



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:49 AM UTC

PDB ID : 2CE7 / pdb_00002ce7
Title : EDTA treated
Authors : Bieniossek, C.; Baumann, U.
Deposited on : 2006-02-03
Resolution : 2.44 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

<https://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

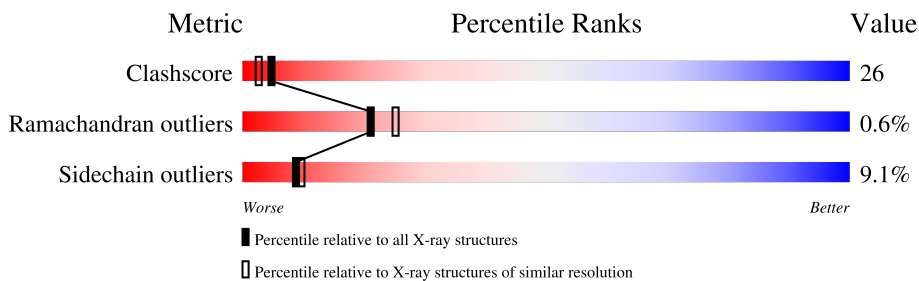
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)

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	476	61% 20% • 14%
1	B	476	57% 25% • 14%
1	C	476	48% 35% 5% 12%
1	D	476	57% 26% • 13%
1	E	476	57% 23% • 15%
1	F	476	49% 33% 5% 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19564 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 CELL DIVISION PROTEIN FTSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	Total 3160	C 1996	N 559	O 595	S 10	0	0	1
1	B	411	Total 3191	C 2017	N 560	O 604	S 10	0	0	0
1	C	421	Total 3280	C 2076	N 573	O 621	S 10	0	0	0
1	D	413	Total 3212	C 2032	N 562	O 608	S 10	0	0	0
1	E	406	Total 3144	C 1986	N 557	O 591	S 10	0	0	1
1	F	412	Total 3204	C 2024	N 564	O 606	S 10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	ALA	LYS	engineered mutation	UNP Q9WZ49
B	410	LEU	LYS	engineered mutation	UNP Q9WZ49
B	415	ALA	LYS	engineered mutation	UNP Q9WZ49
C	415	ALA	LYS	engineered mutation	UNP Q9WZ49
D	410	LEU	LYS	engineered mutation	UNP Q9WZ49
D	415	ALA	LYS	engineered mutation	UNP Q9WZ49
E	410	LEU	LYS	engineered mutation	UNP Q9WZ49
E	415	ALA	LYS	engineered mutation	UNP Q9WZ49
F	415	ALA	LYS	engineered mutation	UNP Q9WZ49

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

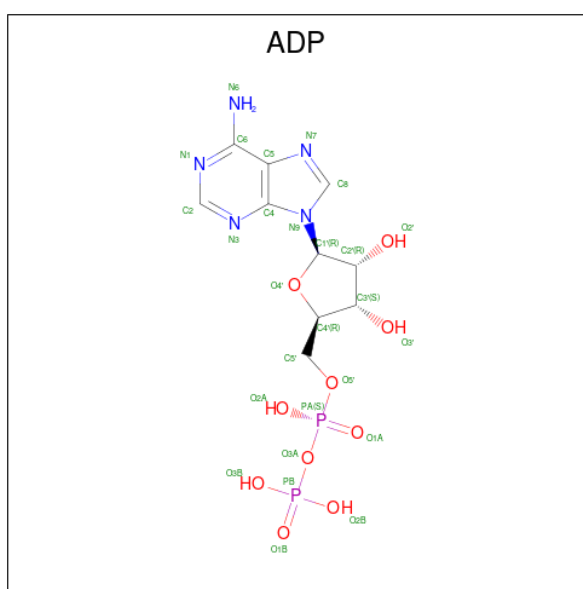
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	33	Total O 33 33	0	0
5	C	26	Total O 26 26	0	0
5	D	33	Total O 33 33	0	0
5	E	38	Total O 38 38	0	0
5	F	23	Total O 23 23	0	0

