



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 05:15 AM EDT

PDB ID : 1G21 / pdb_00001g21
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 3.00 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)
Xtriage (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)	:	2.50

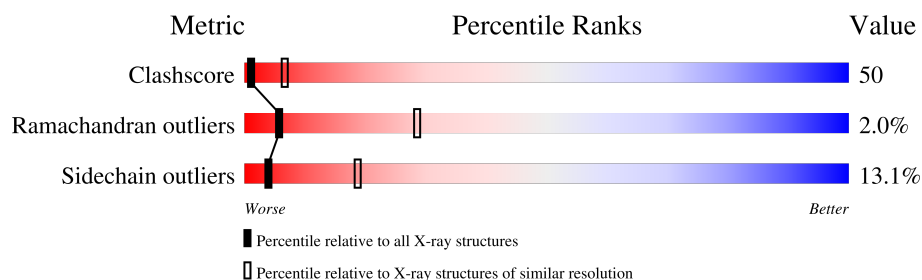
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	492	
1	C	492	
2	B	523	
2	D	523	
3	E	289	
3	F	289	
3	G	289	
3	H	289	

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
5	CFM	A	1496	-	-	X	-
5	CFM	C	3496	-	-	X	-
9	ATP	G	7292	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24237 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4170	2663	704	775	28			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	268	Total	C	N	O	S	109	0	0
			2029	1265	347	397	20			
3	F	267	Total	C	N	O	S	71	0	0
			2020	1260	346	394	20			
3	G	268	Total	C	N	O	S	130	0	0
			2029	1265	347	397	20			
3	H	268	Total	C	N	O	S	116	0	0
			2029	1265	347	397	20			

There are 4 discrepancies between the modelled and reference sequences:

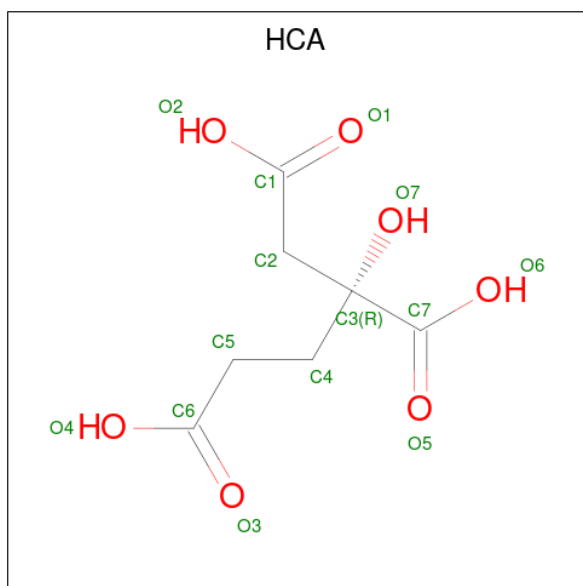
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P00459
F	?	-	LEU	deletion	UNP P00459
G	?	-	LEU	deletion	UNP P00459

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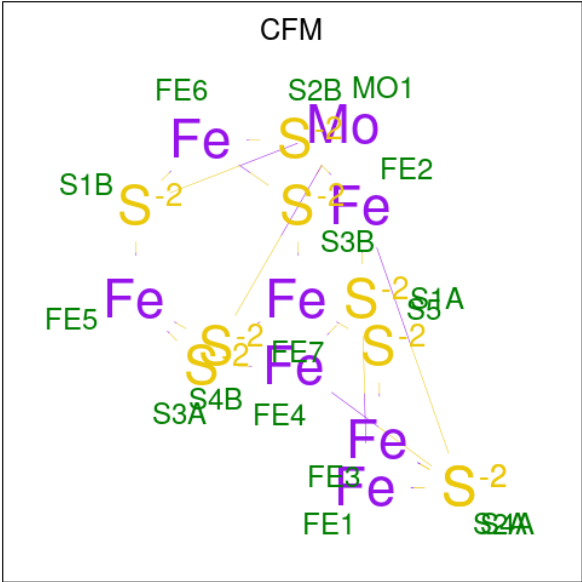
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P00459

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



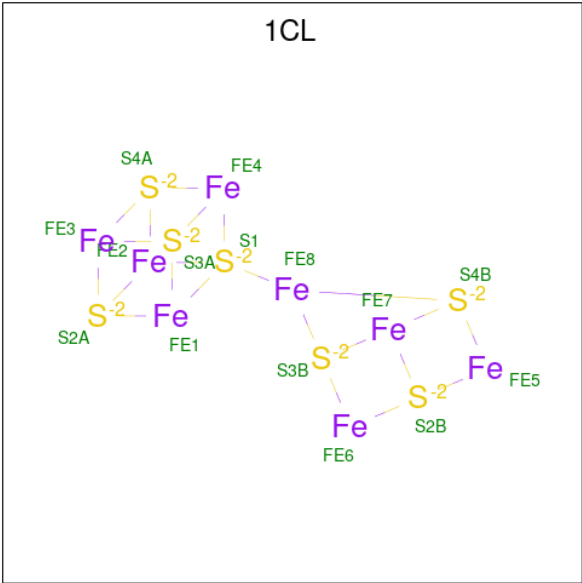
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is FE(8)-S(7) CLUSTER, OXIDIZED (CCD ID: 1CL) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		

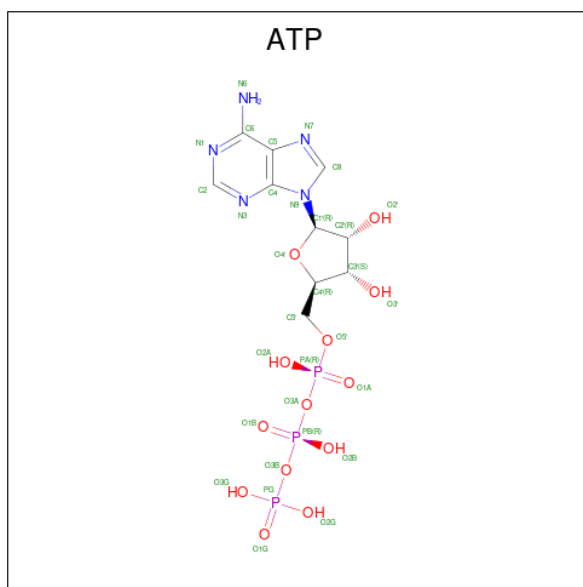
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	G	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		

