wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 02:32 PM JST

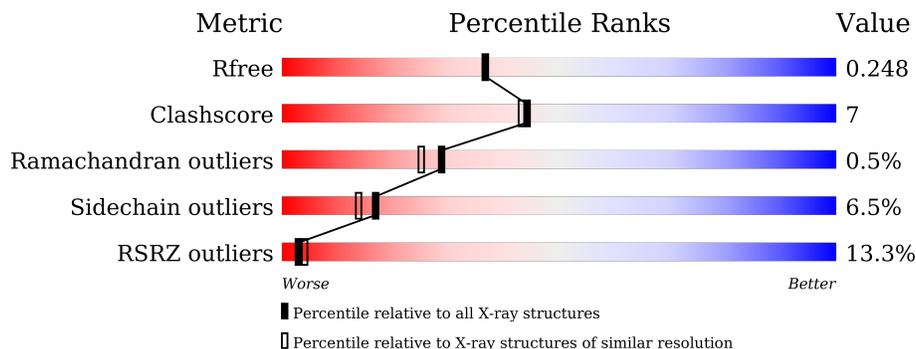|		
PDB ID	:	7CPR
Title	:	glutamine synthetase from Drosophila
Authors	:	Yin, H.S.; Chen, W.T.
Deposited on	:	2020-08-07
Resolution	:	2.12 Å(reported)

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 2.12 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	Percentile Ranks	Value
Rfree		0.248
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		6.5%
RSRZ outliers		13.3%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 <=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	367	15% / 82% 16% •
1	B	367	13% / 79% 18% •
1	C	367	11% / 88% 11% •
1	D	367	10% / 83% 14% ••
1	E	367	12% / 83% 14% ••
1	F	367	11% / 82% 15% •

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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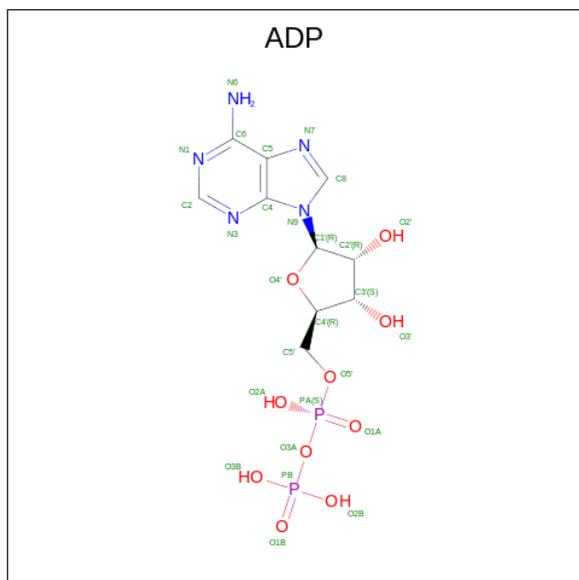| Mol	Chain	Length	Quality of chain
1	G	367	12% ██ 82% ▬▬▬▬ 15% ··
1	H	367	11% ██ 83% ▬▬▬▬ 15% ·
1	I	367	19% ███ 80% ▬▬▬▬ 16% ··
1	J	367	16% ██ 86% ▬▬▬▬ 13% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 29573 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 Glutamine synthetase 2 cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total 2885	C 1807	N 508	O 553	S 17	0	0	0
1	B	366	Total 2884	C 1806	N 507	O 554	S 17	0	0	0
1	C	366	Total 2880	C 1804	N 507	O 552	S 17	0	0	0
1	D	364	Total 2867	C 1797	N 505	O 548	S 17	0	0	0
1	E	365	Total 2872	C 1800	N 506	O 549	S 17	0	0	0
1	F	367	Total 2889	C 1809	N 508	O 555	S 17	0	0	0
1	G	365	Total 2872	C 1800	N 506	O 549	S 17	0	0	0
1	H	366	Total 2876	C 1801	N 506	O 552	S 17	0	0	0
1	I	365	Total 2875	C 1801	N 506	O 551	S 17	0	0	0
1	J	367	Total 2883	C 1806	N 505	O 555	S 17	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	27	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	50	Total	O	0	0
			50	50		

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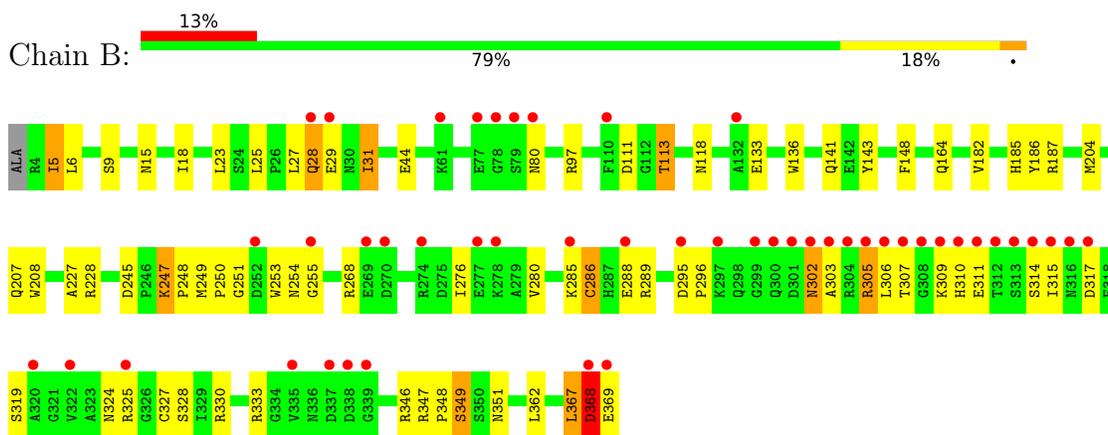| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	34	Total 34	O 34	0	0
3	D	39	Total 39	O 39	0	0
3	E	62	Total 62	O 62	0	0
3	F	56	Total 56	O 56	0	0
3	G	39	Total 39	O 39	0	0
3	H	45	Total 45	O 45	0	0
3	I	62	Total 62	O 62	0	0
3	J	68	Total 68	O 68	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
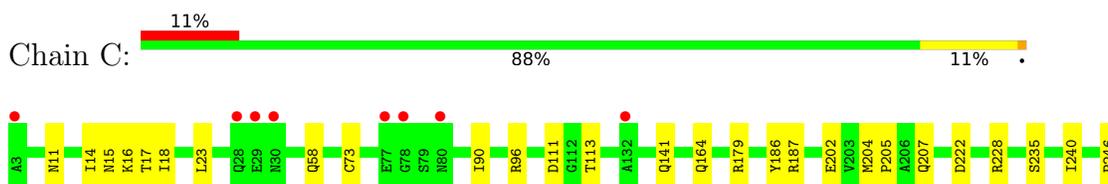
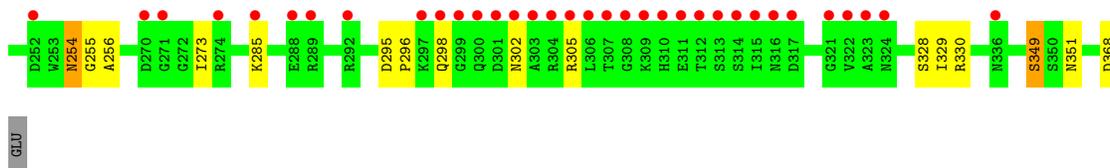• Molecule 1: Glutamine synthetase 2 cytoplasmic
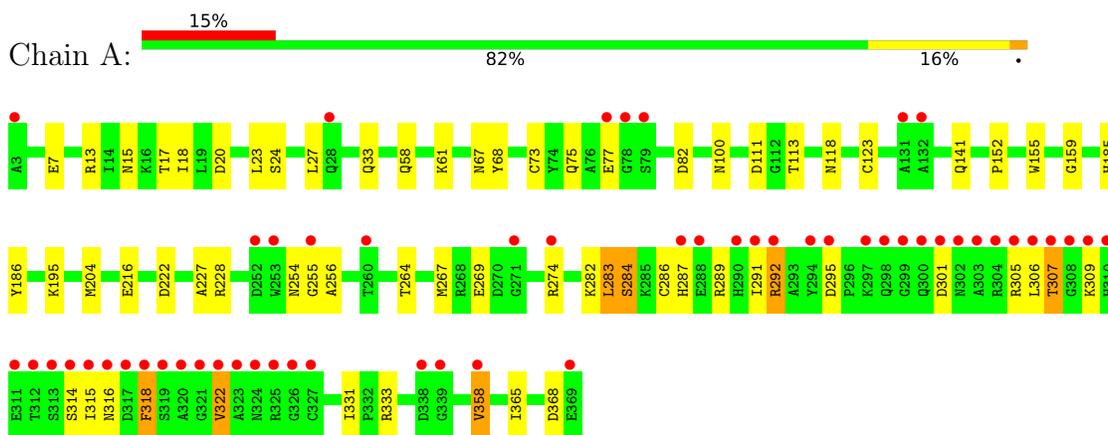
• Molecule 1: Glutamine synthetase 2 cytoplasmic

