



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:25 am BST

PDB ID : 1M34
Title : Nitrogenase Complex From Azotobacter Vinelandii Stabilized By ADP-Tetrafluoroaluminate
Authors : Schmid, B.; Einsle, O.; Chiu, H.-J.; Willing, A.; Yoshida, M.; Howard, J.B.; Rees, D.C.
Deposited on : 2002-06-27
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

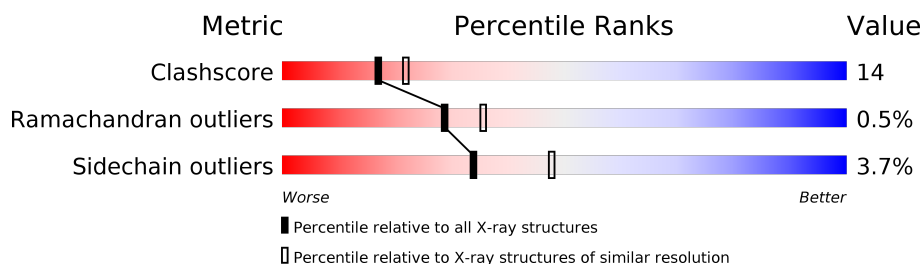
1 Overall quality at a glance

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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 on 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	491	
1	C	491	
1	I	491	
1	K	491	
2	B	522	
2	D	522	
2	J	522	
2	L	522	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	289	
3	F	289	
3	G	289	
3	H	289	
3	M	289	
3	N	289	
3	O	289	
3	P	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
4	HCA	A	2094	X	-	-	-
4	HCA	I	4094	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 50568 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	478	Total	C	N	O	S	0	0	0
			3795	2413	647	710	25			
1	C	478	Total	C	N	O	S	0	0	0
			3795	2413	647	710	25			
1	I	478	Total	C	N	O	S	0	0	0
			3795	2413	647	710	25			
1	K	478	Total	C	N	O	S	0	0	0
			3795	2413	647	710	25			

- 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
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called Nitrogenase Iron Protein 1.

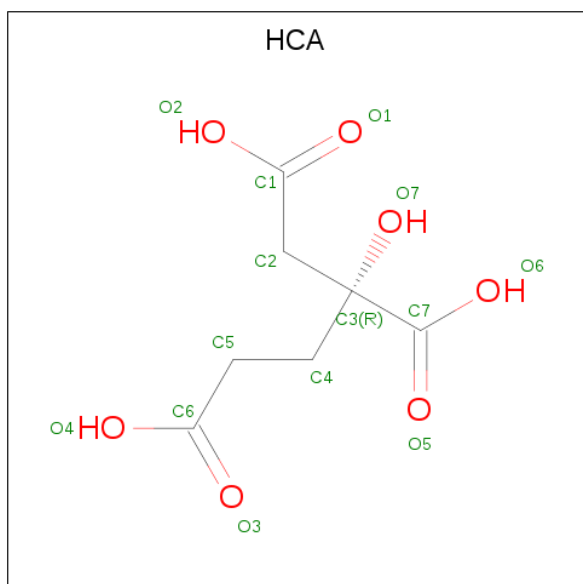
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	F	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	G	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	H	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			

Continued on next page...

Continued from previous page...

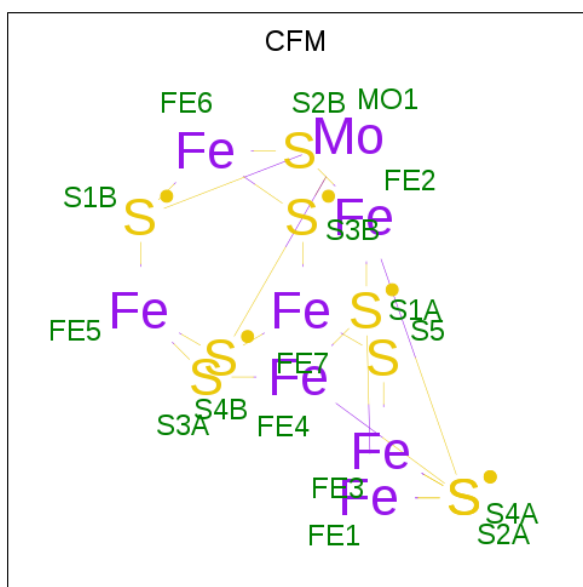
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	N	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	O	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			
3	P	274	Total	C	N	O	S	0	0	0
			2073	1296	353	403	21			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: 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		
4	I	1	Total	C	O	0	0
			14	7	7		
4	K	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (three-letter code: CFM) (formula: Fe_7MoS_9).