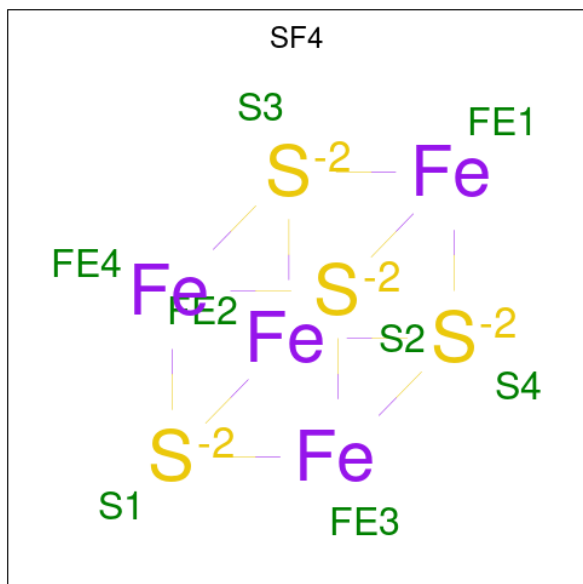
- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



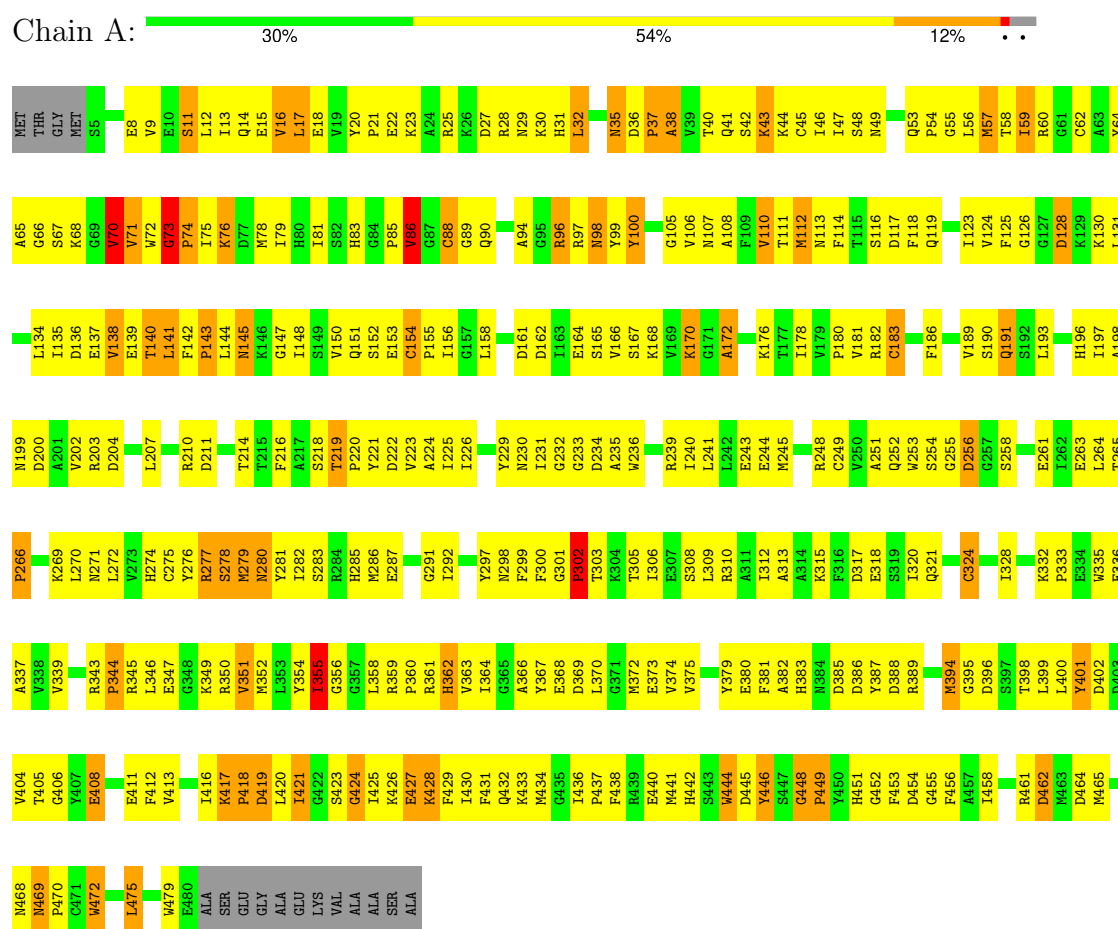
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	F	1	Total	Fe	S	0	0
			8	4	4		
10	G	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

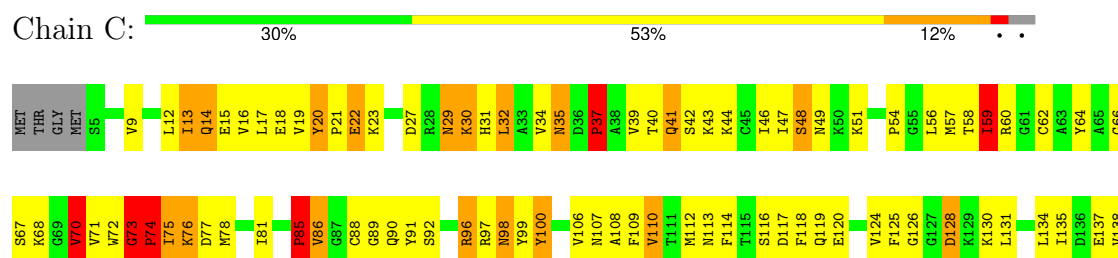
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