• Molecule 1: Glutamine synthetase 2 cytoplasmic

• Molecule 1: Glutamine synthetase 2 cytoplasmic

• Molecule 1: Glutamine synthetase 2 cytoplasmic

• Molecule 1: Glutamine synthetase 2 cytoplasmic

• Molecule 1: Glutamine synthetase 2 cytoplasmic

Chain G:

• Molecule 1: Glutamine synthetase 2 cytoplasmic
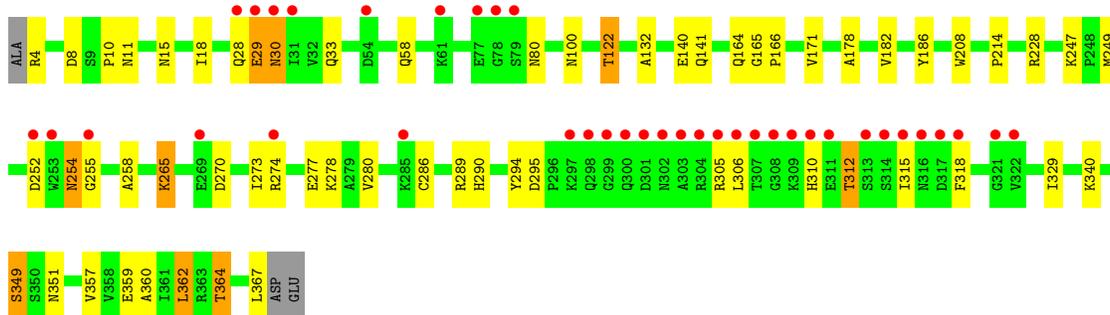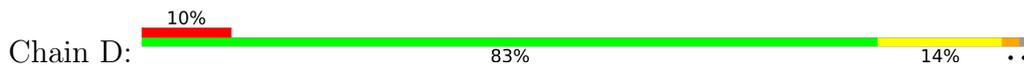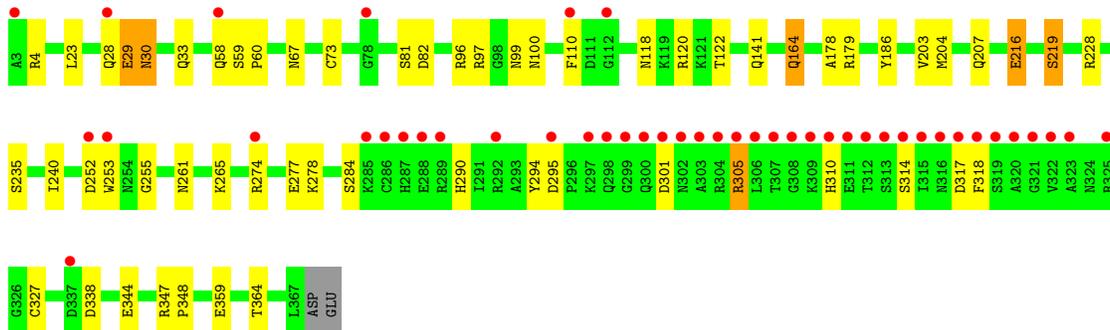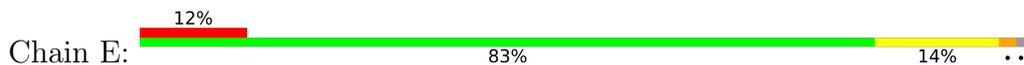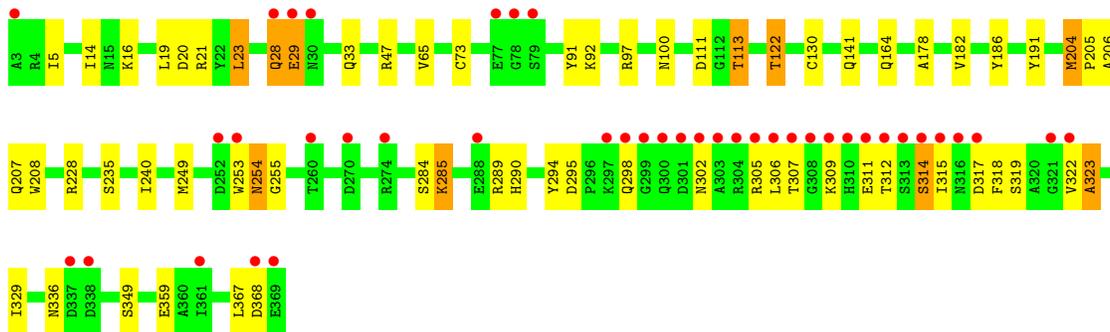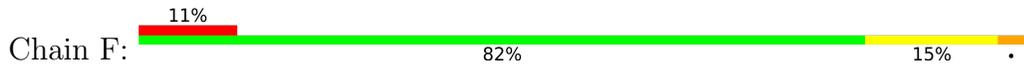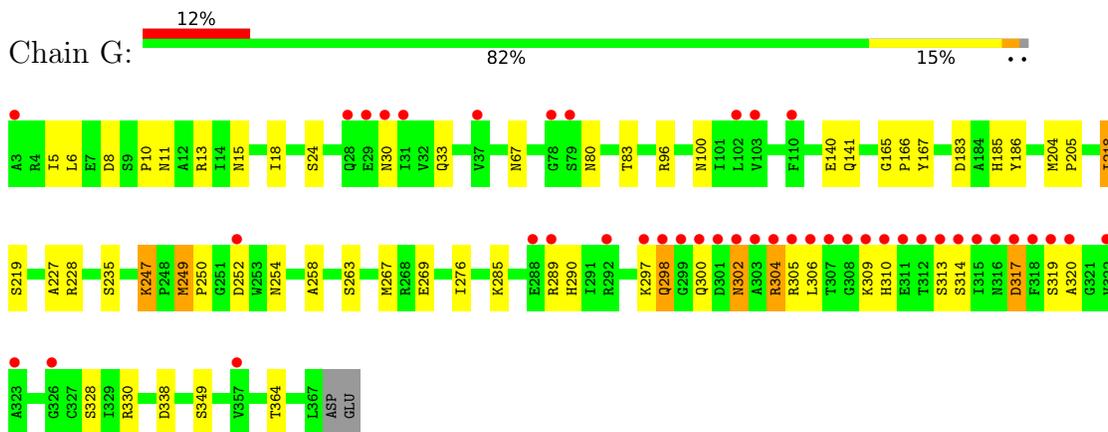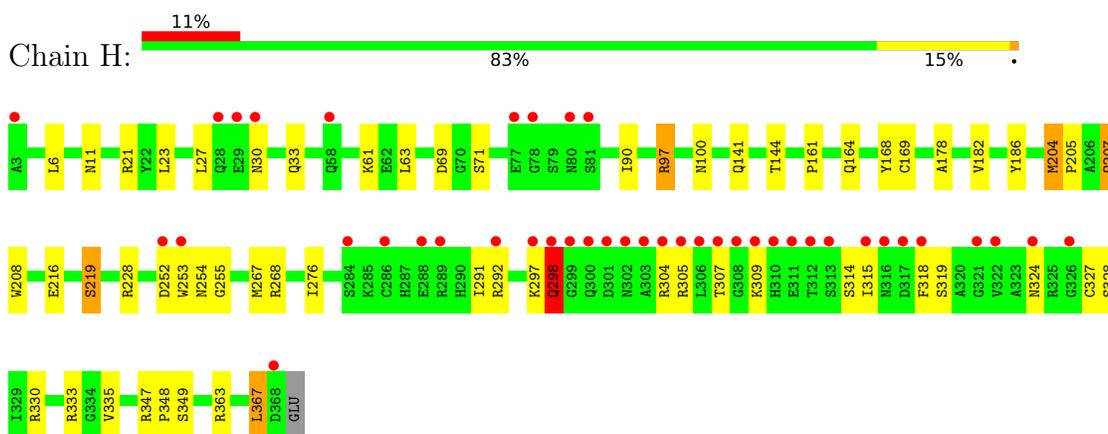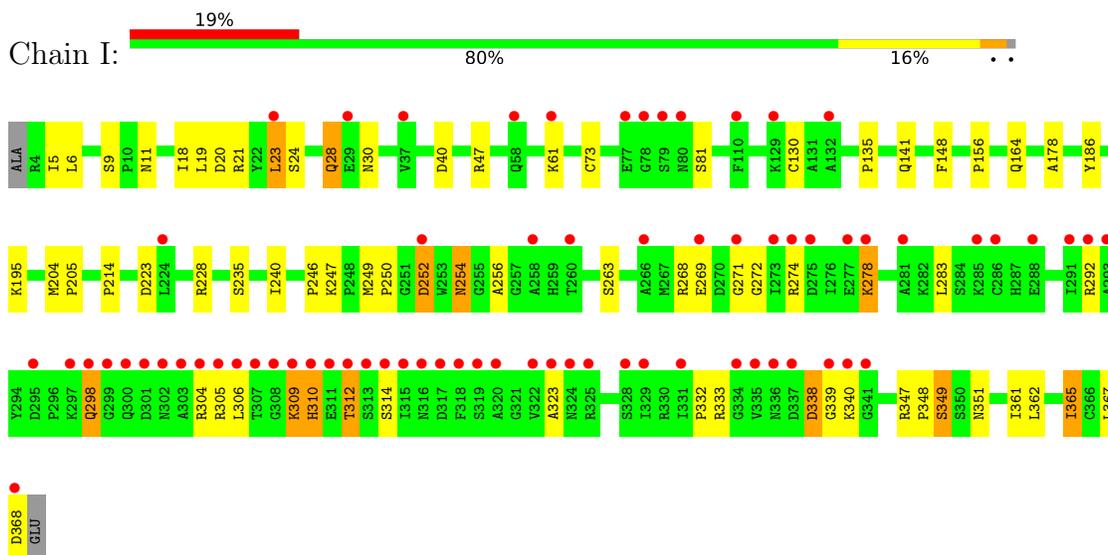
Chain H:

• Molecule 1: Glutamine synthetase 2 cytoplasmic

Chain I:

• Molecule 1: Glutamine synthetase 2 cytoplasmic

Chain J:
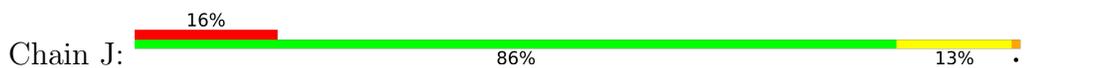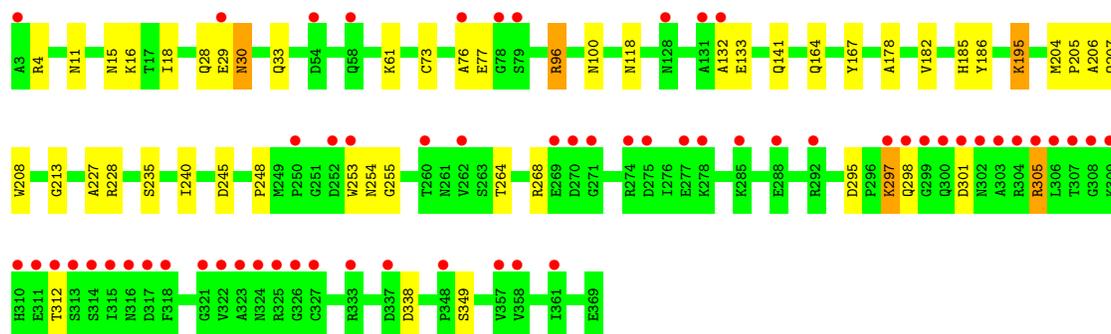
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	229.70Å 102.92Å 206.51Å 90.00° 120.09° 90.00°	Depositor
