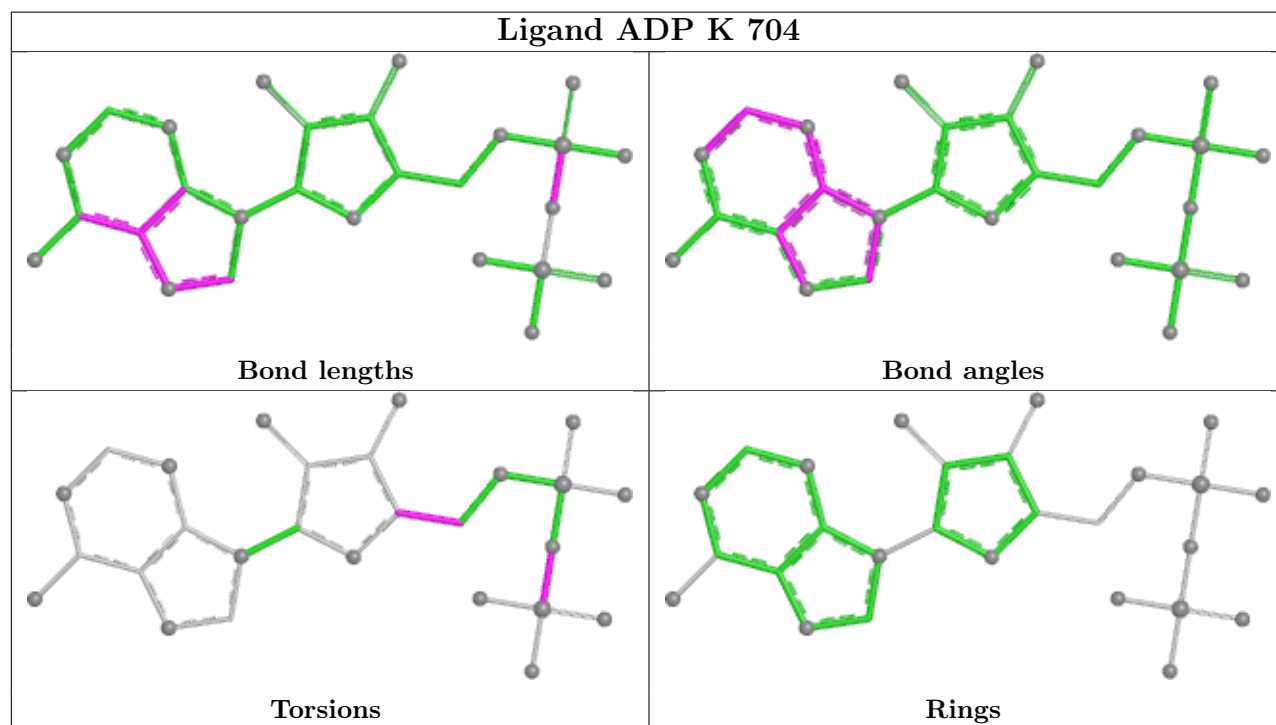
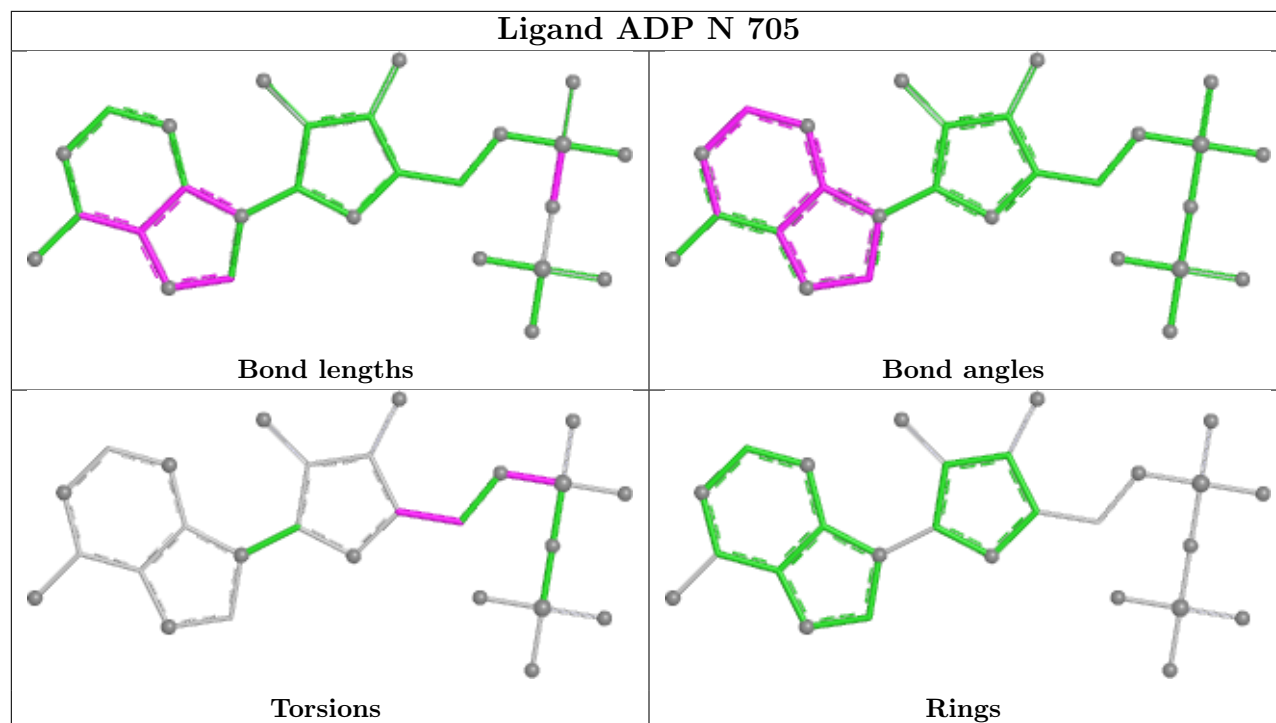
There are no ring outliers.