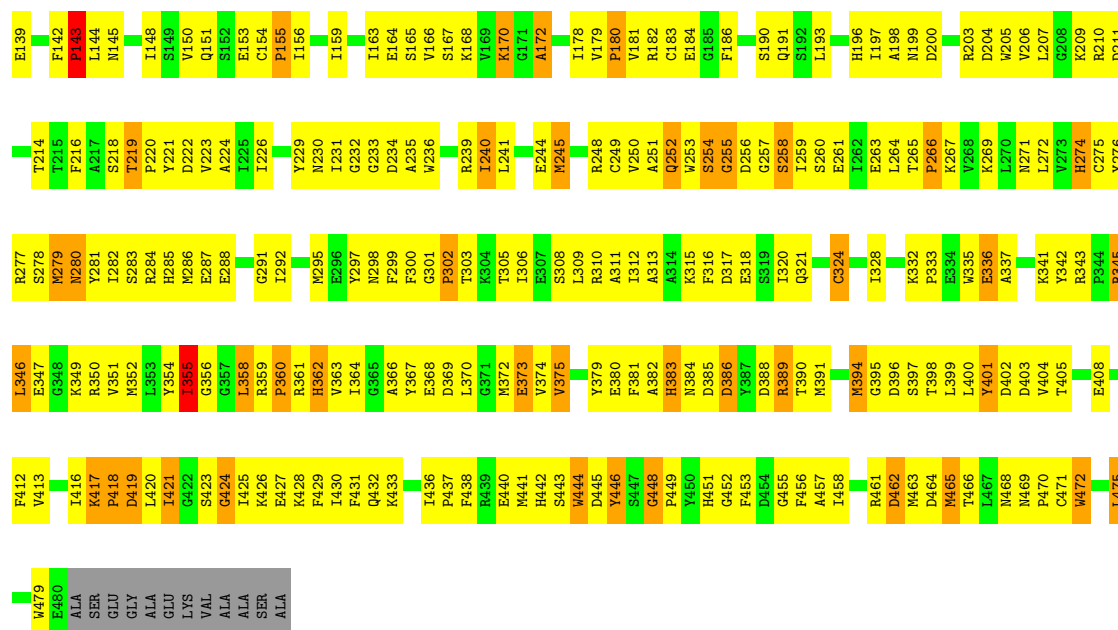
Note EDS was not executed.

• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



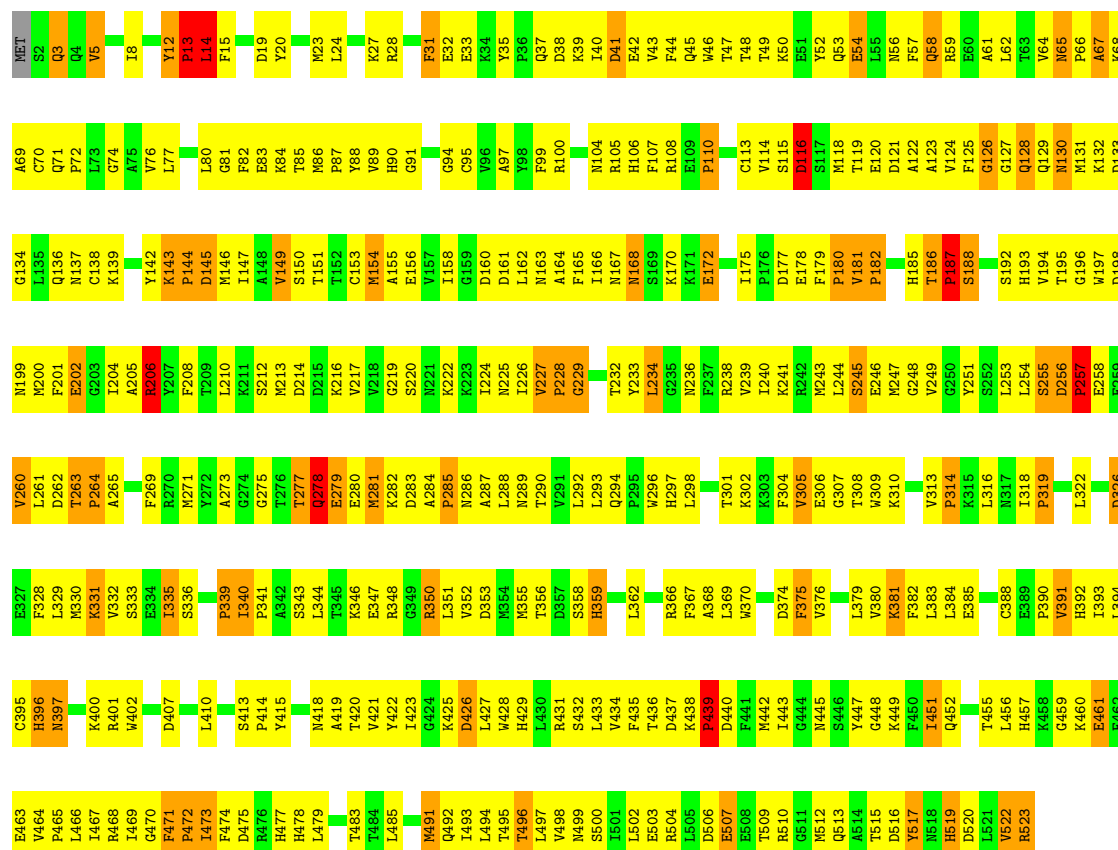
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