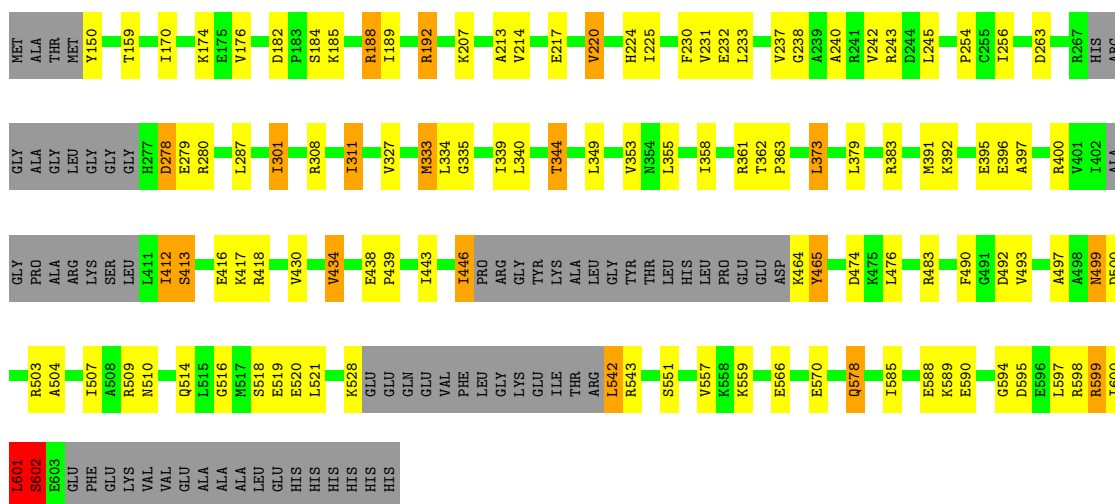
3 Residue-property plots [i](#)

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. 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.

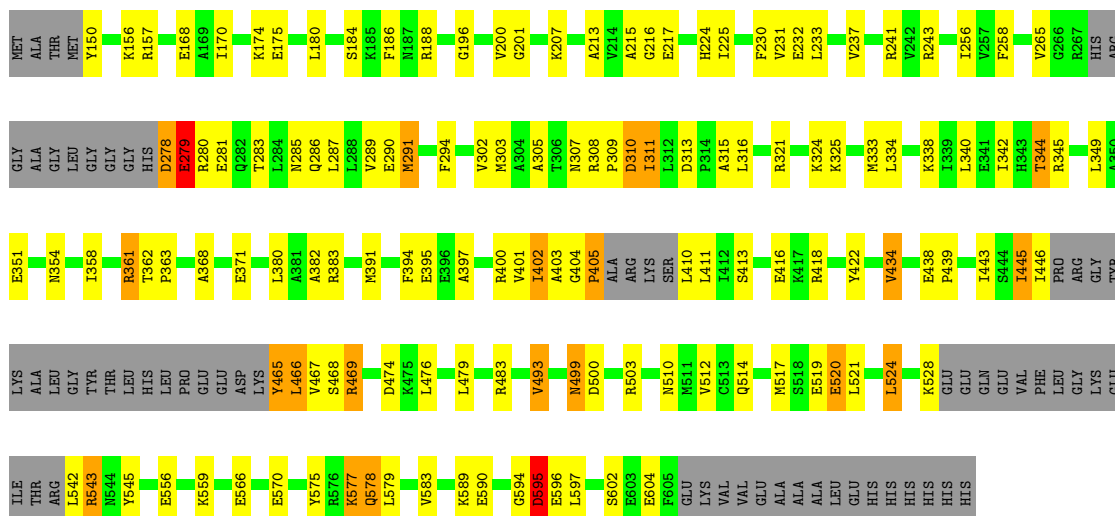
- Molecule 1: CELL DIVISION PROTEIN FTSH