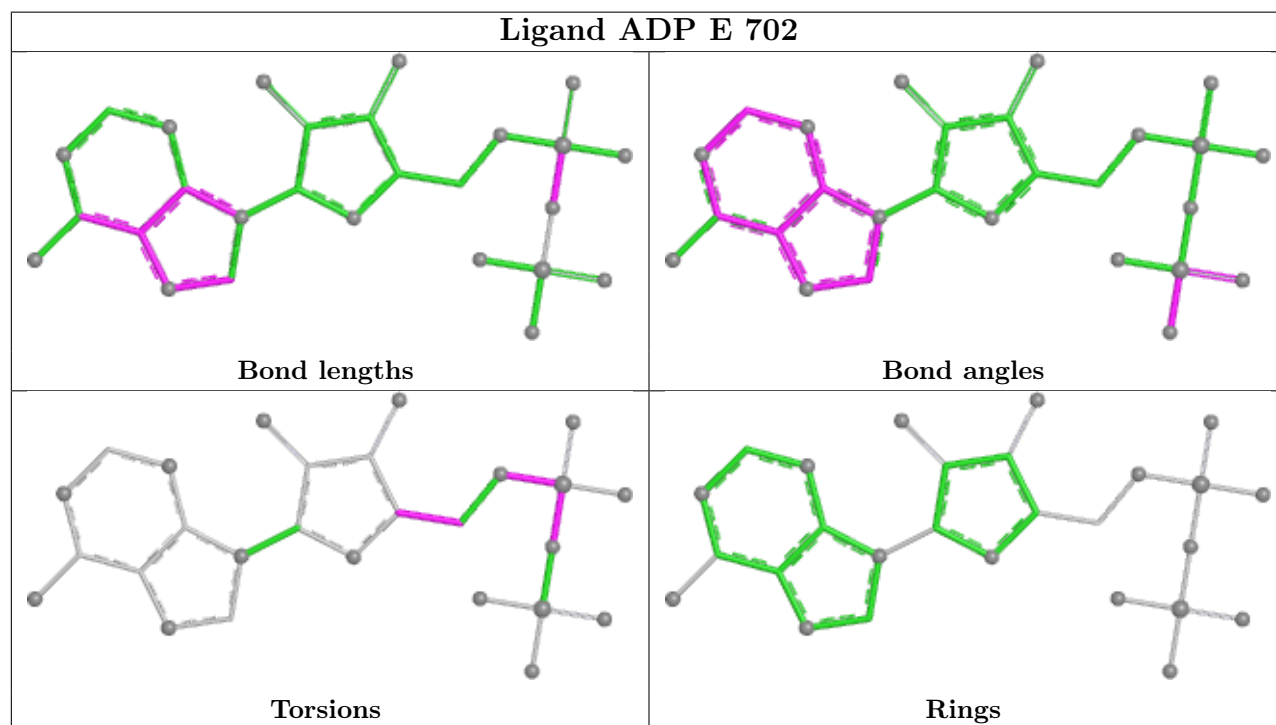
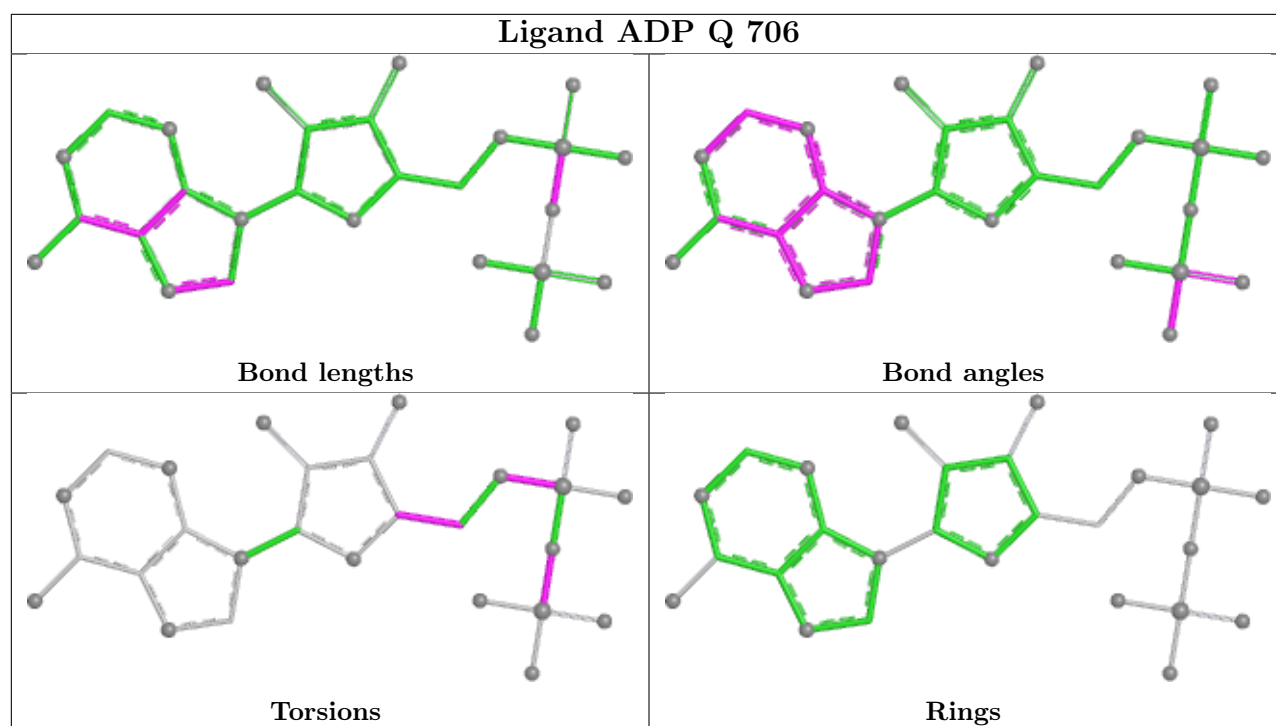
6 monomers are involved in 6 short contacts:

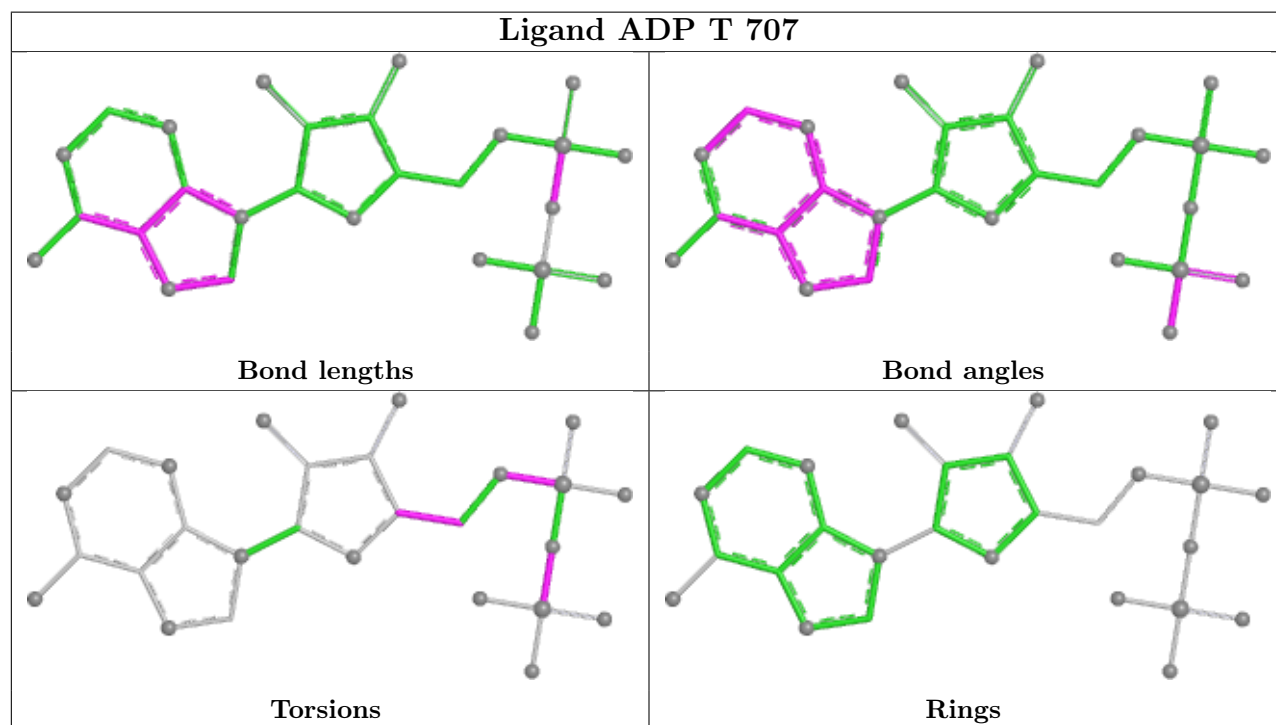
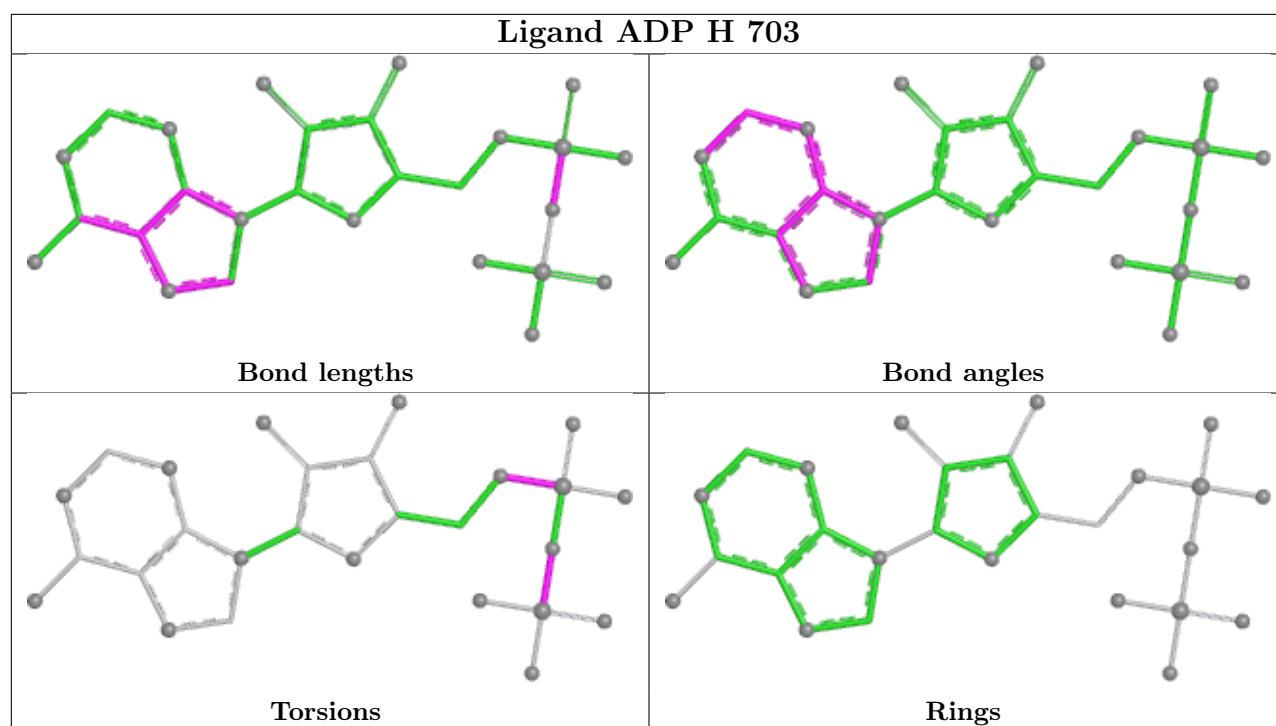
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	906	ASN	1	0
4	D	902	ASN	1	0
4	S	907	ASN	1	0
4	A	901	ASN	1	0
5	T	707	ADP	1	0
5	B	701	ADP	1	0

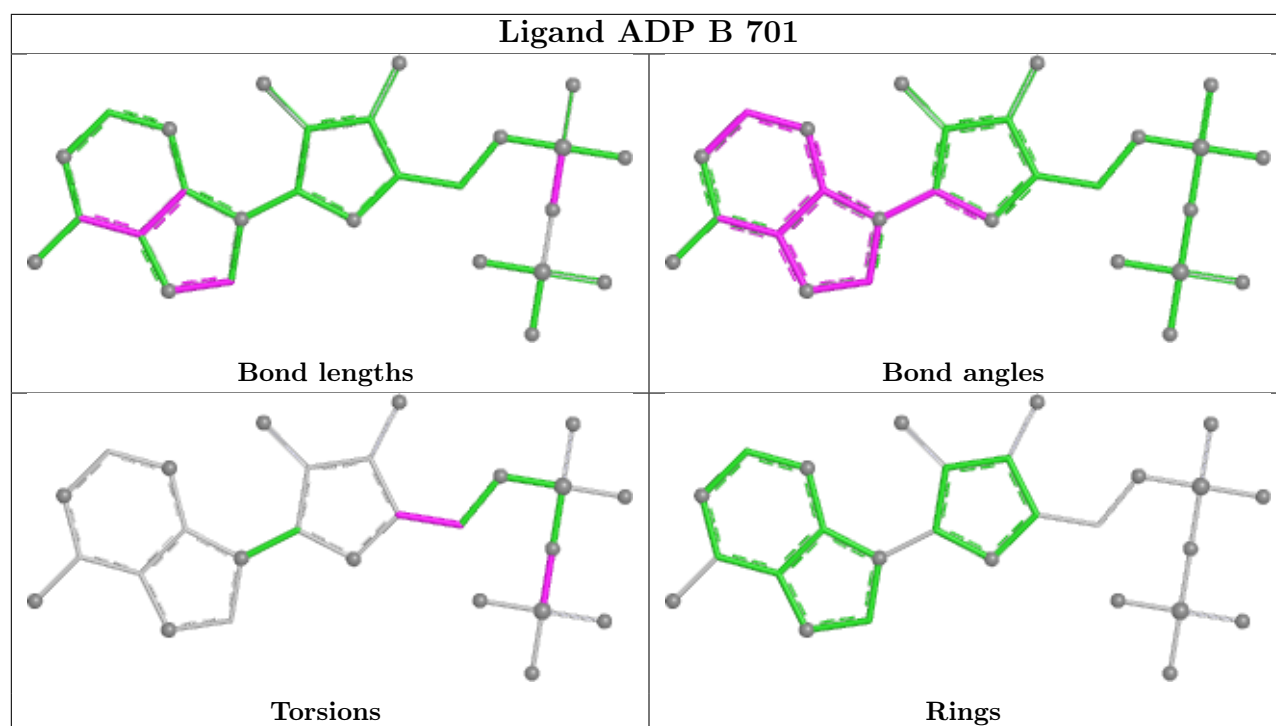
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/478 (100%)	-1.22	0 100 100	23, 44, 71, 79	0
1	D	478/478 (100%)	-1.25	0 100 100	29, 44, 71, 80	0
1	G	478/478 (100%)	-1.26	0 100 100	29, 43, 71, 79	0
1	J	478/478 (100%)	-1.26	0 100 100	28, 43, 71, 79	0