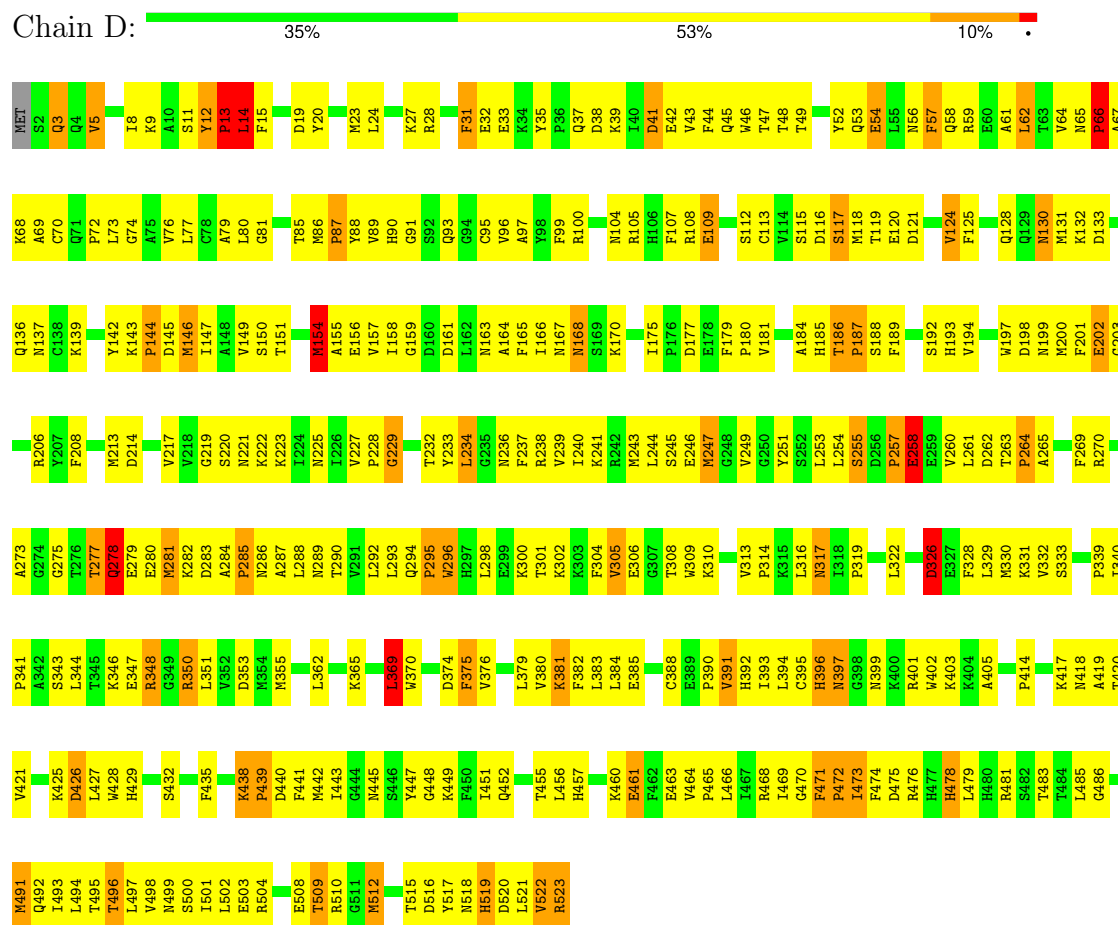


• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

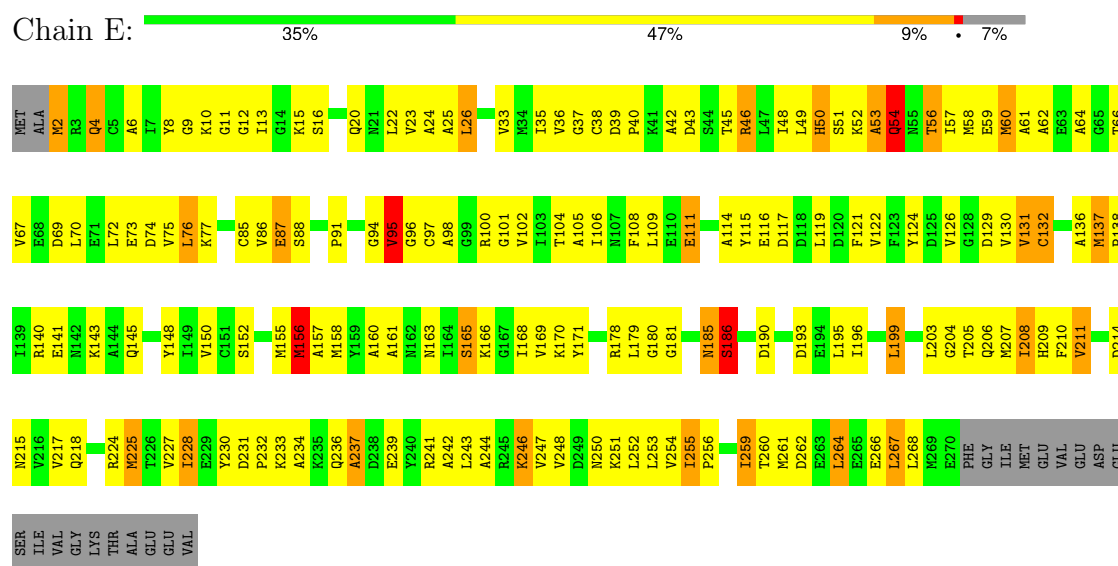
Chain B: 29% 56% 13%



• Molecule 2: NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN

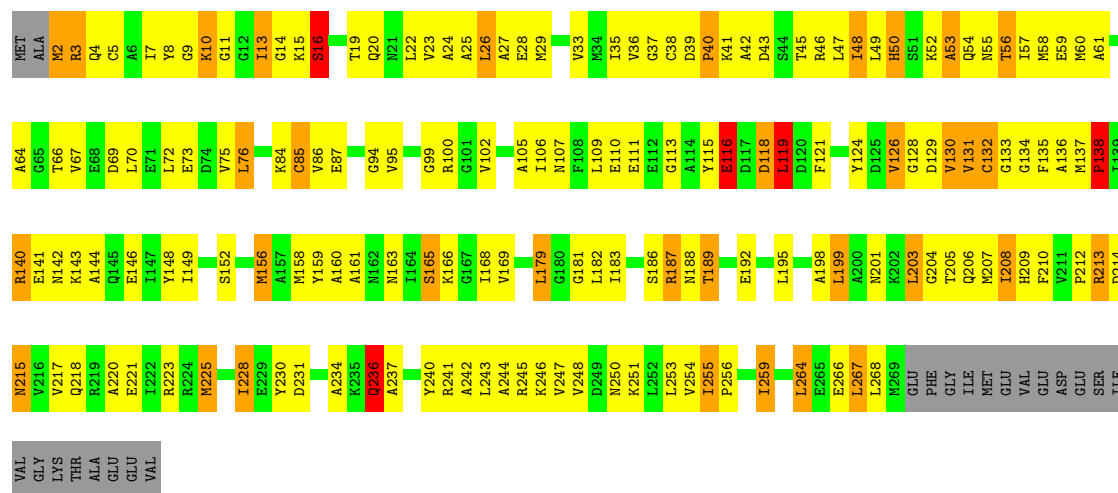


• Molecule 3: NITROGENASE IRON PROTEIN



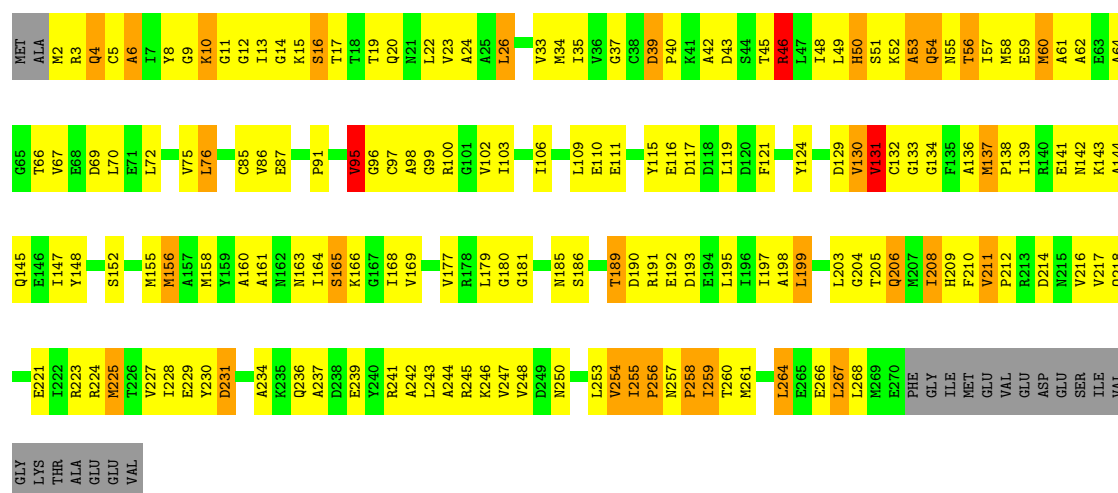
• Molecule 3: NITROGENASE IRON PROTEIN





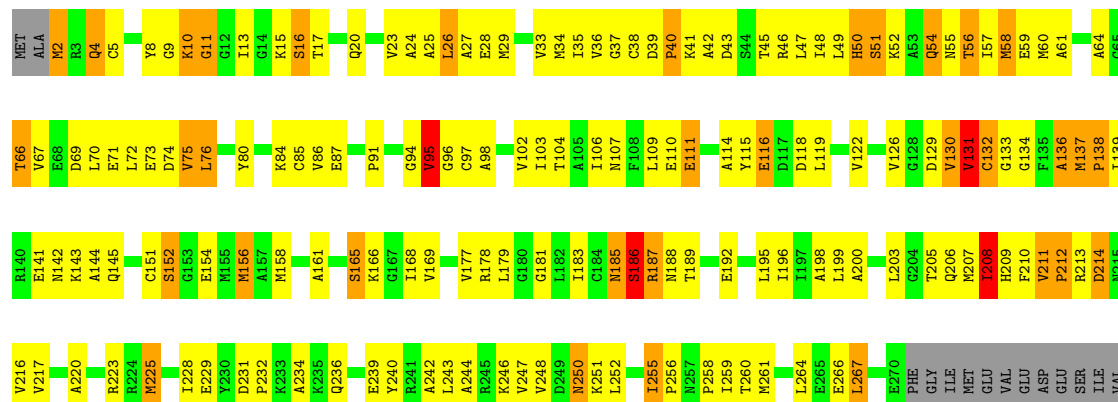
• Molecule 3: NITROGENASE IRON PROTEIN

Chain G: 35% 47% 10% • 7%



• Molecule 3: NITROGENASE IRON PROTEIN

Chain H: 35% 44% 12% • 7%



GLY
LYS
THR
ALA
GLU
GLU
VAL

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	110.50Å 121.50Å 264.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	71.6 (20.00-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24237	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CFM, HCA, SF4, 1CL, CA, ATP, 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	0.67	1/3864 (0.0%)	1.16	38/5212 (0.7%)
1	C	0.60	0/3864	1.17	42/5212 (0.8%)
2	B	0.72	2/4276 (0.0%)	1.51	56/5782 (1.0%)
2	D	0.66	1/4276 (0.0%)	1.42	40/5782 (0.7%)
3	E	0.68	0/2052	1.25	22/2764 (0.8%)
3	F	0.73	1/2043 (0.0%)	1.27	16/2752 (0.6%)
3	G	0.64	0/2052	1.15	18/2764 (0.7%)
3	H	0.71	2/2052 (0.1%)	1.23	20/2764 (0.7%)
All	All	0.67	7/24479 (0.0%)	1.30	252/33032 (0.8%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	156	MET	SD-CE	-8.37	1.58	1.79
1	A	57	MET	SD-CE	-7.88	1.59	1.79
2	D	109	GLU	C-N	-6.80	1.24	1.33
2	B	13	PRO	CA-CB	-6.58	1.44	1.53
2	B	257	PRO	N-CA	5.62	1.54	1.47

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	TYR	CA-C-N	46.49	177.95	119.84
2	B	12	TYR	C-N-CA	46.49	177.95	119.84
2	D	12	TYR	CA-C-N	43.69	174.45	119.84
2	D	12	TYR	C-N-CA	43.69	174.45	119.84
2	D	12	TYR	C-N-CD	-12.75	72.71	125.00

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	3776	0	3709	469	0