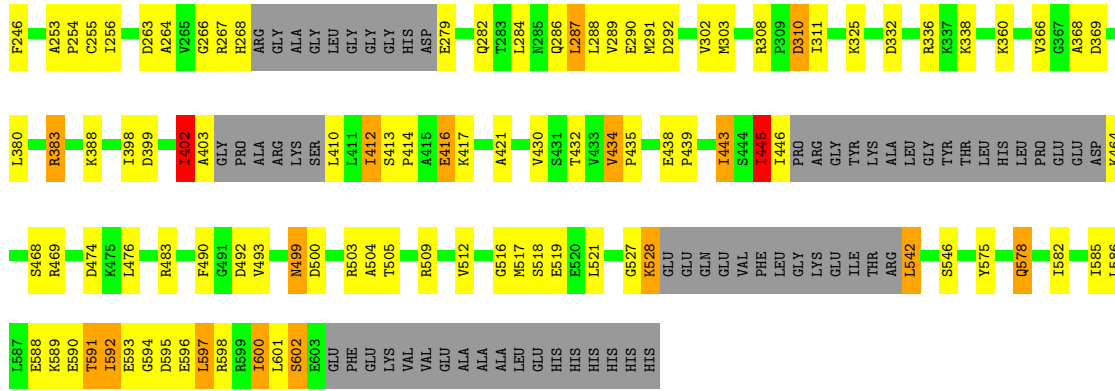
Chain A:  61% 20% 14%



- Molecule 1: CELL DIVISION PROTEIN FTSH

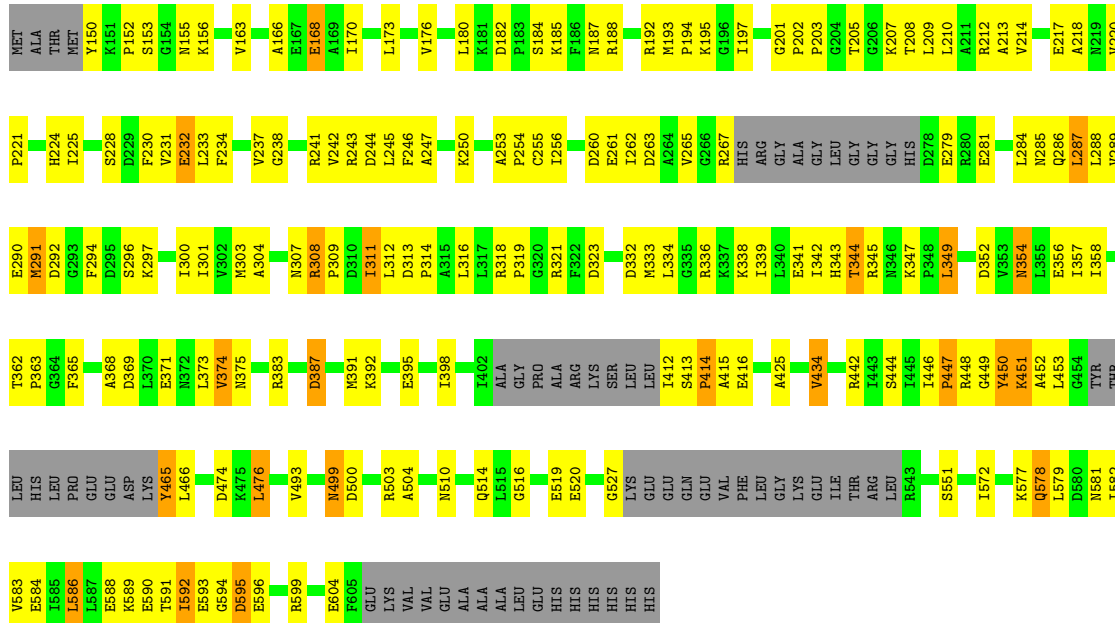
Chain B:  57% 25% 14%





● Molecule 1: CELL DIVISION PROTEIN FTSH

Chain F: 49% 33% 5% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.09Å 165.09Å 235.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.44	Depositor
% Data completeness (in resolution range)	100.0 (25.00-2.44)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	19564	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: 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	0.97	1/3202 (0.0%)	0.85	0/4314
1	B	0.91	0/3233	0.82	1/4356 (0.0%)
1	C	0.78	0/3328	0.81	2/4488 (0.0%)
1	D	0.87	0/3256	0.80	1/4388 (0.0%)
1	E	0.93	1/3185 (0.0%)	0.83	1/4291 (0.0%)
1	F	0.70	0/3248	0.78	0/4376
All	All	0.87	2/19452 (0.0%)	0.82	5/26213 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	602	SER	C-N	-6.63	1.24	1.33
1	A	602	SER	C-N	-6.42	1.24	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PRO	N-CA-CB	7.37	111.11	103.00
1	E	445	ILE	N-CA-C	-6.78	106.39	112.90
1	C	446	ILE	CA-C-N	6.03	127.37	119.84
1	C	446	ILE	C-N-CA	6.03	127.37	119.84
1	D	445	ILE	CB-CA-C	-5.37	104.08	111.65

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	449	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3160	0	3240	113	0
1	B	3191	0	3261	134	0
1	C	3280	0	3346	230	0
1	D	3212	0	3283	132	0
1	E	3144	0	3231	158	0
1	F	3204	0	3270	242	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	5	0
3	C	27	0	12	5	0
3	D	27	0	12	6	0
3	E	27	0	12	6	0
3	F	27	0	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	46	0	0	6	0
5	B	33	0	0	4	0
5	C	26	0	0	10	0
5	D	33	0	0	7	0
5	E	38	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	23	0	0	6	0
All	All	19564	0	19703	999	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 999 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:340:LEU:O	1:C:344:THR:HG22	1.24	1.34
1:C:594:GLY:N	5:C:2024:HOH:O	1.60	1.29
1:A:446:ILE:HG22	5:A:2024:HOH:O	1.19	1.27
1:C:519:GLU:HA	5:C:2018:HOH:O	1.34	1.22
1:E:231:VAL:HG12	1:E:232:GLU:OE2	1.38	1.20