1	M	478/478 (100%)	-1.26	0 100 100	29, 43, 71, 79	0
1	P	478/478 (100%)	-1.25	0 100 100	28, 43, 71, 79	0
1	S	478/478 (100%)	-1.24	0 100 100	29, 44, 71, 79	0
1	V	478/478 (100%)	-1.22	0 100 100	29, 44, 71, 79	0
2	B	410/478 (85%)	-1.15	0 100 100	28, 54, 85, 103	0
2	E	410/478 (85%)	-1.13	0 100 100	29, 54, 85, 103	0
2	H	410/478 (85%)	-1.19	0 100 100	29, 54, 85, 103	0
2	K	410/478 (85%)	-1.17	0 100 100	29, 54, 85, 103	0
2	N	410/478 (85%)	-1.17	0 100 100	29, 54, 85, 103	0
2	Q	410/478 (85%)	-1.18	0 100 100	28, 54, 85, 103	0
2	T	410/478 (85%)	-1.18	0 100 100	28, 54, 85, 103	0
2	W	410/478 (85%)	-1.16	0 100 100	29, 54, 85, 103	0
3	C	91/94 (96%)	-1.22	0 100 100	39, 50, 64, 68	0
3	F	91/94 (96%)	-1.21	0 100 100	39, 50, 64, 67	0
3	I	91/94 (96%)	-1.24	0 100 100	39, 50, 64, 68	0
3	L	91/94 (96%)	-1.22	0 100 100	39, 50, 64, 67	0
3	O	91/94 (96%)	-1.19	0 100 100	39, 50, 64, 68	0
3	R	91/94 (96%)	-1.21	0 100 100	39, 50, 64, 67	0
3	U	91/94 (96%)	-1.20	0 100 100	39, 50, 64, 68	0
3	X	91/94 (96%)	-1.25	0 100 100	39, 50, 64, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7832/8400 (93%)	-1.21	0 100 100	23, 47, 79, 103	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

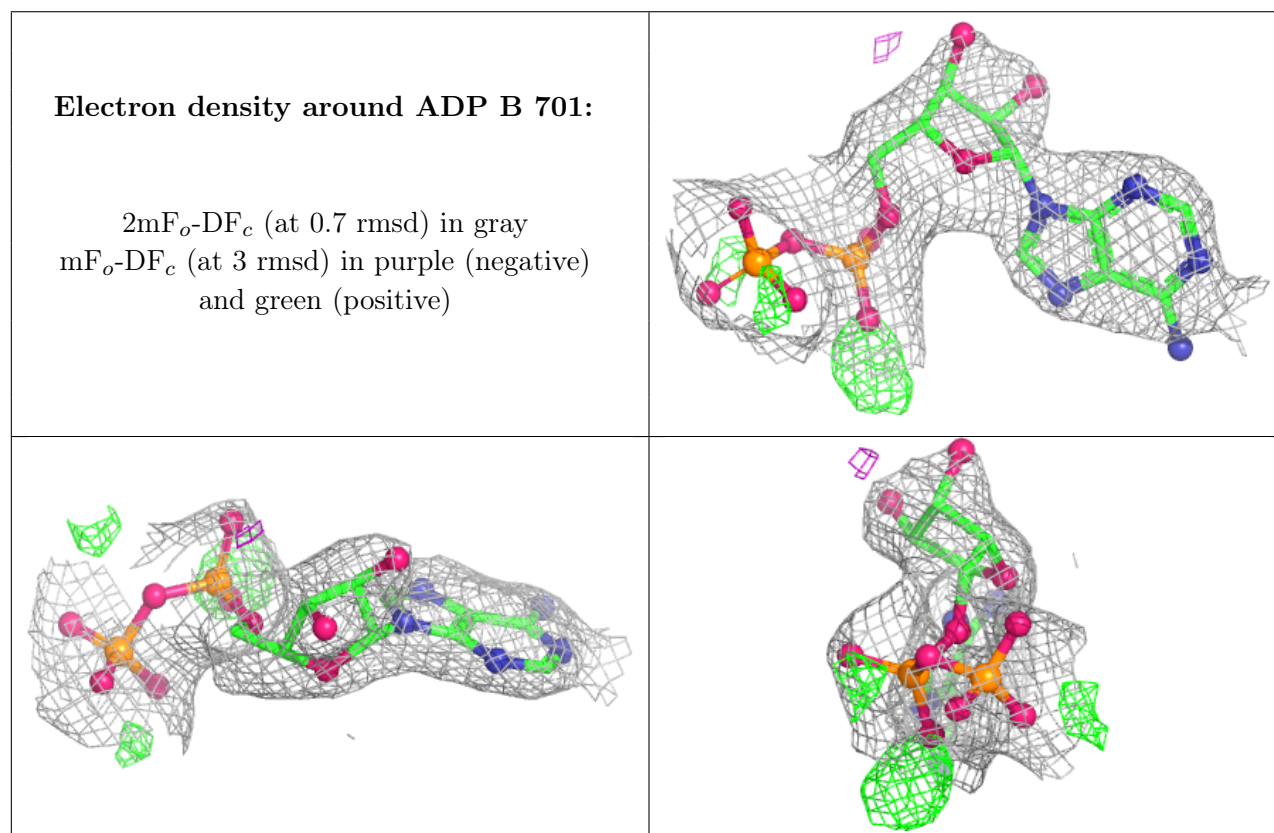
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	W	808	1/1	0.97	0.05	18,18,18,18	0
4	ASN	D	902	8/9	0.98	0.04	39,40,40,41	0