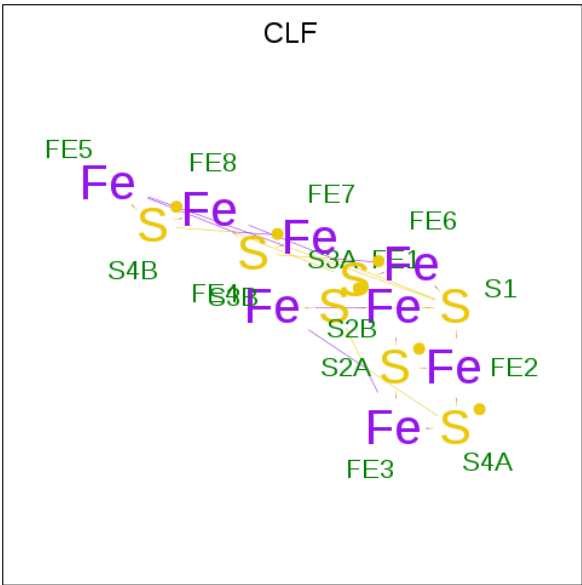


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	I	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	K	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	Ca	0	0
			1	1		
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	J	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe₈S₇).

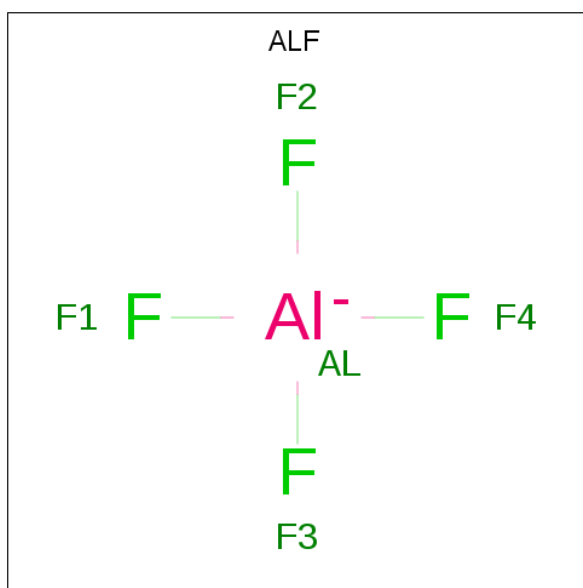


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			15	8	7		
7	D	1	Total	Fe	S	0	0
			15	8	7		
7	J	1	Total	Fe	S	0	0
			15	8	7		
7	L	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

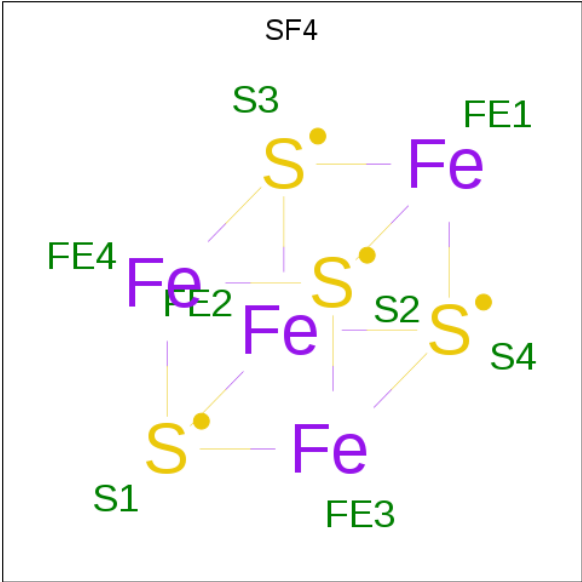
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Mg	0	0
			1	1		
8	G	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		
8	N	1	Total	Mg	0	0
			1	1		
8	O	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		
8	M	1	Total	Mg	0	0
			1	1		

- Molecule 9 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



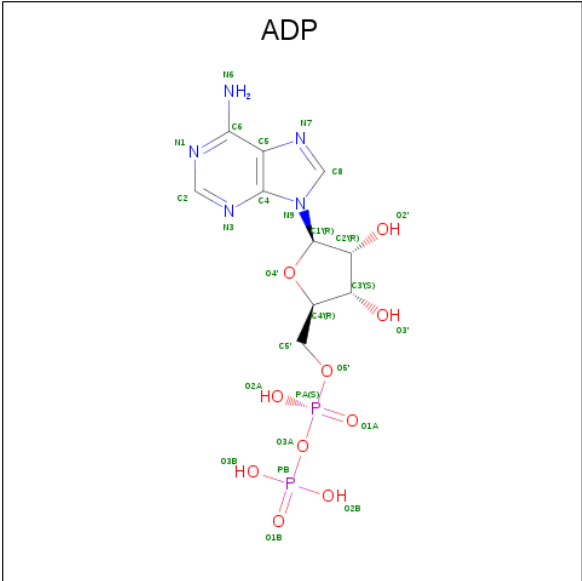
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	Al	F	0	0
			5	1	4		
9	F	1	Total	Al	F	0	0
			5	1	4		
9	G	1	Total	Al	F	0	0
			5	1	4		
9	H	1	Total	Al	F	0	0
			5	1	4		
9	M	1	Total	Al	F	0	0
			5	1	4		
9	N	1	Total	Al	F	0	0
			5	1	4		
9	O	1	Total	Al	F	0	0
			5	1	4		
9	P	1	Total	Al	F	0	0
			5	1	4		