Resolution (Å)	178.68 – 2.12 27.37 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.6 (178.68-2.12) 96.6 (27.37-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.198 , 0.246 0.203 , 0.248	Depositor DCC
R_{free} test set	11245 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29573	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.76	1/2957 (0.0%)	0.89	4/4013 (0.1%)
1	B	0.75	0/2956	0.86	0/4011
1	C	0.82	1/2952 (0.0%)	0.86	5/4006 (0.1%)
1	D	0.87	0/2939	0.93	1/3988 (0.0%)
1	E	0.80	2/2944 (0.1%)	0.89	4/3995 (0.1%)
1	F	0.84	2/2961 (0.1%)	0.91	1/4018 (0.0%)
1	G	0.88	1/2944 (0.0%)	0.91	3/3995 (0.1%)
1	H	0.81	0/2948	0.91	4/4002 (0.1%)
1	I	0.75	0/2947	0.87	2/3999 (0.1%)
1	J	0.71	1/2955 (0.0%)	0.80	1/4011 (0.0%)
All	All	0.80	8/29503 (0.0%)	0.88	25/40038 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	CYS	CB-SG	-7.50	1.69	1.82
1	F	73	CYS	CB-SG	-6.97	1.70	1.82
1	J	73	CYS	CB-SG	-6.96	1.70	1.82
1	A	73	CYS	CB-SG	-6.31	1.71	1.82
1	G	235	SER	CB-OG	-5.61	1.34	1.42