1	C	3776	0	3709	507	0
2	B	4170	0	4076	458	0
2	D	4170	0	4076	485	0
3	E	2029	0	2040	158	0
3	F	2020	0	2034	172	0
3	G	2029	0	2041	166	0
3	H	2029	0	2041	162	0
4	A	14	0	6	1	0
4	C	14	0	6	2	0
5	A	17	0	0	4	0
5	C	17	0	0	7	0
6	A	15	0	0	1	0
6	D	15	0	0	3	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	E	31	0	12	4	0
9	F	31	0	12	6	0
9	G	31	0	12	11	0
9	H	31	0	12	6	0
10	F	8	0	0	0	0
10	G	8	0	0	0	0
All	All	24237	0	23786	2341	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 50.

The worst 5 of 2341 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)
3:F:39:ASP:OD1	3:F:40:PRO:HD2	1.28	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:GLY:HA2	2:D:118:MET:CE	1.62	1.28
1:C:124:VAL:HG21	3:H:58:MET:CE	1.70	1.21
1:A:355:ILE:HG23	1:A:356:GLY:H	0.99	1.15
1:A:75:ILE:HG21	1:A:78:MET:HE3	1.27	1.14

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	474/492 (96%)	420 (89%)	47 (10%)	7 (2%)	8	35
1	C	474/492 (96%)	415 (88%)	52 (11%)	7 (2%)	8	35
2	B	520/523 (99%)	470 (90%)	43 (8%)	7 (1%)	9	38
2	D	520/523 (99%)	450 (86%)	60 (12%)	10 (2%)	6	30
3	E	266/289 (92%)	232 (87%)	29 (11%)	5 (2%)	6	30
3	F	265/289 (92%)	232 (88%)	25 (9%)	8 (3%)	3	19
3	G	266/289 (92%)	225 (85%)	33 (12%)	8 (3%)	3	19
3	H	266/289 (92%)	234 (88%)	24 (9%)	8 (3%)	3	19
All	All	3051/3186 (96%)	2678 (88%)	313 (10%)	60 (2%)	6	28

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	13	PRO
2	B	391	VAL
2	D	13	PRO
2	D	439	PRO
3	E	53	ALA

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	405/415 (98%)	364 (90%)	41 (10%)	7	29
1	C	405/415 (98%)	351 (87%)	54 (13%)	4	18
2	B	453/455 (100%)	396 (87%)	57 (13%)	4	20
2	D	453/455 (100%)	407 (90%)	46 (10%)	7	29
3	E	216/233 (93%)	181 (84%)	35 (16%)	2	12
3	F	215/233 (92%)	180 (84%)	35 (16%)	2	12
3	G	216/233 (93%)	181 (84%)	35 (16%)	2	12
3	H	216/233 (93%)	182 (84%)	34 (16%)	2	13
All	All	2579/2672 (96%)	2242 (87%)	337 (13%)	4	19