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	Fe	S	0	0
			8	4	4		
10	G	1	Total	Fe	S	0	0
			8	4	4		
10	M	1	Total	Fe	S	0	0
			8	4	4		
10	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
11	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	128	Total	O	0	0
			128	128		
12	B	178	Total	O	0	0
			178	178		
12	C	151	Total	O	0	0
			151	151		
12	D	171	Total	O	0	0
			171	171		
12	E	41	Total	O	0	0
			41	41		
12	F	39	Total	O	0	0
			39	39		
12	G	56	Total	O	0	0
			56	56		
12	H	26	Total	O	0	0
			26	26		
12	I	190	Total	O	0	0
			190	190		
12	J	207	Total	O	0	0
			207	207		
12	K	109	Total	O	0	0
			109	109		
12	L	170	Total	O	0	0
			170	170		

Continued on next page...

Continued from previous page...

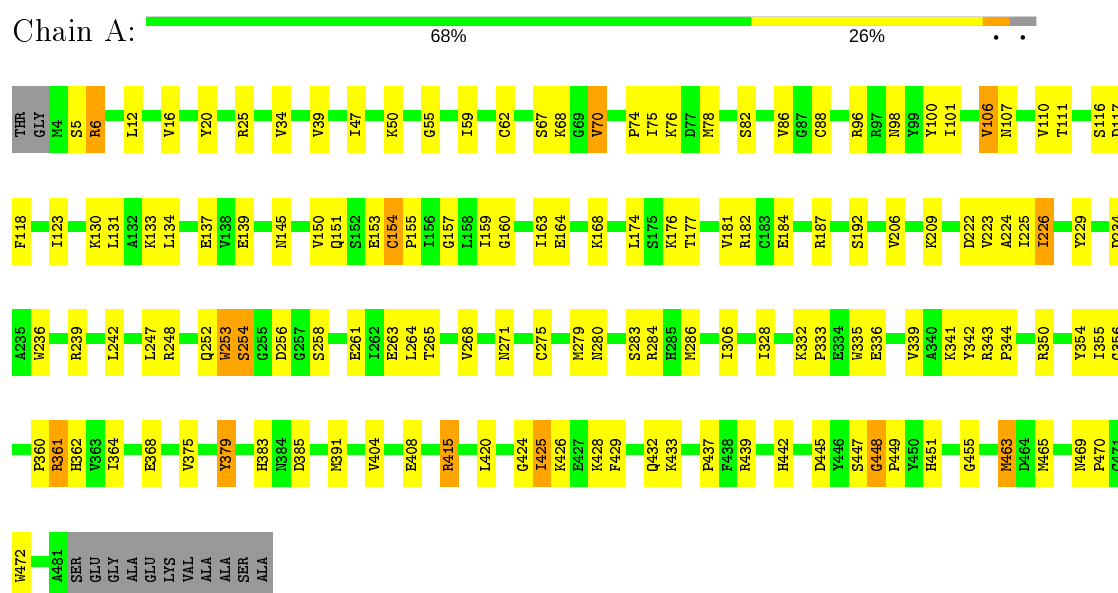
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	62	Total 62	O 62	0	0
12	N	41	Total 41	O 41	0	0
12	O	30	Total 30	O 30	0	0
12	P	25	Total 25	O 25	0	0

3 Residue-property plots

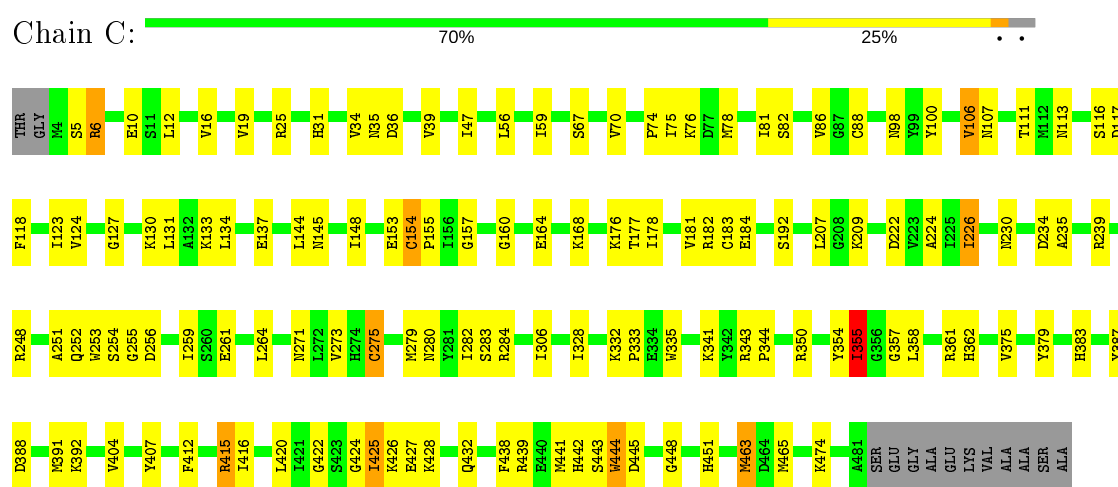
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