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	96	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	H	268	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	E	179	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	222	ASP	CB-CG-OD1	5.80	123.52	118.30
1	G	96	ARG	NE-CZ-NH2	-5.80	117.40	120.30

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	2885	0	2764	48	0
1	B	2884	0	2763	56	0
1	C	2880	0	2762	23	0
1	D	2867	0	2753	37	0
1	E	2872	0	2758	41	0
1	F	2889	0	2768	48	0
1	G	2872	0	2758	32	0
1	H	2876	0	2751	44	0
1	I	2875	0	2757	38	0
1	J	2883	0	2757	34	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
3	A	65	0	0	1	0
3	B	50	0	0	1	0
3	C	34	0	0	0	0
3	D	39	0	0	0	0
3	E	62	0	0	1	0
3	F	56	0	0	1	0
3	G	39	0	0	0	0
3	H	45	0	0	4	0
3	I	62	0	0	0	0
3	J	68	0	0	2	0
All	All	29573	0	27711	374	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 7.

The worst 5 of 374 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:F:204:MET:HB2	1:F:207:GLN:OE1	1.71	0.90
1:E:122:THR:HG22	1:E:359:GLU:OE1	1.77	0.85
1:H:204:MET:HB2	3:H:502:HOH:O	1.78	0.83
1:A:307:THR:OG1	1:A:315:ILE:HG22	1.77	0.82
1:F:204:MET:CE	1:F:253:TRP:CZ3	2.62	0.82

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	365/367 (100%)	343 (94%)	20 (6%)	2 (0%)	29	25
1	B	364/367 (99%)	341 (94%)	18 (5%)	5 (1%)	11	6
1	C	364/367 (99%)	348 (96%)	15 (4%)	1 (0%)	41	40
1	D	362/367 (99%)	345 (95%)	17 (5%)	0	100	100
1	E	363/367 (99%)	340 (94%)	22 (6%)	1 (0%)	41	40
1	F	365/367 (100%)	344 (94%)	18 (5%)	3 (1%)	19	14
1	G	363/367 (99%)	348 (96%)	14 (4%)	1 (0%)	41	40
1	H	364/367 (99%)	345 (95%)	18 (5%)	1 (0%)	41	40
1	I	363/367 (99%)	341 (94%)	20 (6%)	2 (1%)	25	20
1	J	365/367 (100%)	342 (94%)	22 (6%)	1 (0%)	41	40
All	All	3638/3670 (99%)	3437 (94%)	184 (5%)	17 (0%)	29	25

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	286	CYS
1	B	368	ASP
1	C	298	GLN
1	F	298	GLN

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	308/309 (100%)	287 (93%)	21 (7%)	16	12
1	B	309/309 (100%)	282 (91%)	27 (9%)	10	6
1	C	308/309 (100%)	297 (96%)	11 (4%)	35	35
1	D	307/309 (99%)	285 (93%)	22 (7%)	14	11
1	E	307/309 (99%)	287 (94%)	20 (6%)	17	14
1	F	309/309 (100%)	287 (93%)	22 (7%)	14	11
1	G	307/309 (99%)	284 (92%)	23 (8%)	13	10
1	H	307/309 (99%)	290 (94%)	17 (6%)	21	18
1	I	308/309 (100%)	283 (92%)	25 (8%)	11	8
1	J	308/309 (100%)	296 (96%)	12 (4%)	32	32
All	All	3078/3090 (100%)	2878 (94%)	200 (6%)	17	14

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	295	ASP
1	G	317	ASP
1	J	349	SER
1	F	314	SER
1	G	249	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	290	HIS
1	H	11	ASN
1	F	336	ASN
1	G	141	GLN
1	H	200	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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 Counts	RMSZ	#$|Z| > 2$	Bond angles Counts	RMSZ	#$|Z| > 2$
2	ADP	A	401	-	24,29,29	0.96	0	29,45,45	1.30	3 (10%)
2	ADP	F	401	-	24,29,29	0.93	2 (8%)	29,45,45	1.49	4 (13%)
2	ADP	C	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	D	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	B	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
2	ADP	I	401	-	24,29,29	0.96	0	29,45,45	1.31	3 (10%)
2	ADP	J	401	-	24,29,29	0.96	2 (8%)	29,45,45	1.30	3 (10%)
2	ADP	G	401	-	24,29,29	0.95	0	29,45,45	1.34	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	H	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
2	ADP	E	401	-	24,29,29	0.91	0	29,45,45	1.70	4 (13%)

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	ADP	A	401	-	-	5/12/32/32	0/3/3/3
2	ADP	F	401	-	-	5/12/32/32	0/3/3/3
2	ADP	C	401	-	-	4/12/32/32	0/3/3/3
2	ADP	D	401	-	-	2/12/32/32	0/3/3/3
2	ADP	B	401	-	-	0/12/32/32	0/3/3/3
2	ADP	I	401	-	-	5/12/32/32	0/3/3/3
2	ADP	J	401	-	-	2/12/32/32	0/3/3/3
2	ADP	G	401	-	-	5/12/32/32	0/3/3/3
2	ADP	H	401	-	-	0/12/32/32	0/3/3/3
2	ADP	E	401	-	-	5/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	ADP	C5-C4	2.73	1.48	1.40
2	H	401	ADP	C5-C4	2.52	1.47	1.40
2	C	401	ADP	C5-C4	2.50	1.47	1.40
2	B	401	ADP	C5-C4	2.47	1.47	1.40
2	J	401	ADP	C5-C4	2.26	1.46	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	ADP	O4'-C1'-C2'	-5.04	99.56	106.93
2	F	401	ADP	N3-C2-N1	-4.93	120.97	128.68
2	E	401	ADP	N3-C2-N1	-4.10	122.27	128.68
2	J	401	ADP	N3-C2-N1	-4.05	122.35	128.68
2	H	401	ADP	PA-O3A-PB	-3.61	120.44	132.83