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	397/476 (83%)	383 (96%)	9 (2%)	5 (1%)	9 9
1	B	401/476 (84%)	385 (96%)	13 (3%)	3 (1%)	18 21
1	C	413/476 (87%)	392 (95%)	20 (5%)	1 (0%)	43 53
1	D	403/476 (85%)	387 (96%)	15 (4%)	1 (0%)	43 53
1	E	396/476 (83%)	380 (96%)	15 (4%)	1 (0%)	36 44
1	F	402/476 (84%)	381 (95%)	17 (4%)	4 (1%)	12 13
All	All	2412/2856 (84%)	2308 (96%)	89 (4%)	15 (1%)	21 25

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	602	SER
1	B	595	ASP
1	F	414	PRO
1	A	601	LEU

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	337/390 (86%)	310 (92%)	27 (8%)	11	13
1	B	339/390 (87%)	307 (91%)	32 (9%)	8	9
1	C	349/390 (90%)	315 (90%)	34 (10%)	8	8
1	D	342/390 (88%)	314 (92%)	28 (8%)	10	12
1	E	335/390 (86%)	304 (91%)	31 (9%)	8	9
1	F	340/390 (87%)	306 (90%)	34 (10%)	7	7
All	All	2042/2340 (87%)	1856 (91%)	186 (9%)	9	10

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	520	GLU
1	E	519	GLU
1	D	593	GLU
1	E	383	ARG
1	E	600	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	286	GLN
1	F	307	ASN
1	F	499	ASN
1	C	544	ASN

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Mol	Chain	Res	Type
1	C	514	GLN

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
3	ADP	E	1604	4	28,29,29	1.20	3 (10%)	43,45,45	1.94	11 (25%)
3	ADP	A	1604	4	28,29,29	1.36	3 (10%)	43,45,45	1.92	11 (25%)
3	ADP	D	1608	4	28,29,29	1.46	5 (17%)	43,45,45	1.93	10 (23%)
3	ADP	C	1608	4	28,29,29	1.38	4 (14%)	43,45,45	1.87	10 (23%)
3	ADP	F	1607	4	28,29,29	1.46	5 (17%)	43,45,45	1.93	10 (23%)
3	ADP	B	1607	4	28,29,29	1.43	6 (21%)	43,45,45	1.89	10 (23%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	E	1604	4	-	3/16/32/32	0/3/3/3
3	ADP	A	1604	4	-	2/16/32/32	0/3/3/3
3	ADP	D	1608	4	-	2/16/32/32	0/3/3/3
3	ADP	C	1608	4	-	2/16/32/32	0/3/3/3
3	ADP	F	1607	4	-	3/16/32/32	0/3/3/3
3	ADP	B	1607	4	-	2/16/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1604	ADP	C5-C4	4.35	1.46	1.39
3	F	1607	ADP	C5-C4	4.23	1.46	1.39
3	C	1608	ADP	C5-C4	4.17	1.46	1.39
3	E	1604	ADP	C5-C4	3.47	1.45	1.39
3	D	1608	ADP	C5-C4	3.46	1.45	1.39

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1607	ADP	C5-C4-N3	-5.74	118.81	126.72
3	D	1608	ADP	C5-C4-N3	-5.63	118.97	126.72
3	E	1604	ADP	C5-C4-N3	-5.62	118.98	126.72
3	C	1608	ADP	C5-C4-N3	-5.55	119.07	126.72
3	A	1604	ADP	C5-C4-N3	-5.48	119.17	126.72

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1604	ADP	C5'-O5'-PA-O3A
3	F	1607	ADP	C5'-O5'-PA-O1A
3	F	1607	ADP	C5'-O5'-PA-O2A
3	F	1607	ADP	C5'-O5'-PA-O3A
3	E	1604	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 30 short contacts:

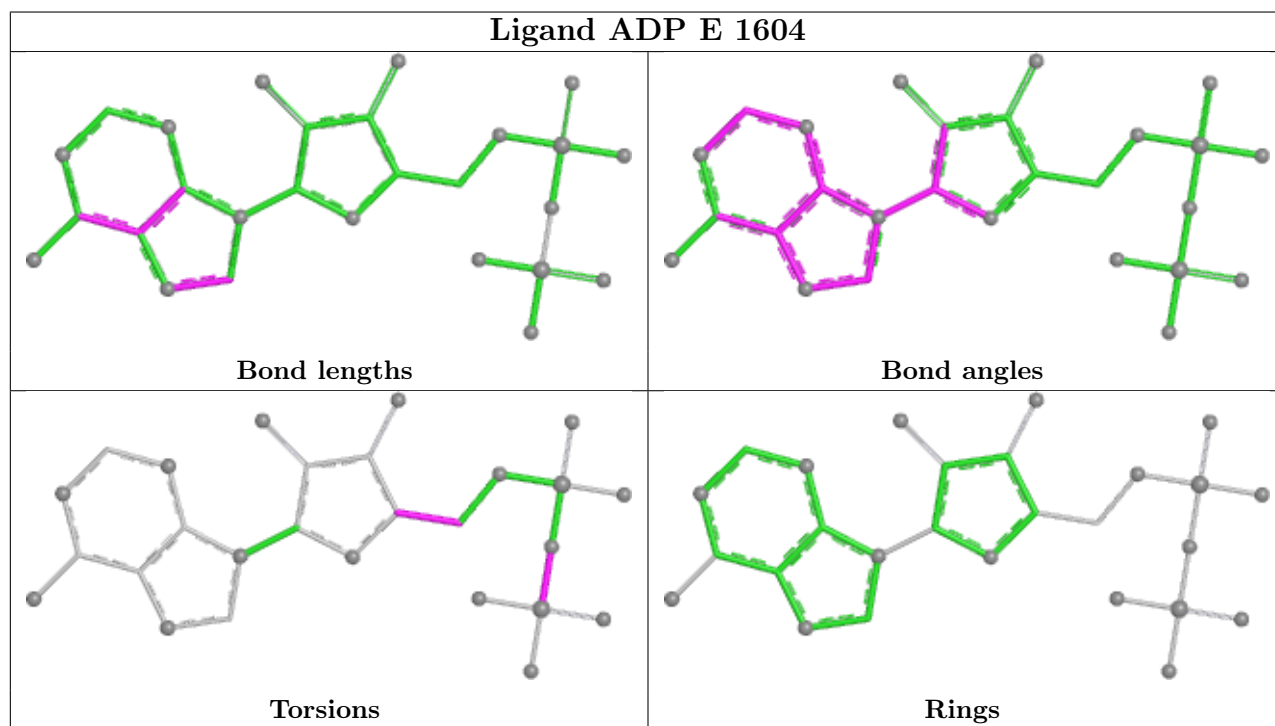
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1604	ADP	6	0