5 of 337 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	266	GLU
3	G	145	GLN
3	F	26	LEU
3	F	228	ILE
3	G	264	LEU

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

Mol	Chain	Res	Type
2	D	199	ASN
3	E	55	ASN
2	D	268	GLN
2	D	396	HIS
3	E	236	GLN

5.3.3 RNA ⓘ

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, 6 are monoatomic - leaving 12 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
9	ATP	E	5292	8	32,33,33	1.58	4 (12%)	48,52,52	1.07	2 (4%)
4	HCA	C	3494	5	13,13,13	2.35	4 (30%)	15,18,18	2.55	7 (46%)
10	SF4	G	7290	3	0,12,12	-	-	-	-	-
5	CFM	A	1496	4,1	0,24,24	-	-	-	-	-
9	ATP	G	7292	8	32,33,33	1.82	6 (18%)	48,52,52	1.11	3 (6%)
4	HCA	A	1494	5	13,13,13	2.52	5 (38%)	15,18,18	2.03	4 (26%)
9	ATP	H	8292	8	32,33,33	1.51	4 (12%)	48,52,52	1.05	4 (8%)
9	ATP	F	6292	8	32,33,33	1.57	3 (9%)	48,52,52	1.18	4 (8%)
6	1CL	A	1498	2,1	0,22,22	-	-	-	-	-
10	SF4	F	5290	3	0,12,12	-	-	-	-	-
6	1CL	D	3498	2,1	0,22,22	-	-	-	-	-
5	CFM	C	3496	4,1	0,24,24	-	-	-	-	-

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
9	ATP	E	5292	8	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	C	3494	5	-	5/17/17/17	-
10	SF4	G	7290	3	-	-	0/6/5/5
9	ATP	G	7292	8	-	9/22/38/38	0/3/3/3
9	ATP	H	8292	8	-	3/22/38/38	0/3/3/3
9	ATP	F	6292	8	-	7/22/38/38	0/3/3/3
6	1CL	A	1498	2,1	-	-	0/10/8/8
10	SF4	F	5290	3	-	-	0/6/5/5
6	1CL	D	3498	2,1	-	-	0/10/8/8
4	HCA	A	1494	5	-	8/17/17/17	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1494	HCA	O5-C7	6.99	1.44	1.22
4	C	3494	HCA	O5-C7	6.73	1.43	1.22
9	E	5292	ATP	PB-O3A	-6.22	1.52	1.59
9	H	8292	ATP	PB-O3A	-5.46	1.53	1.59
9	G	7292	ATP	PB-O3A	-5.32	1.53	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	O6-C7-C3	5.46	123.62	113.14
4	A	1494	HCA	O6-C7-C3	4.55	121.86	113.14
4	C	3494	HCA	O7-C3-C4	-3.79	102.81	108.88
4	C	3494	HCA	O2-C1-C2	3.50	125.44	114.35
4	A	1494	HCA	O5-C7-C3	-3.43	115.44	122.09

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

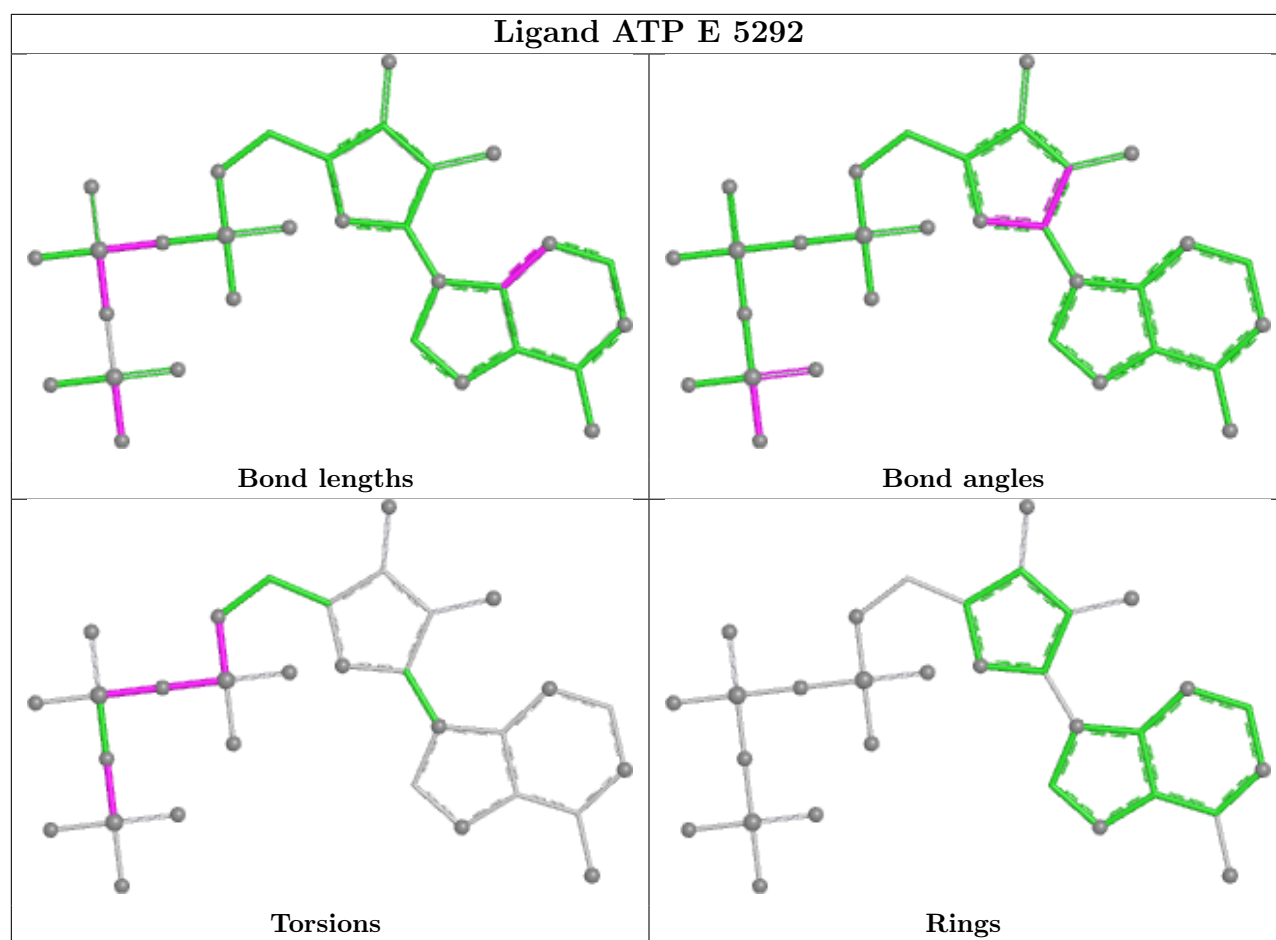
Mol	Chain	Res	Type	Atoms
4	A	1494	HCA	C2-C3-C4-C5
4	A	1494	HCA	C7-C3-C4-C5
4	A	1494	HCA	O7-C3-C4-C5
4	C	3494	HCA	C2-C3-C4-C5
4	C	3494	HCA	C7-C3-C4-C5