4	ASN	G	903	8/9	0.98	0.06	28,30,31,31	0
4	ASN	P	906	8/9	0.98	0.05	28,32,33,34	0
5	ADP	B	701	27/27	0.98	0.05	46,49,65,66	27
5	ADP	E	702	27/27	0.98	0.05	59,60,72,73	27
5	ADP	H	703	27/27	0.98	0.04	44,48,63,65	27
5	ADP	K	704	27/27	0.98	0.05	40,41,64,66	27
5	ADP	Q	706	27/27	0.98	0.05	44,46,65,66	27
5	ADP	T	707	27/27	0.98	0.05	51,52,70,71	27
5	ADP	W	708	27/27	0.98	0.05	48,50,68,70	27
6	MG	E	802	1/1	0.98	0.03	19,19,19,19	0
6	MG	H	803	1/1	0.98	0.03	10,10,10,10	0
6	MG	N	805	1/1	0.98	0.04	16,16,16,16	0
4	ASN	A	901	8/9	0.98	0.04	33,33,36,36	0
4	ASN	S	907	8/9	0.99	0.03	28,32,33,33	0
6	MG	B	801	1/1	0.99	0.03	10,10,10,10	0
4	ASN	V	908	8/9	0.99	0.04	29,30,31,32	0
5	ADP	N	705	27/27	0.99	0.05	49,52,63,65	27

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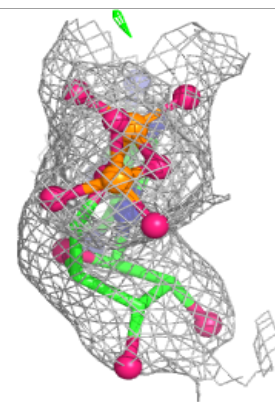
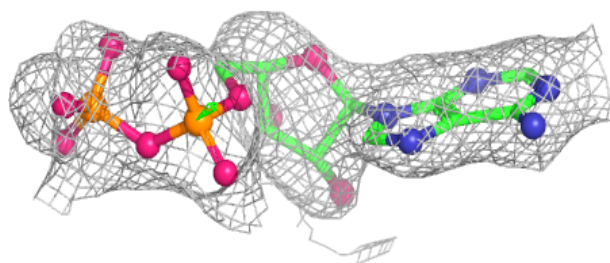
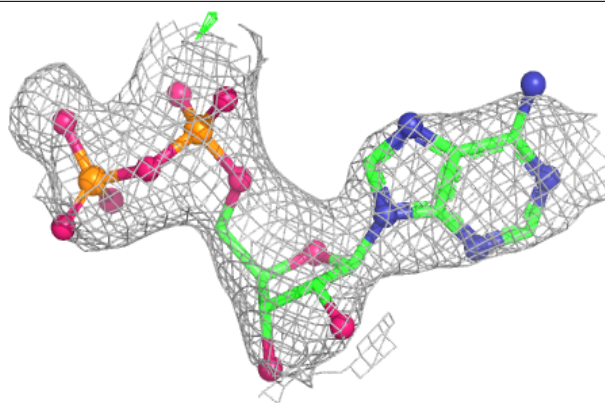
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	K	804	1/1	0.99	0.03	11,11,11,11	0
4	ASN	M	905	8/9	0.99	0.03	32,33,34,36	0
6	MG	Q	806	1/1	0.99	0.04	21,21,21,21	0
6	MG	T	807	1/1	0.99	0.03	15,15,15,15	0
4	ASN	J	904	8/9	0.99	0.03	26,28,29,29	0
7	ZN	B	901	1/1	1.00	0.01	37,37,37,37	0
7	ZN	E	902	1/1	1.00	0.02	40,40,40,40	0
7	ZN	H	903	1/1	1.00	0.01	33,33,33,33	0
7	ZN	K	904	1/1	1.00	0.01	29,29,29,29	0
7	ZN	N	905	1/1	1.00	0.01	36,36,36,36	0