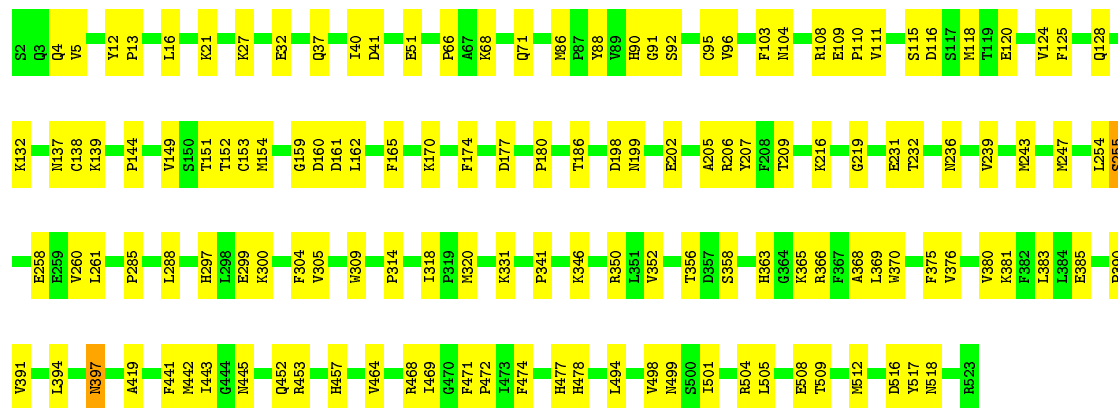


• Molecule 1: Nitrogenase Molybdenum-Iron Protein alpha chain



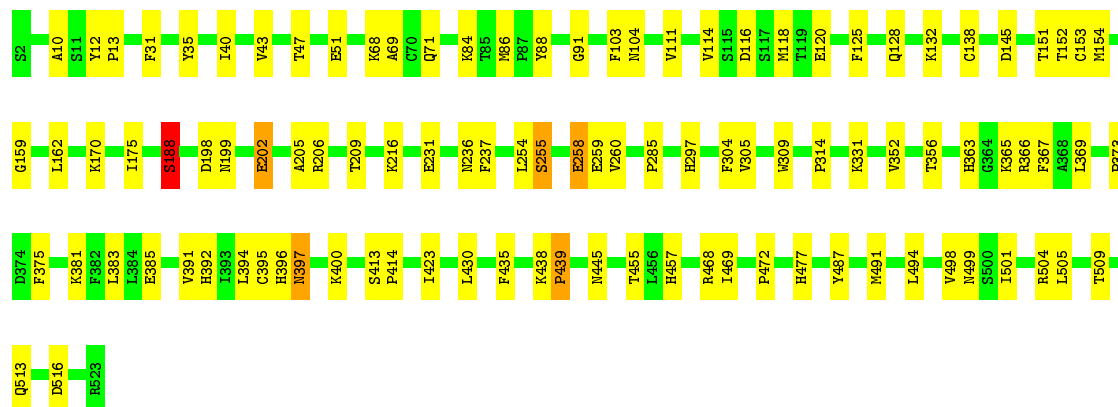
• Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain D: 74% 26%



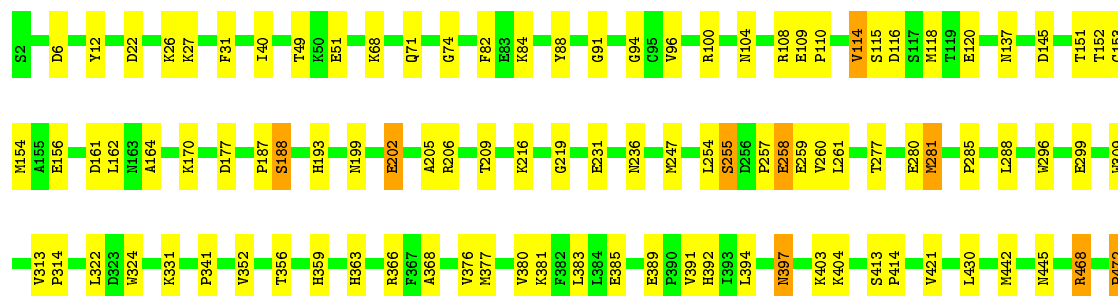
• Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain J: 80% 19%



• Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

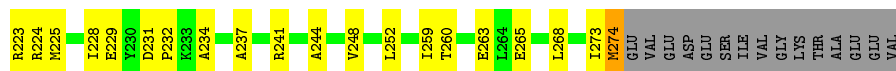
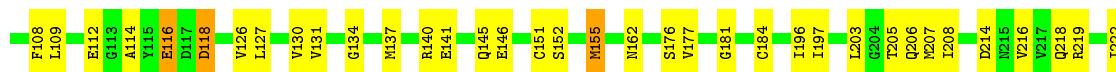
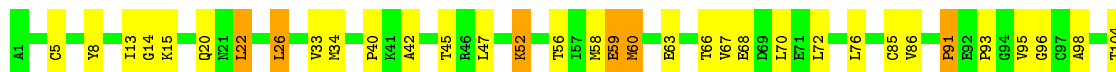
Chain L: 79% 20%





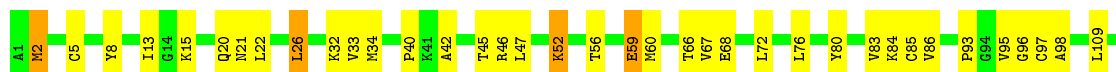
• Molecule 3: Nitrogenase Iron Protein 1

Chain E: 64% 28% 5%



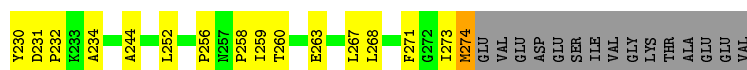
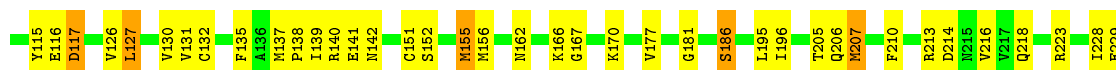
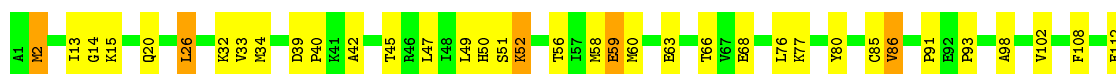
• Molecule 3: Nitrogenase Iron Protein 1

Chain F: 63% 29% 5%



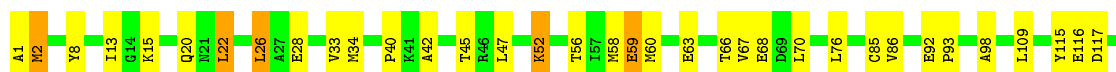
• Molecule 3: Nitrogenase Iron Protein 1

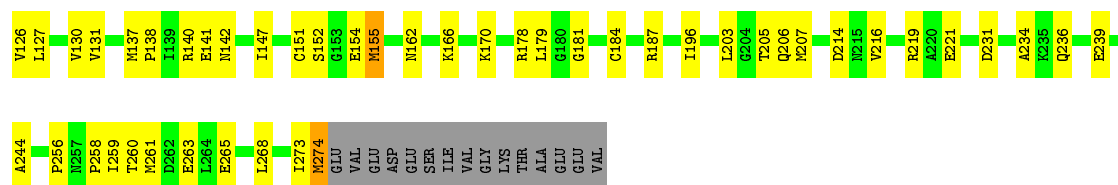
Chain G: 63% 28% 5%



• Molecule 3: Nitrogenase Iron Protein 1

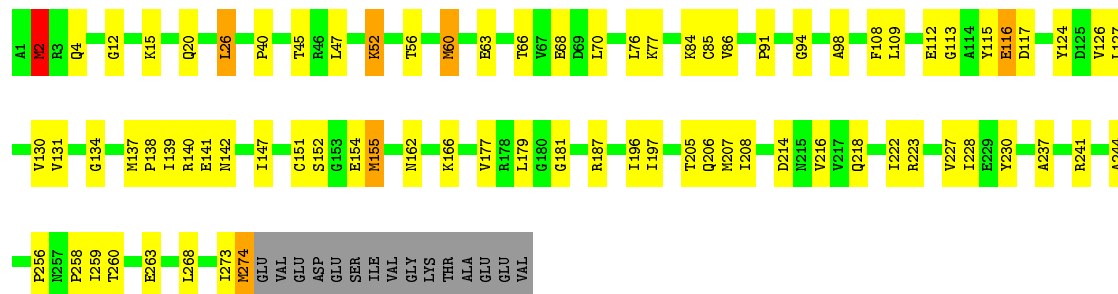
Chain H: 67% 26% 5%





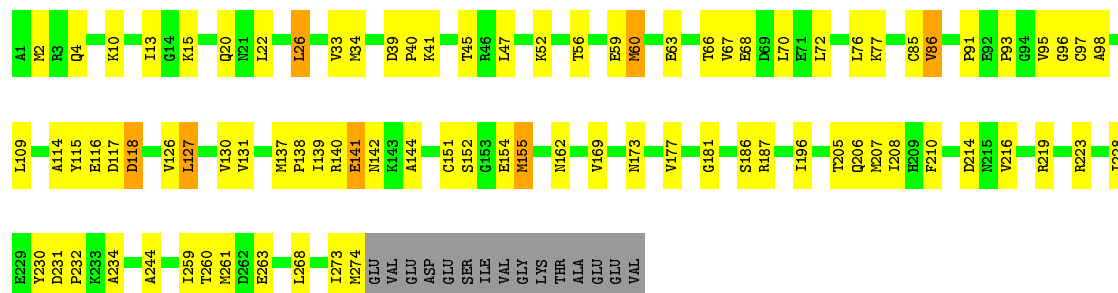
• Molecule 3: Nitrogenase Iron Protein 1