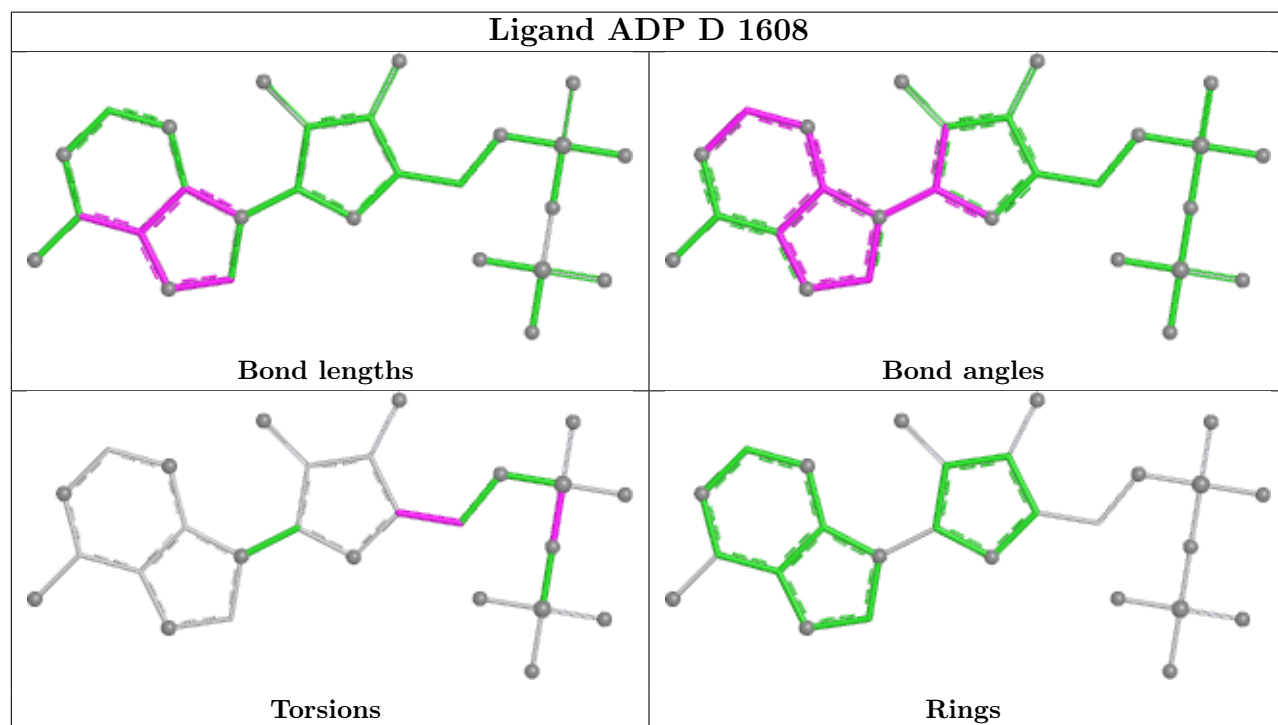
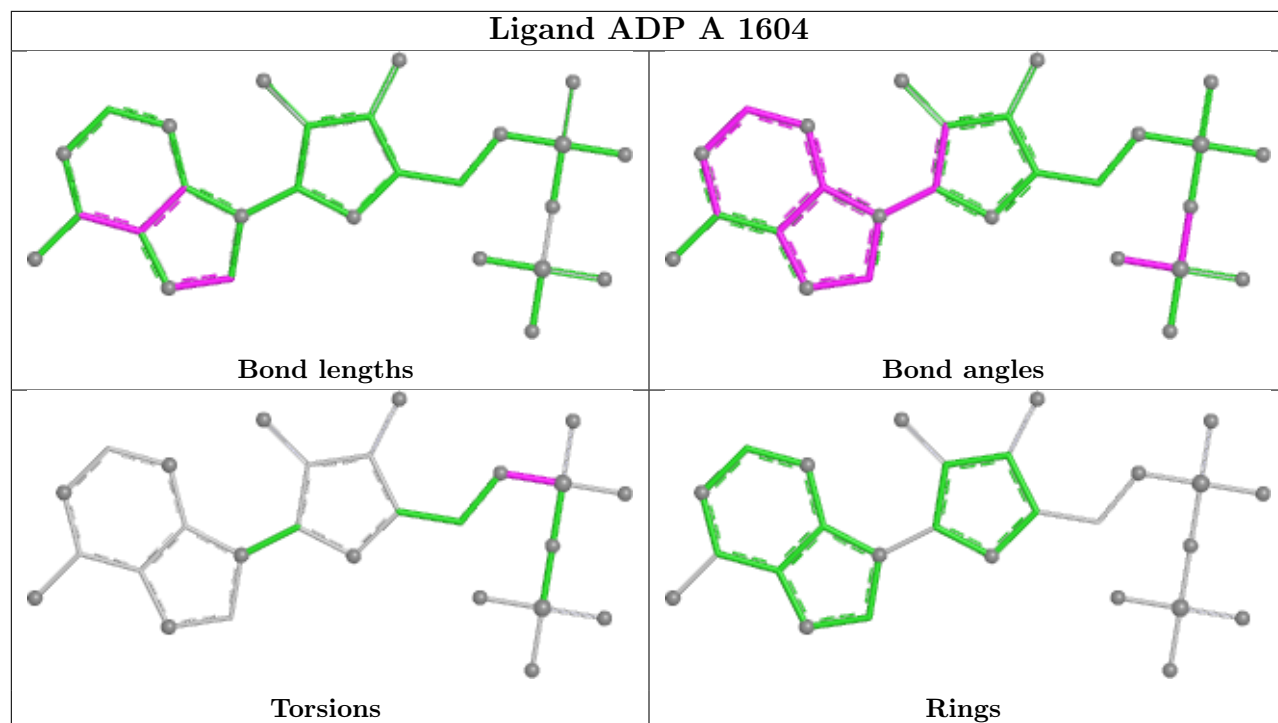
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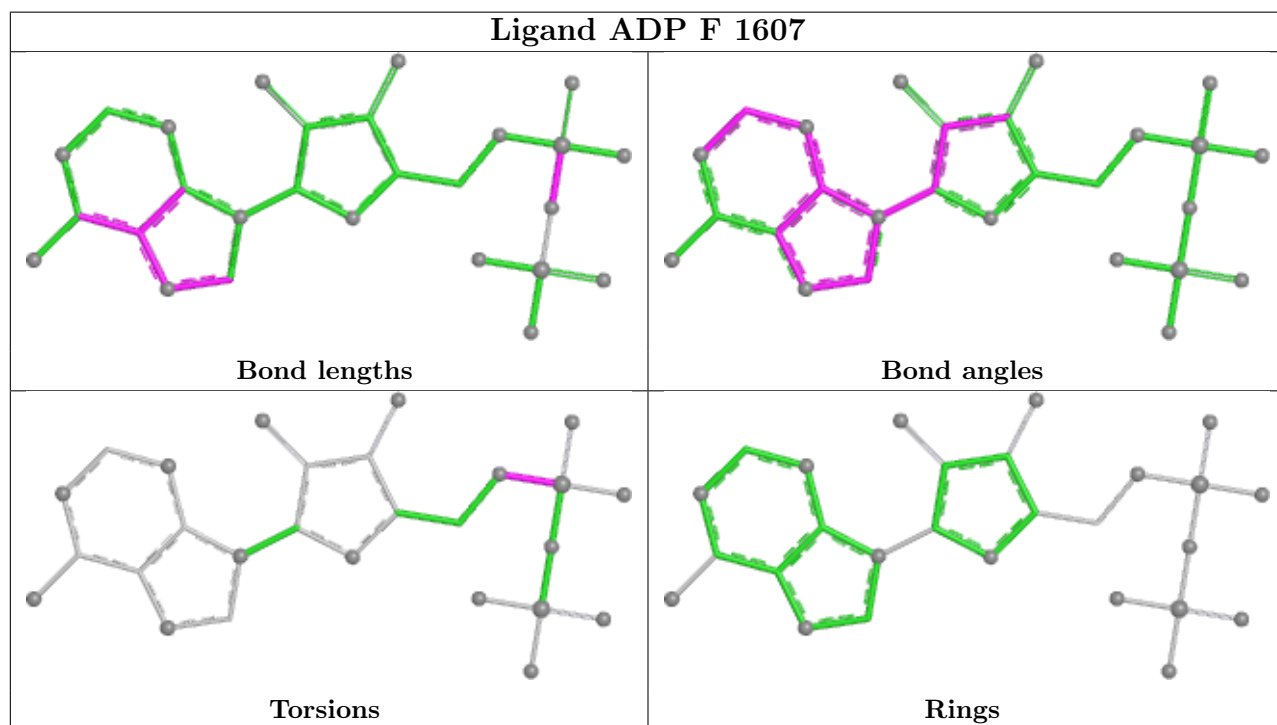