7	ZN	Q	906	1/1	1.00	0.01	30,30,30,30	0
7	ZN	T	907	1/1	1.00	0.01	37,37,37,37	0
7	ZN	W	908	1/1	1.00	0.02	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

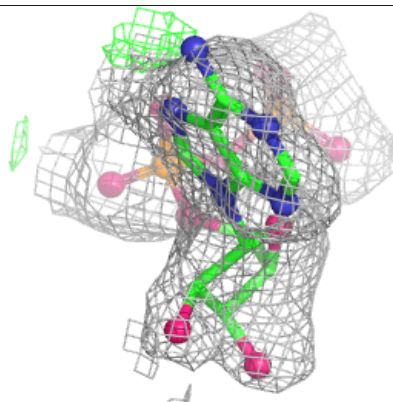
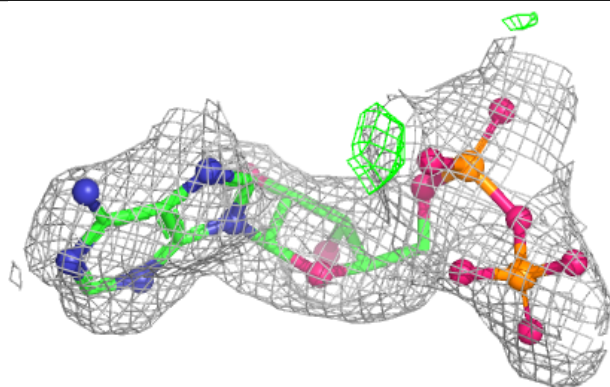
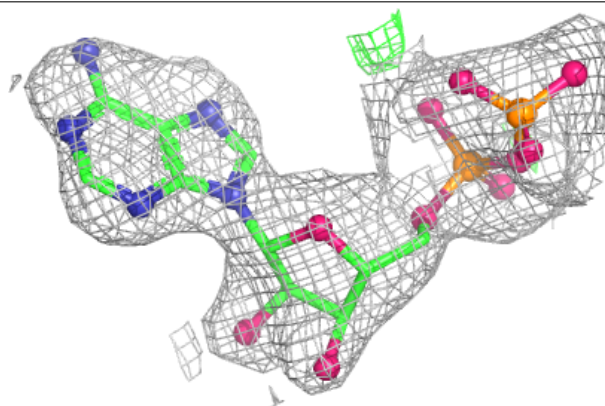


Electron density around ADP E 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

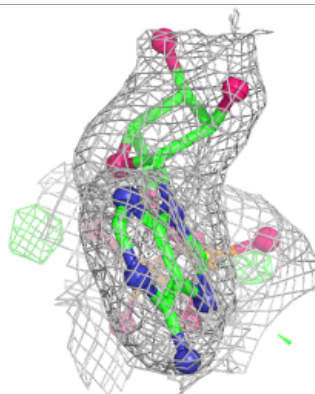
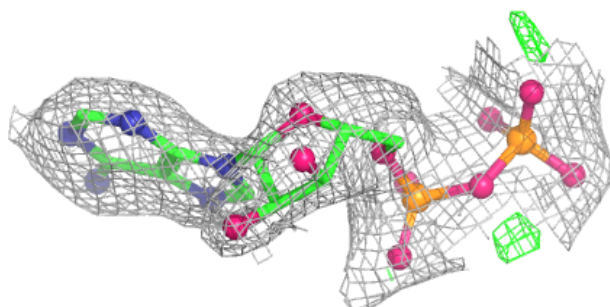
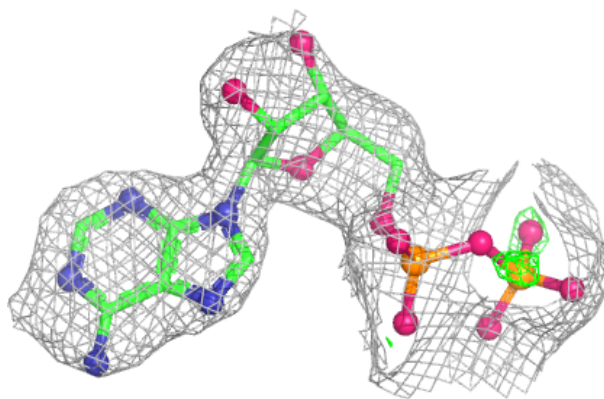
**Electron density around ADP H 703:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

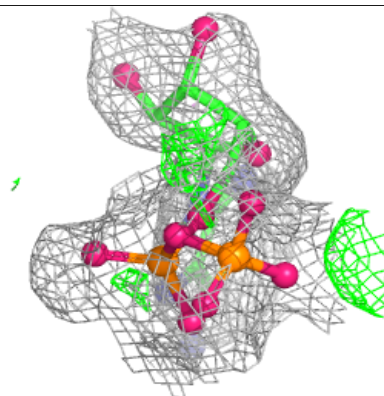
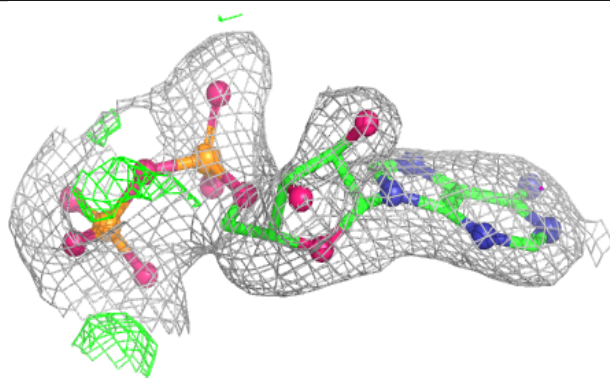