There are no chirality outliers.
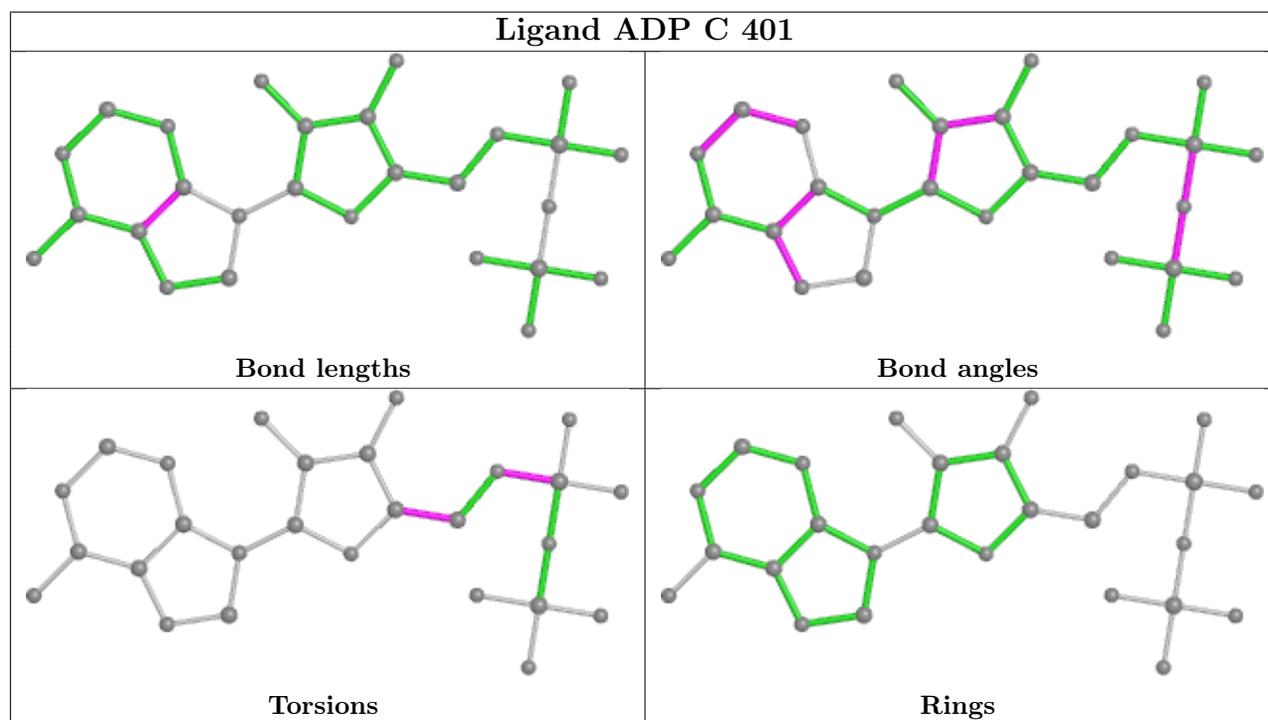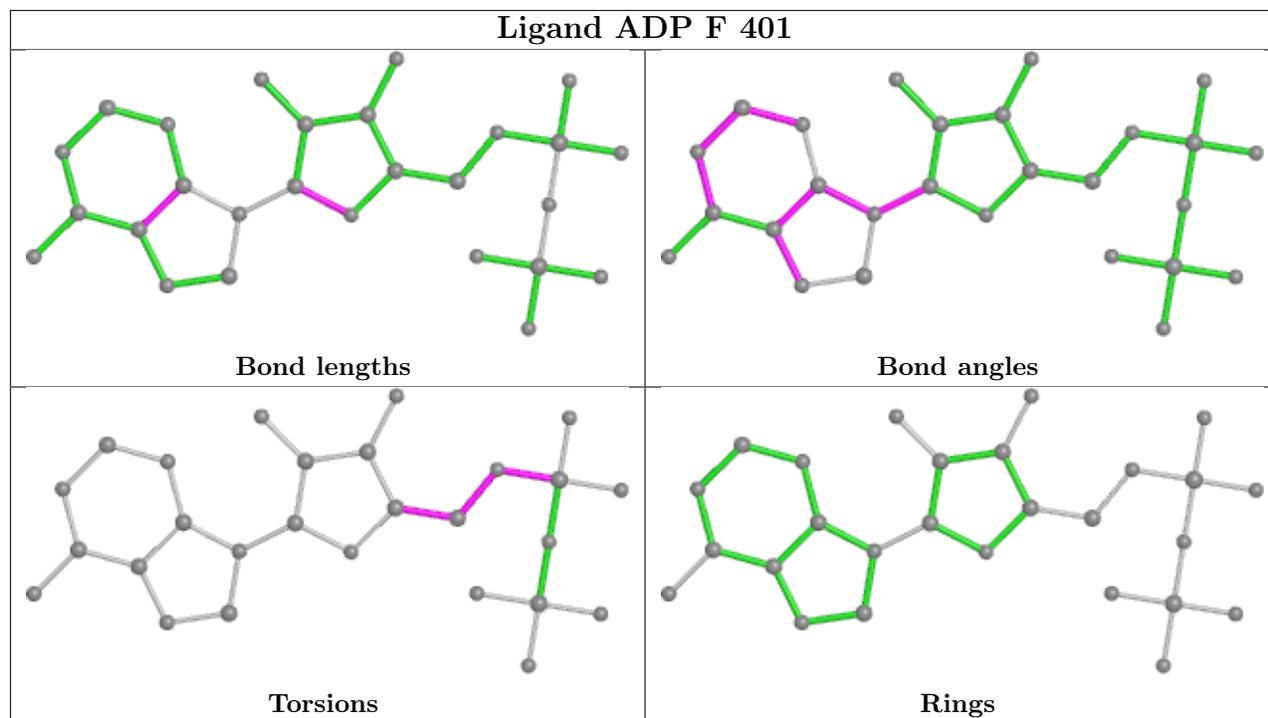
5 of 33 torsion outliers are listed below:

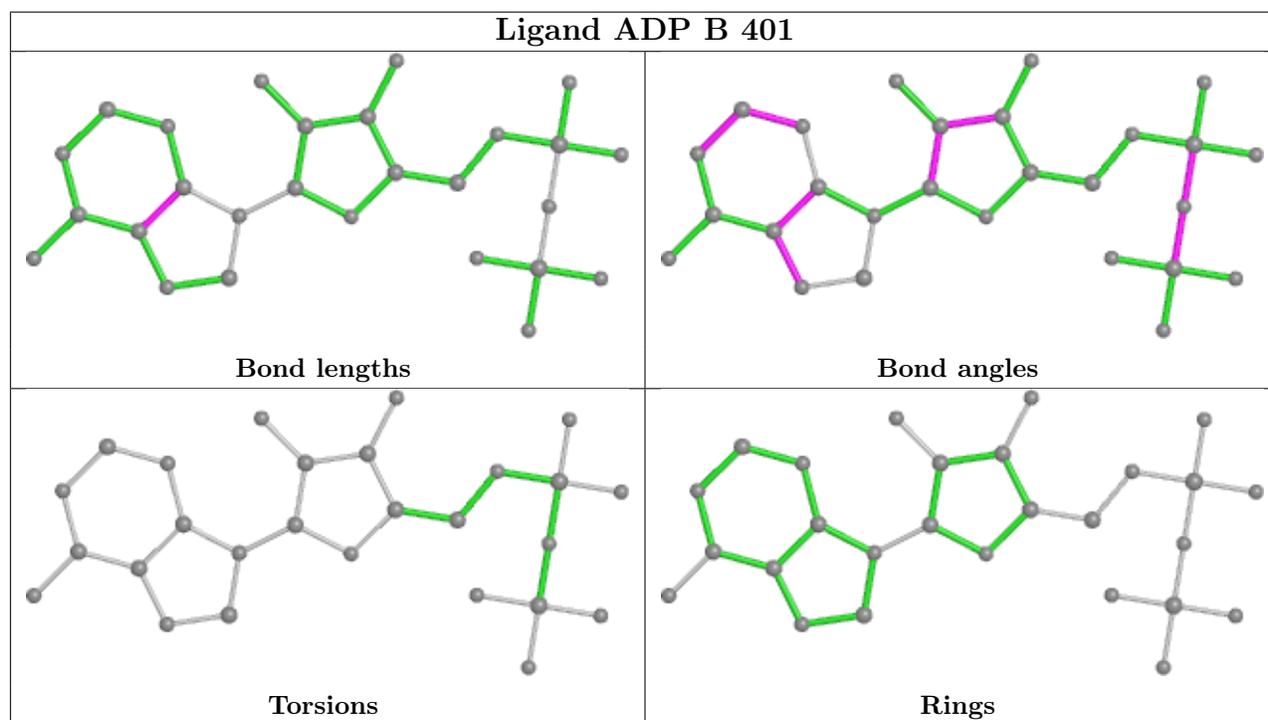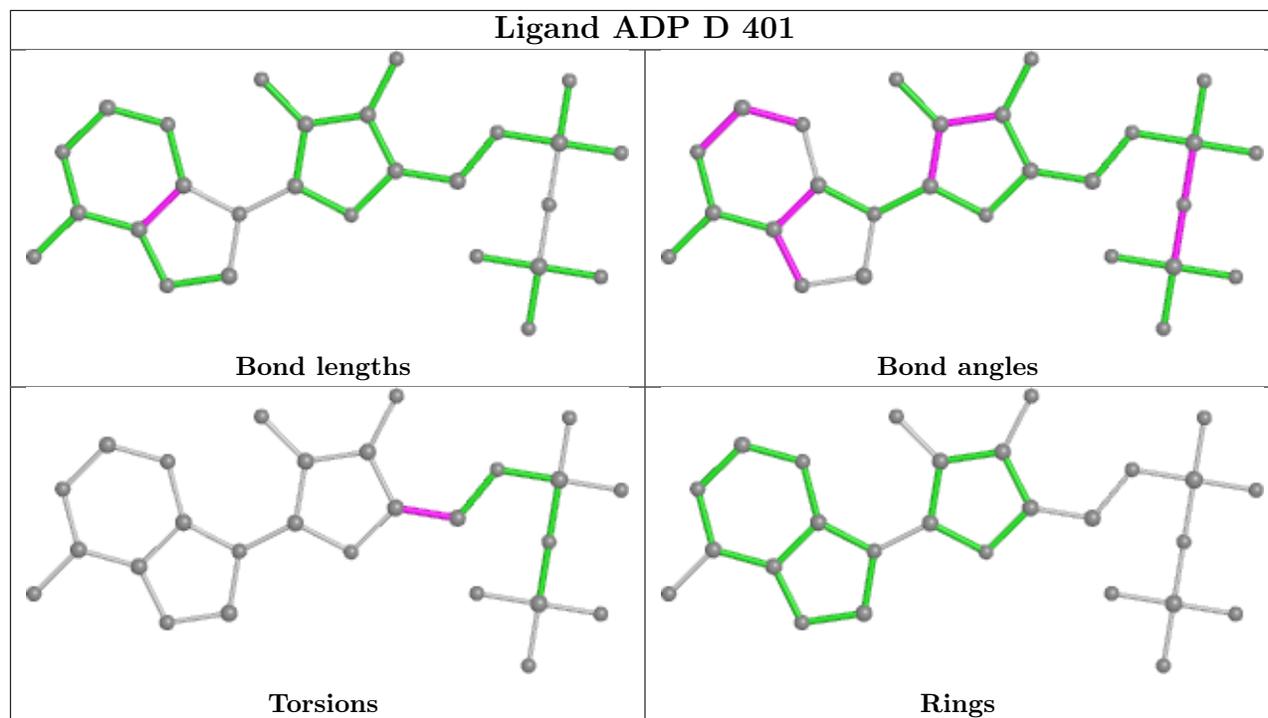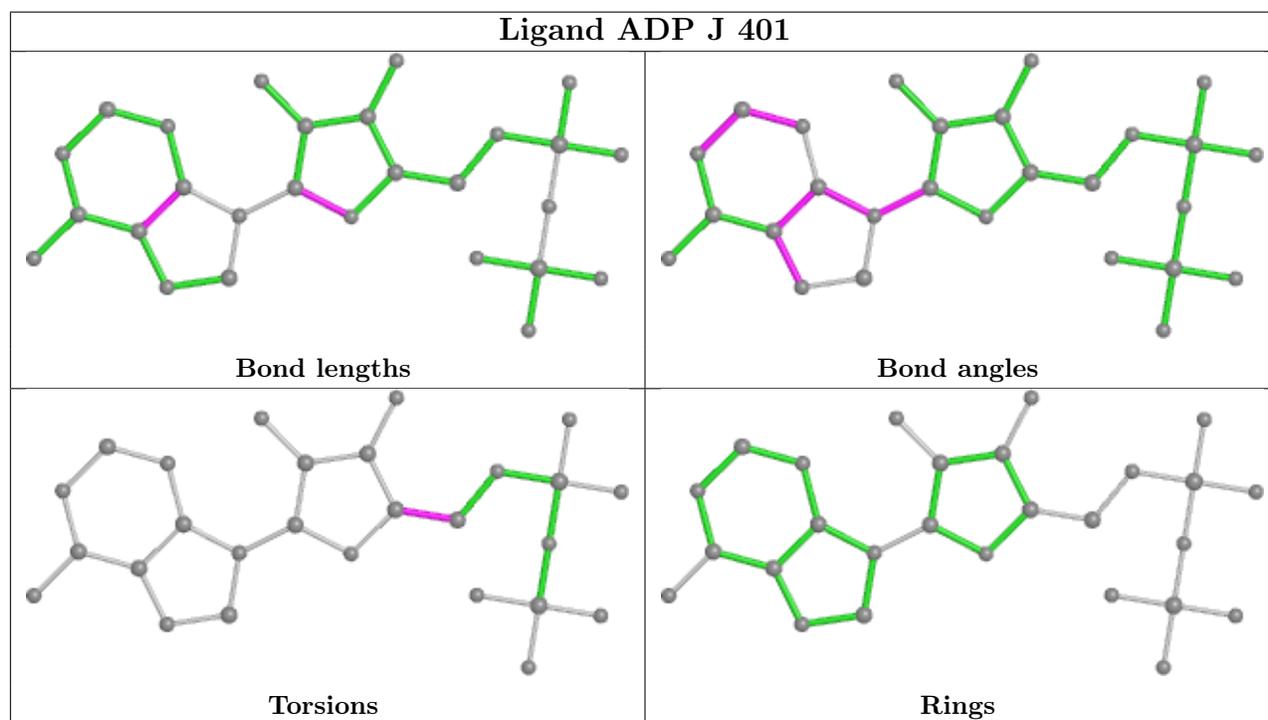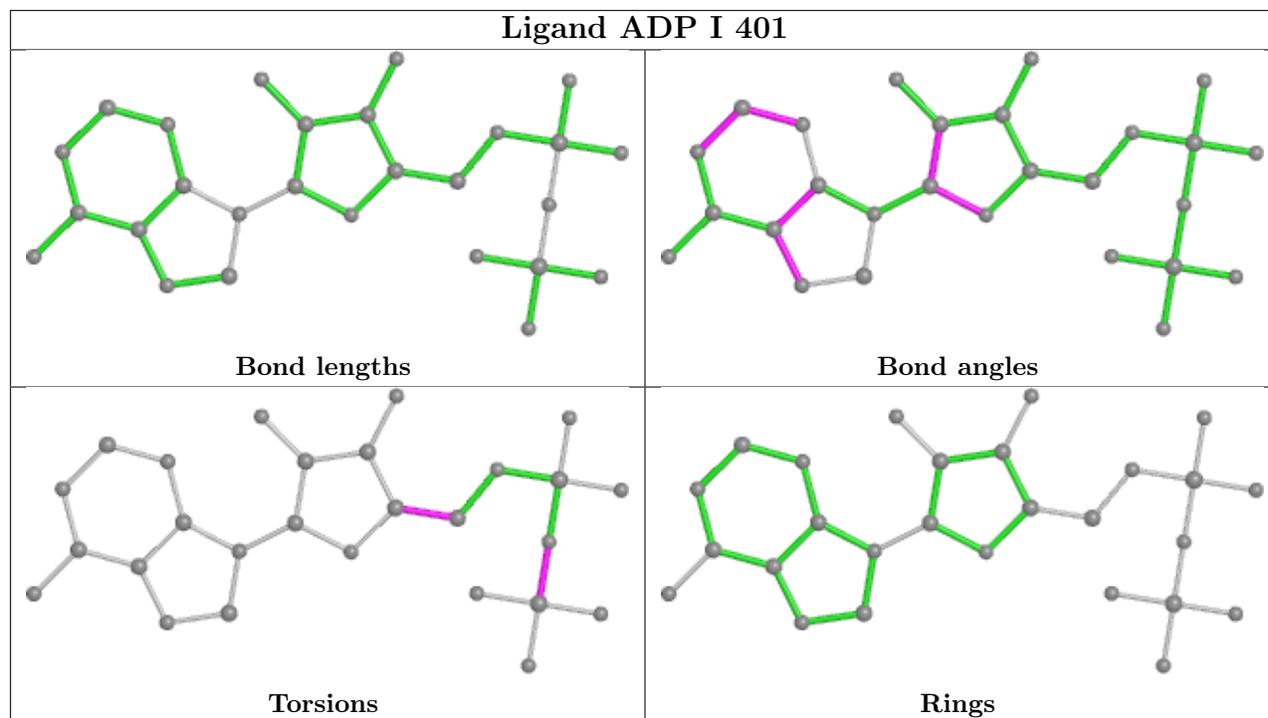| Mol	Chain	Res	Type	Atoms
2	C	401	ADP	C5'-O5'-PA-O1A
2	C	401	ADP	C3'-C4'-C5'-O5'