Chain M: 67% 25% 5%



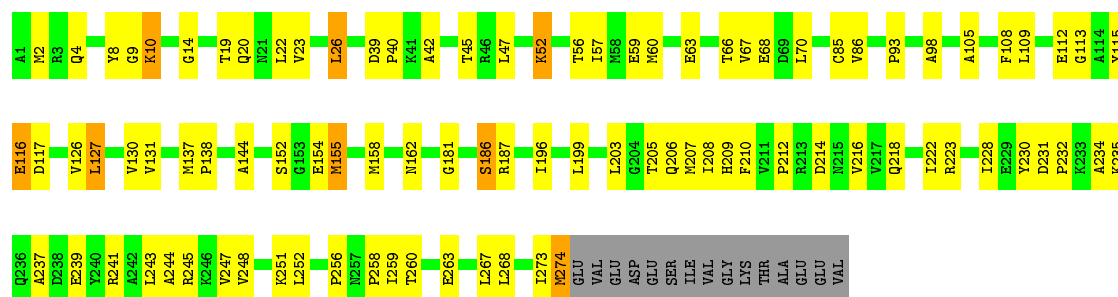
• Molecule 3: Nitrogenase Iron Protein 1

Chain N: 65% 27% 5%



• Molecule 3: Nitrogenase Iron Protein 1

Chain O: 63% 29% 5%



• Molecule 3: Nitrogenase Iron Protein 1

Chain P: 65% 28% 5%

A1	M2	Y8	K15	Q20	R21	L22	L26	M29	V33	M34	G37	C38	D39	P40	T45	R46	L47	K52	T56	I57	M58	E59	M60	T66	V67	E68	L72	L76	K84	C85	V86	E87	P93	G94	V95	G96	C97	A98	T104	A105	F108	L109
E112	G113	A114	Y115	E116	D117	D118	L127	V130	V131	M137	P138	E141	M142	I149	M155	N162	K170	L179	G180	G181	C184	I196	T205	Q206	M207	R213	D214	N215	V216	V217	Q218	R219	I222	R223	I228	E229	Y230	D231	P232	K233	A234	A244
R245	V248	P256	R257	P258	I259	T260	E263	L267	L268	I273	M274	GLU	VAL	GLU	ASP	GLU	GLU	SER	ILE	VAL	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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	326.10 Å 75.80 Å 312.20 Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	50568	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: MG, CFM, ADP, ALF, CLF, HCA, CA, SF4

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	0.47	2/3883 (0.1%)	0.72	6/5236 (0.1%)
1	C	0.41	1/3883 (0.0%)	0.68	4/5236 (0.1%)
1	I	0.40	0/3883	0.69	0/5236
1	K	0.41	0/3883	0.66	0/5236
2	B	0.53	3/4280 (0.1%)	0.66	2/5786 (0.0%)
2	D	0.42	1/4280 (0.0%)	0.66	1/5786 (0.0%)
2	J	0.51	2/4280 (0.0%)	0.66	2/5786 (0.0%)
2	L	0.42	1/4280 (0.0%)	0.64	1/5786 (0.0%)
3	E	0.37	0/2097	0.64	0/2824
3	F	0.34	0/2097	0.61	0/2824
3	G	0.35	0/2097	0.61	0/2824
3	H	0.33	0/2097	0.62	1/2824 (0.0%)
3	M	0.34	0/2097	0.59	0/2824
3	N	0.36	0/2097	0.63	0/2824
3	O	0.32	0/2097	0.59	0/2824
3	P	0.32	0/2097	0.59	0/2824
All	All	0.42	10/49428 (0.0%)	0.65	17/66680 (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	A	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	439	PRO	N-CD	-18.12	1.22	1.47
2	B	66	PRO	N-CD	-18.07	1.22	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	CYS	CB-SG	-7.10	1.70	1.82
1	A	154	CYS	CB-SG	-6.75	1.70	1.82
2	J	188	SER	CB-OG	6.52	1.50	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	95	CYS	CA-CB-SG	-10.50	95.10	114.00
2	J	188	SER	CA-CB-OG	9.37	136.50	111.20
2	L	188	SER	CA-CB-OG	8.06	132.97	111.20
2	B	95	CYS	CA-CB-SG	-7.95	99.69	114.00
1	A	253	TRP	C-N-CA	6.28	137.40	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	TYR	Sidechain