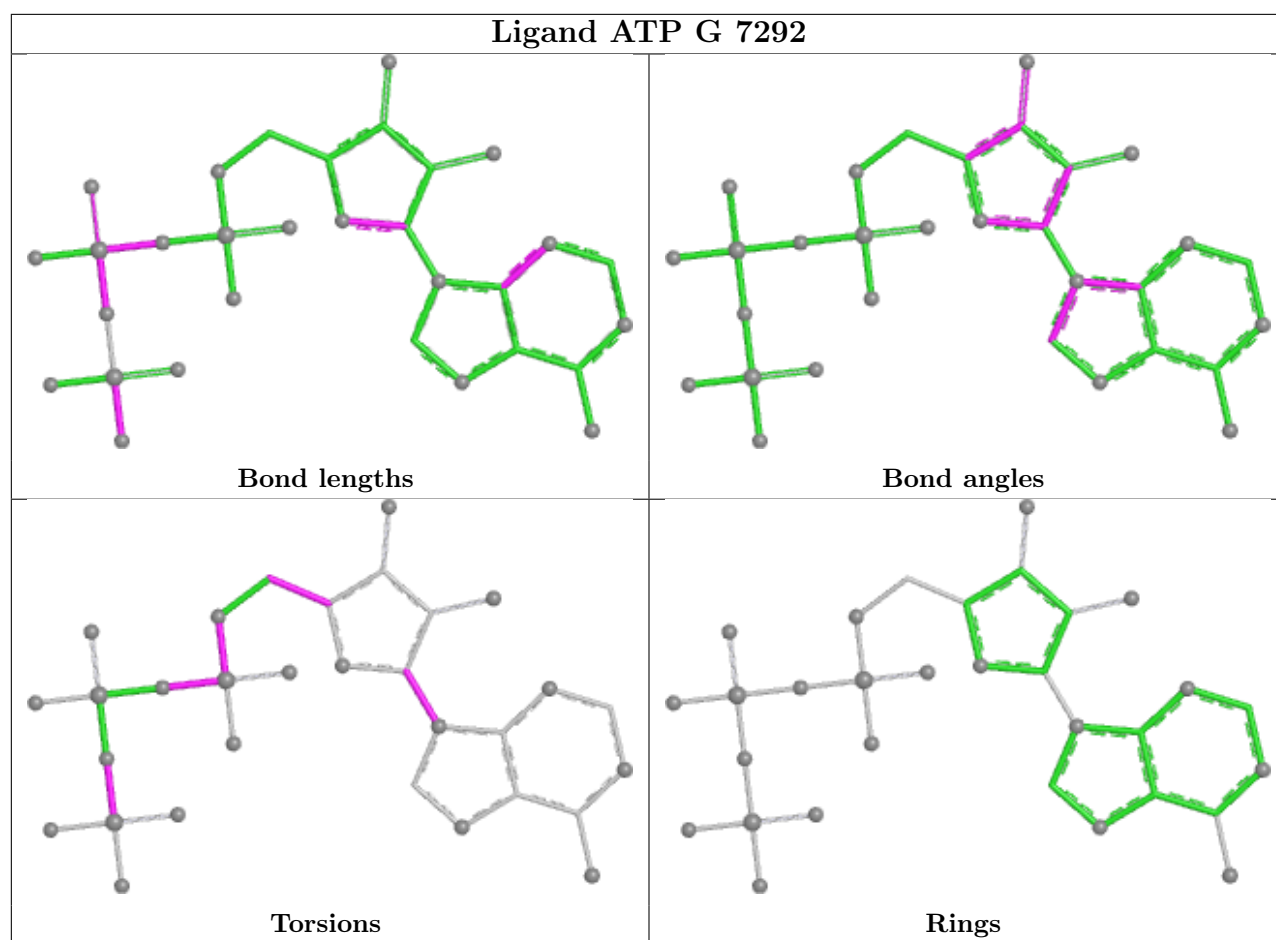
There are no ring outliers.