2	F	401	ADP	C5'-O5'-PA-O1A
2	F	401	ADP	C5'-O5'-PA-O3A
2	F	401	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.
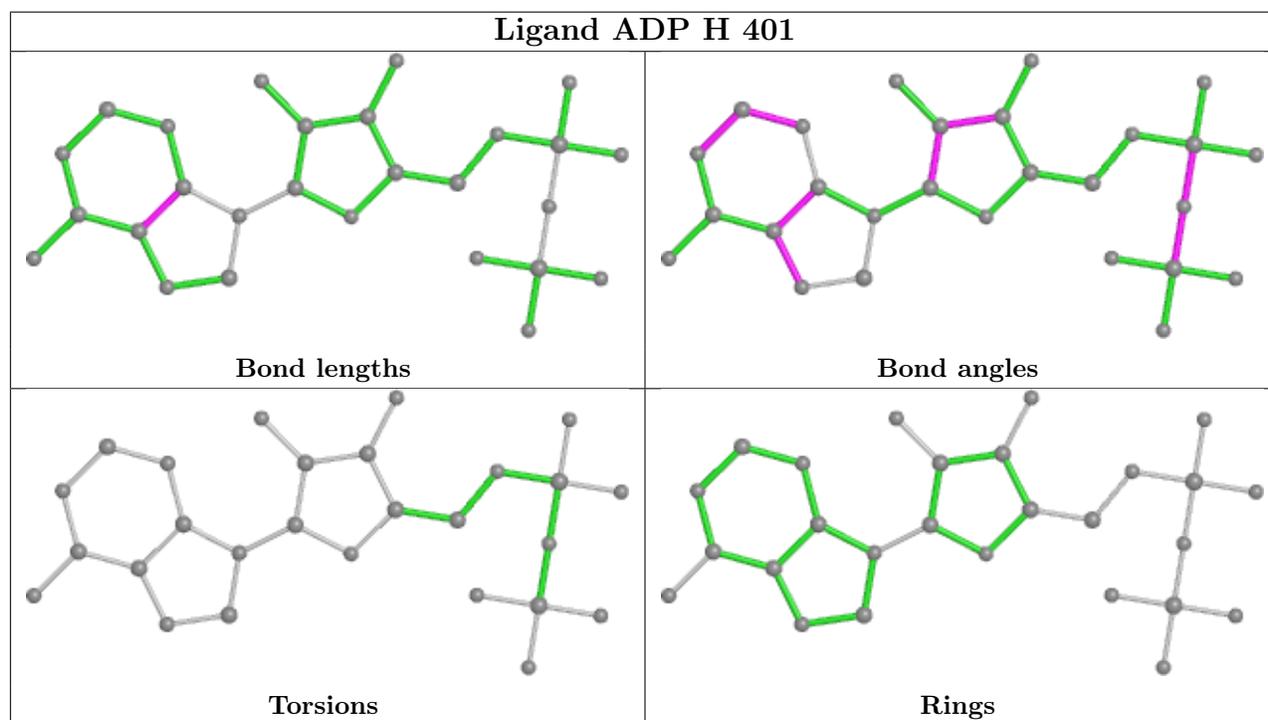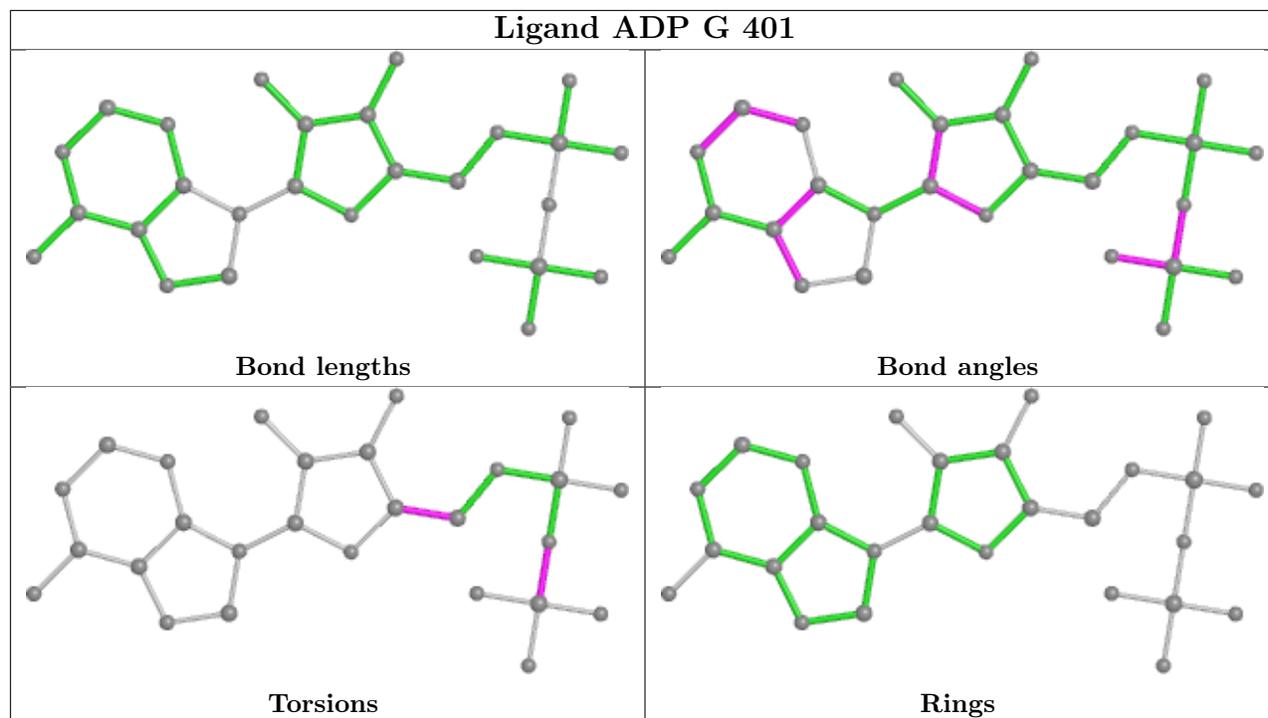
No monomer is involved in short contacts.