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	3795	0	3734	115	0
1	C	3795	0	3734	106	0
1	I	3795	0	3734	127	0
1	K	3795	0	3734	125	0
2	B	4174	0	4088	100	0
2	D	4174	0	4088	113	0
2	J	4174	0	4087	86	0
2	L	4174	0	4087	93	0
3	E	2073	0	2092	81	0
3	F	2073	0	2089	74	0
3	G	2073	0	2092	85	0
3	H	2073	0	2092	80	1
3	M	2073	0	2091	72	0
3	N	2073	0	2091	71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2073	0	2091	84	1
3	P	2073	0	2092	73	0
4	A	14	0	7	0	0
4	C	14	0	7	0	0
4	I	14	0	7	0	0
4	K	14	0	7	0	0
5	A	17	0	0	1	0
5	C	17	0	0	0	0
5	I	17	0	0	1	0
5	K	17	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	B	15	0	0	0	0
7	D	15	0	0	0	0
7	J	15	0	0	1	0
7	L	15	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
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	E	5	0	0	0	0
9	F	5	0	0	0	0
9	G	5	0	0	0	0
9	H	5	0	0	0	0
9	M	5	0	0	0	0
9	N	5	0	0	0	0
9	O	5	0	0	0	0
9	P	5	0	0	0	0
10	E	8	0	0	0	0
10	G	8	0	0	0	0
10	M	8	0	0	0	0
10	O	8	0	0	0	0
11	E	27	0	12	2	0
11	F	27	0	12	0	0
11	G	27	0	12	2	0
11	H	27	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	27	0	12	1	0
11	N	27	0	12	0	0
11	O	27	0	12	2	0
11	P	27	0	12	1	0
12	A	128	0	0	1	0
12	B	178	0	0	1	0
12	C	151	0	0	1	0
12	D	171	0	0	1	0
12	E	41	0	0	0	0
12	F	39	0	0	0	0
12	G	56	0	0	0	0
12	H	26	0	0	0	0
12	I	190	0	0	1	0
12	J	207	0	0	0	0
12	K	109	0	0	2	0
12	L	170	0	0	0	0
12	M	62	0	0	0	0
12	N	41	0	0	0	0
12	O	30	0	0	0	0
12	P	25	0	0	0	0
All	All	50568	0	48140	1356	1

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 14.

The worst 5 of 1356 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:I:31:HIS:CE1	1:I:47:ILE:CD1	2.29	1.14
2:D:209:THR:HG21	2:D:309:TRP:HE1	1.09	1.14
1:I:31:HIS:CE1	1:I:47:ILE:HD13	1.85	1.12
1:I:47:ILE:HD12	1:I:47:ILE:O	1.51	1.09
3:M:130:VAL:HG23	3:N:93:PRO:HB3	1.34	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:GLU:OE2	3:O:251:LYS:CD[3_546]	2.17	0.03

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	476/491 (97%)	450 (94%)	24 (5%)	2 (0%)	34	42
1	C	476/491 (97%)	448 (94%)	25 (5%)	3 (1%)	25	31
1	I	476/491 (97%)	450 (94%)	24 (5%)	2 (0%)	34	42
1	K	476/491 (97%)	447 (94%)	25 (5%)	4 (1%)	19	23
2	B	520/522 (100%)	500 (96%)	19 (4%)	1 (0%)	47	58
2	D	520/522 (100%)	503 (97%)	16 (3%)	1 (0%)	47	58
2	J	520/522 (100%)	499 (96%)	19 (4%)	2 (0%)	34	42
2	L	520/522 (100%)	496 (95%)	23 (4%)	1 (0%)	47	58
3	E	272/289 (94%)	254 (93%)	18 (7%)	0	100	100
3	F	272/289 (94%)	256 (94%)	14 (5%)	2 (1%)	22	26
3	G	272/289 (94%)	256 (94%)	13 (5%)	3 (1%)	14	15
3	H	272/289 (94%)	251 (92%)	20 (7%)	1 (0%)	34	42
3	M	272/289 (94%)	258 (95%)	12 (4%)	2 (1%)	22	26
3	N	272/289 (94%)	258 (95%)	12 (4%)	2 (1%)	22	26
3	O	272/289 (94%)	254 (93%)	14 (5%)	4 (2%)	10	10
3	P	272/289 (94%)	253 (93%)	18 (7%)	1 (0%)	34	42
All	All	6160/6364 (97%)	5833 (95%)	296 (5%)	31 (0%)	29	35

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	116	GLU
3	O	116	GLU
1	A	5	SER
1	A	448	GLY
1	C	5	SER