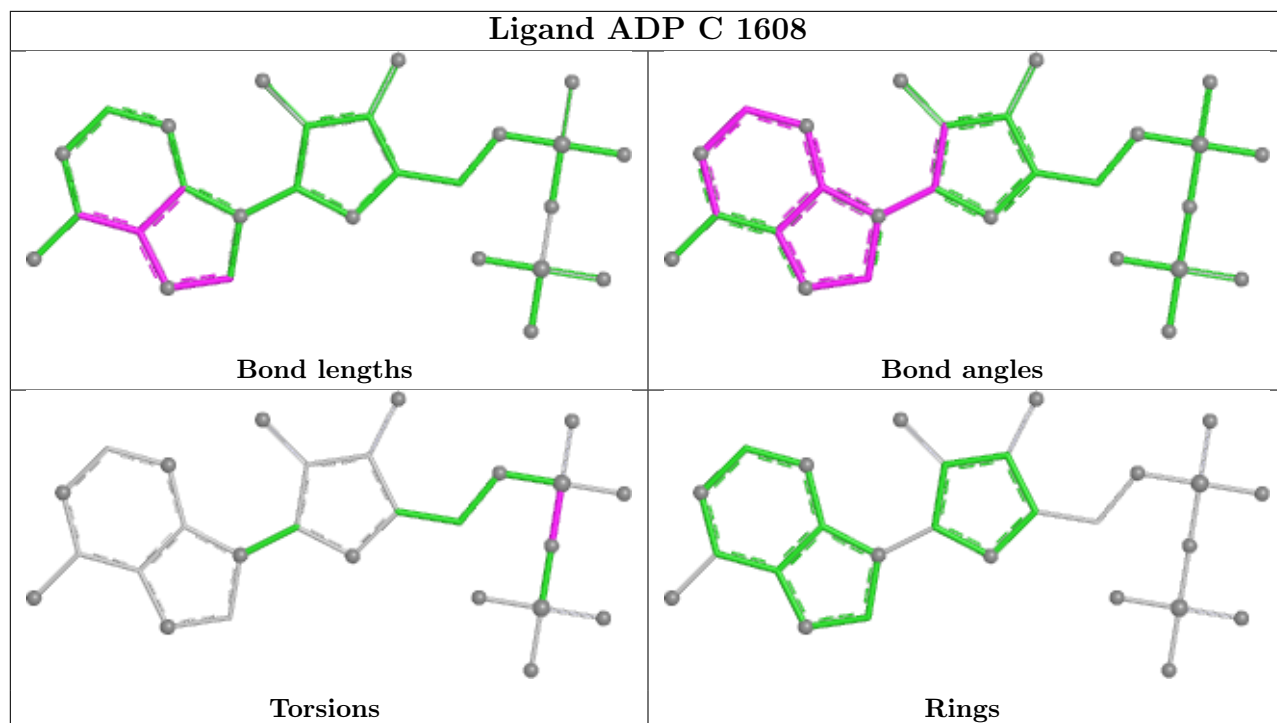
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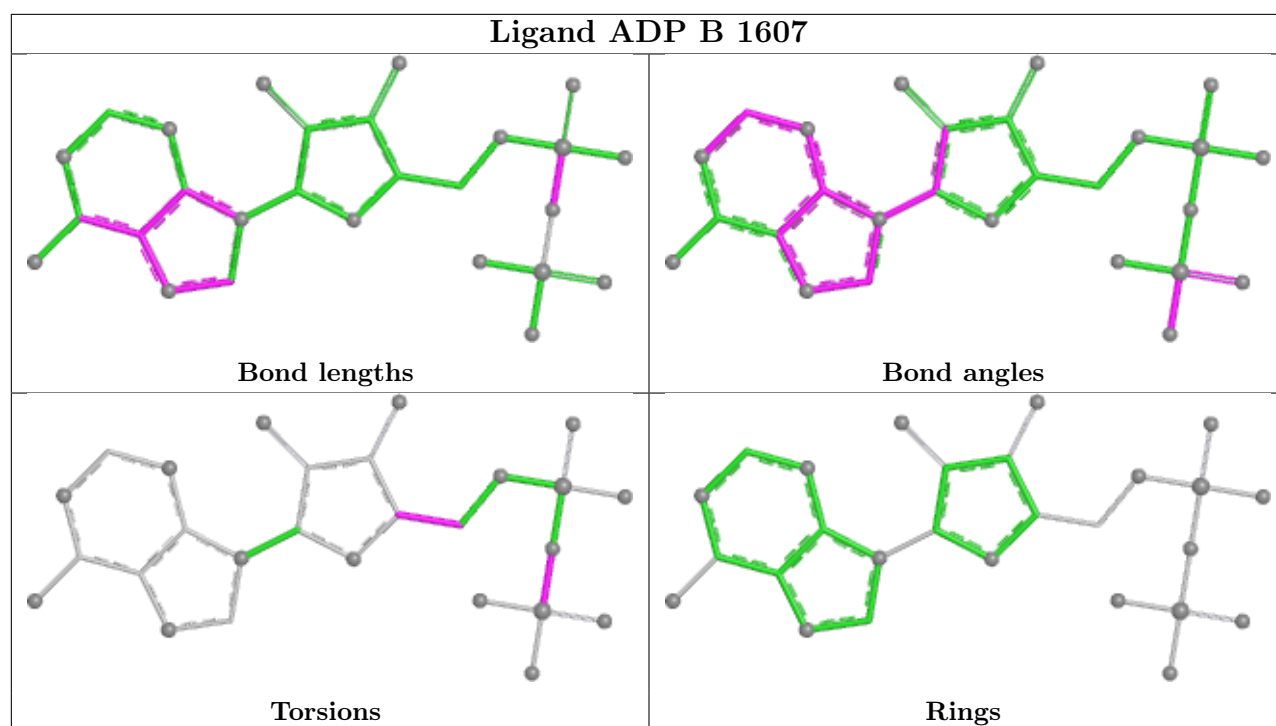
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1604	ADP	3	0
3	D	1608	ADP	6	0
3	C	1608	ADP	5	0
3	F	1607	ADP	5	0
3	B	1607	ADP	5	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.