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 then 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.

Ligand ADP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP I 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP J 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 401

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 401
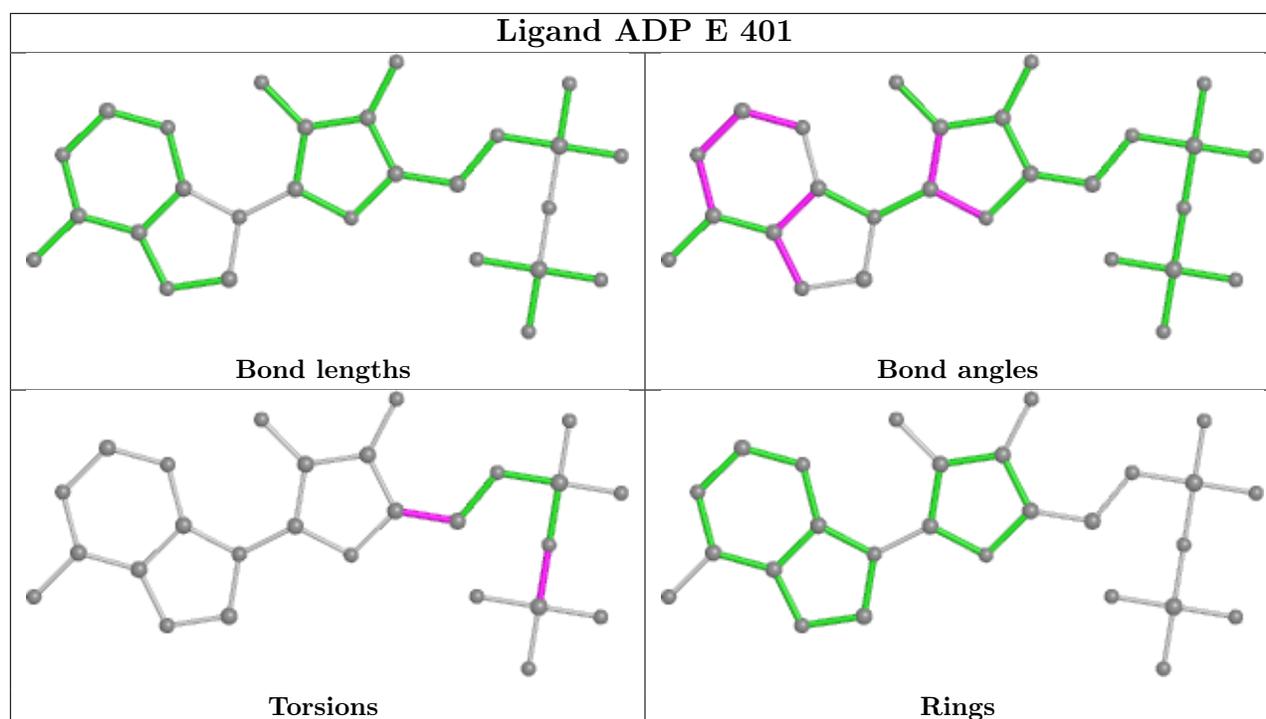

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	367/367 (100%)	0.74	55 (14%)	2	3	24, 46, 127, 170	0
1	B	366/367 (99%)	0.55	48 (13%)	3	4	23, 46, 110, 166	0
1	C	366/367 (99%)	0.43	42 (11%)	4	6	23, 39, 102, 150	0
1	D	364/367 (99%)	0.20	38 (10%)	6	8	23, 36, 96, 126	0
1	E	365/367 (99%)	0.61	45 (12%)	4	5	24, 42, 125, 183	0
1	F	367/367 (100%)	0.40	41 (11%)	5	6	24, 39, 101, 136	0
1	G	365/367 (99%)	0.50	43 (11%)	4	5	21, 37, 114, 155	0
1	H	366/367 (99%)	0.44	42 (11%)	4	6	22, 41, 116, 190	0
1	I	365/367 (99%)	0.73	71 (19%)	1	1	24, 47, 109, 163	0
1	J	367/367 (100%)	0.72	60 (16%)	1	2	26, 48, 118, 157	0
All	All	3658/3670 (99%)	0.53	485 (13%)	3	4	21, 42, 114, 190	0

The worst 5 of 485 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	312	THR	19.8
1	G	318	PHE	19.0
1	E	310	HIS	14.7
1	E	307	THR	13.8
1	E	302	ASN	13.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

LIGAND-RSR INFOmissingINFO

6.5 Other polymers ⓘ

There are no such residues in this entry.