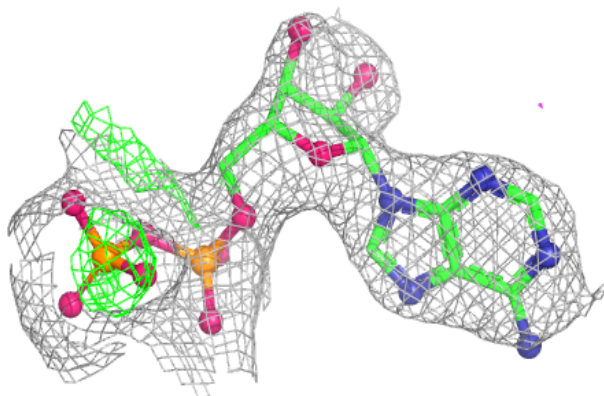


Electron density around ADP K 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

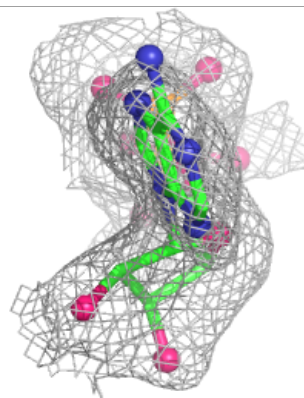
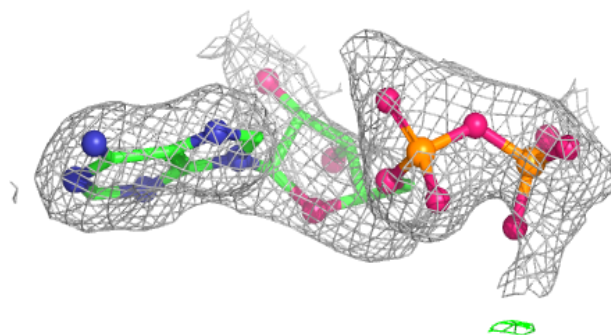
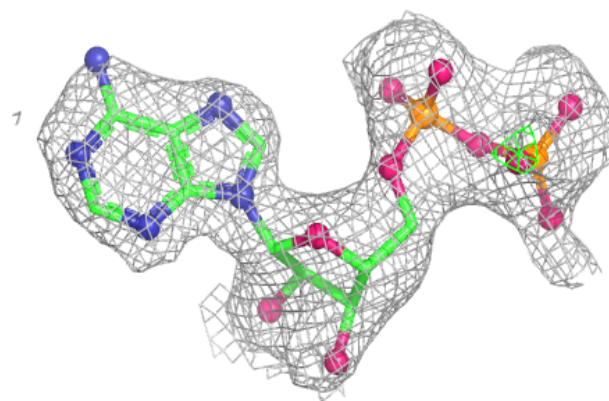
**Electron density around ADP Q 706:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

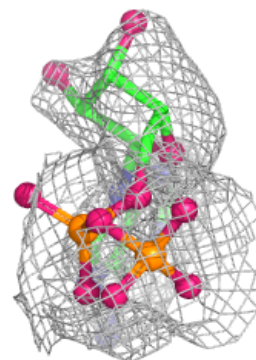
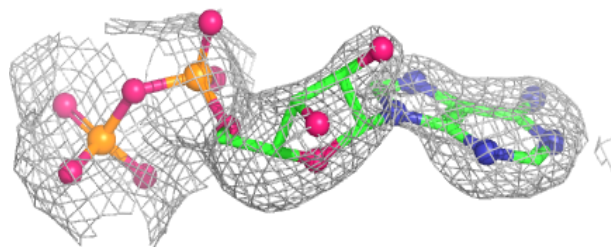
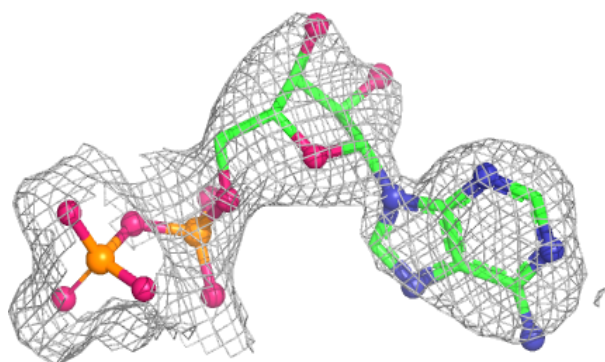


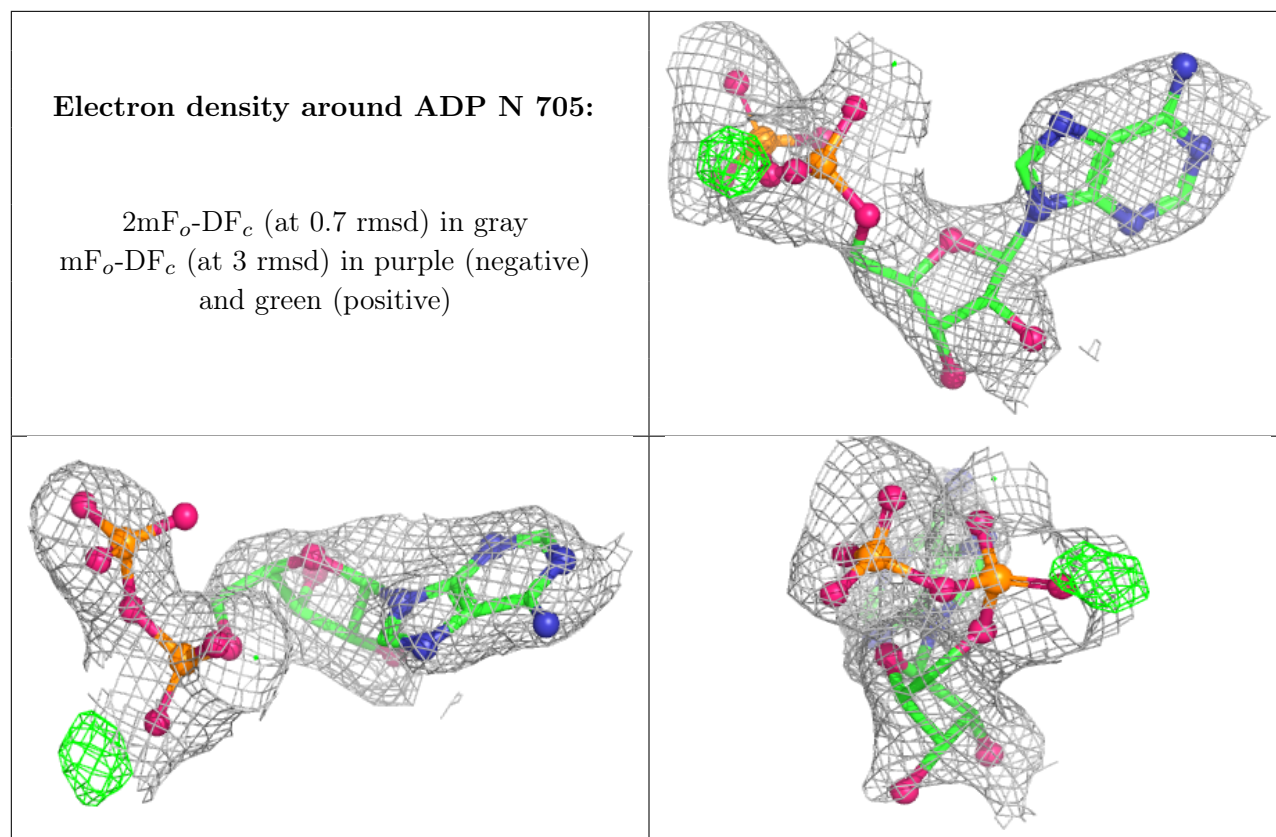
Electron density around ADP T 707:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP W 708:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.