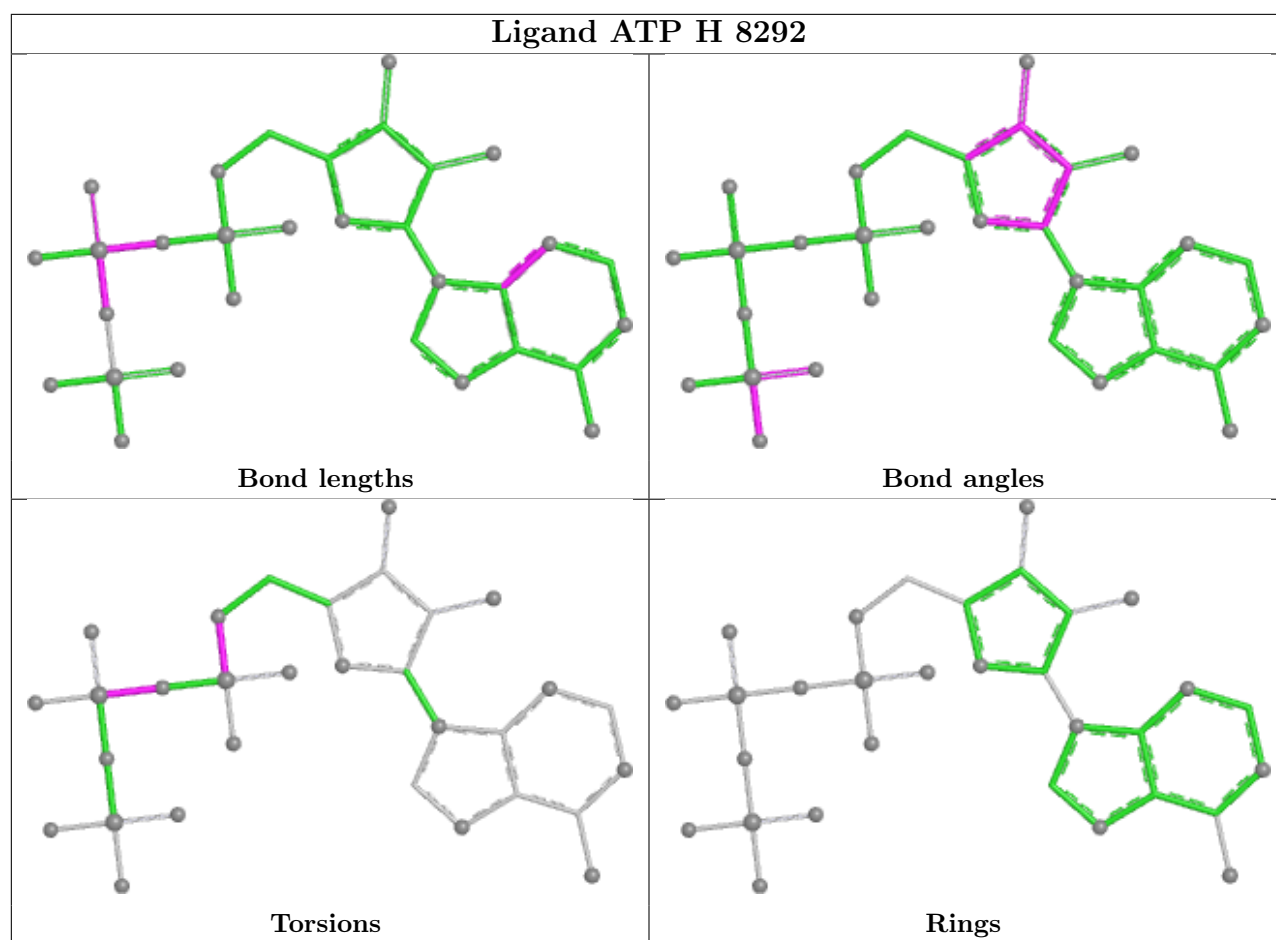
10 monomers are involved in 45 short contacts:

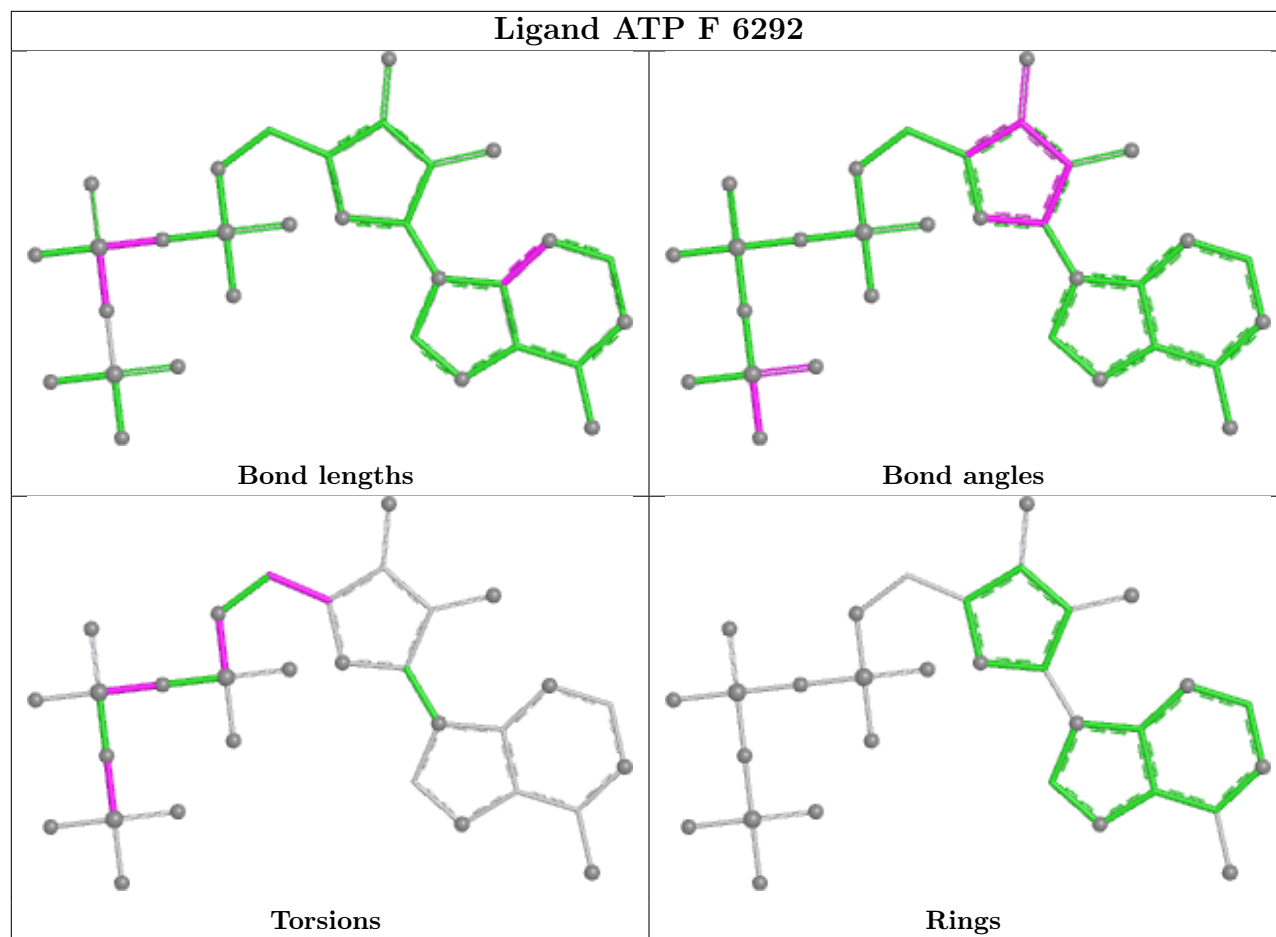
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	5292	ATP	4	0
4	C	3494	HCA	2	0
5	A	1496	CFM	4	0
9	G	7292	ATP	11	0
4	A	1494	HCA	1	0
9	H	8292	ATP	6	0
9	F	6292	ATP	6	0
6	A	1498	1CL	1	0
6	D	3498	1CL	3	0
5	C	3496	CFM	7	0

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.