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	407/414 (98%)	392 (96%)	15 (4%)	34	48
1	C	407/414 (98%)	390 (96%)	17 (4%)	30	42
1	I	407/414 (98%)	389 (96%)	18 (4%)	28	39
1	K	407/414 (98%)	390 (96%)	17 (4%)	30	42
2	B	454/454 (100%)	439 (97%)	15 (3%)	38	53
2	D	454/454 (100%)	445 (98%)	9 (2%)	55	72
2	J	454/454 (100%)	444 (98%)	10 (2%)	52	69
2	L	454/454 (100%)	439 (97%)	15 (3%)	38	53
3	E	220/233 (94%)	207 (94%)	13 (6%)	19	27
3	F	220/233 (94%)	212 (96%)	8 (4%)	35	49
3	G	220/233 (94%)	209 (95%)	11 (5%)	24	34
3	H	220/233 (94%)	212 (96%)	8 (4%)	35	49
3	M	220/233 (94%)	213 (97%)	7 (3%)	39	54
3	N	220/233 (94%)	208 (94%)	12 (6%)	21	30
3	O	220/233 (94%)	214 (97%)	6 (3%)	44	61
3	P	220/233 (94%)	211 (96%)	9 (4%)	30	43
All	All	5204/5336 (98%)	5014 (96%)	190 (4%)	34	48

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	155	MET
1	I	264	LEU
3	O	26	LEU
3	H	2	MET
1	I	6	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	215	ASN
1	I	383	HIS
3	O	162	ASN
3	H	4	GLN
3	H	206	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 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	$\# Z > 2$
11	ADP	E	3091	8	24,29,29	1.28	3 (12%)	29,45,45	1.33	4 (13%)
7	CLF	L	4298	1,2	0,24,24	0.00	-	-		
11	ADP	N	5191	8	24,29,29	1.30	2 (8%)	29,45,45	1.32	4 (13%)
7	CLF	D	2298	1,2	0,24,24	0.00	-	-		
11	ADP	O	5291	8	24,29,29	1.34	3 (12%)	29,45,45	1.32	5 (17%)
9	ALF	H	3393	-	0,4,4	0.00	-	-		
9	ALF	N	5193	-	0,4,4	0.00	-	-		
5	CFM	I	4096	1	0,24,24	0.00	-	-		
9	ALF	G	3293	-	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HCA	A	2094	-	4,13,13	2.75	2 (50%)	4,18,18	7.49	3 (75%)
9	ALF	E	3093	-	0,4,4	0.00	-	-	-	-
9	ALF	O	5293	-	0,4,4	0.00	-	-	-	-
5	CFM	K	4296	1	0,24,24	0.00	-	-	-	-
9	ALF	F	3193	-	0,4,4	0.00	-	-	-	-
4	HCA	I	4094	-	4,13,13	2.76	2 (50%)	4,18,18	7.48	3 (75%)
5	CFM	A	2096	1	0,24,24	0.00	-	-	-	-
11	ADP	F	3191	8	24,29,29	1.39	4 (16%)	29,45,45	1.17	2 (6%)
7	CLF	J	4098	1,2	0,24,24	0.00	-	-	-	-
5	CFM	C	2296	1	0,24,24	0.00	-	-	-	-
7	CLF	B	2098	1,2	0,24,24	0.00	-	-	-	-
4	HCA	C	2294	-	4,13,13	1.32	0	4,18,18	1.84	1 (25%)
11	ADP	G	3291	8	24,29,29	1.34	3 (12%)	29,45,45	1.34	3 (10%)
9	ALF	P	5393	-	0,4,4	0.00	-	-	-	-
11	ADP	M	5091	8	24,29,29	1.25	3 (12%)	29,45,45	1.30	2 (6%)
10	SF4	E	3090	3	0,12,12	0.00	-	-	-	-
10	SF4	O	5290	3	0,12,12	0.00	-	-	-	-
11	ADP	P	5391	8	24,29,29	1.31	3 (12%)	29,45,45	1.29	2 (6%)
9	ALF	M	5093	-	0,4,4	0.00	-	-	-	-
4	HCA	K	4294	-	4,13,13	2.09	1 (25%)	4,18,18	5.58	2 (50%)
11	ADP	H	3391	8	24,29,29	1.41	4 (16%)	29,45,45	1.28	1 (3%)
10	SF4	G	3290	3	0,12,12	0.00	-	-	-	-
10	SF4	M	5090	3	0,12,12	0.00	-	-	-	-

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
11	ADP	E	3091	8	-	0/12/32/32	0/3/3/3
7	CLF	L	4298	1,2	-	-	0/12/10/10
11	ADP	F	3191	8	-	4/12/32/32	0/3/3/3
11	ADP	P	5391	8	-	0/12/32/32	0/3/3/3
10	SF4	E	3090	3	-	-	0/6/5/5
7	CLF	D	2298	1,2	-	-	0/12/10/10
7	CLF	J	4098	1,2	-	-	0/12/10/10
4	HCA	K	4294	-	-	6/7/17/17	-
11	ADP	O	5291	8	-	0/12/32/32	0/3/3/3
7	CLF	B	2098	1,2	-	-	0/12/10/10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	M	5091	8	-	5/12/32/32	0/3/3/3
4	HCA	A	2094	-	1/1/4/4	6/7/17/17	-
10	SF4	O	5290	3	-	-	0/6/5/5
4	HCA	C	2294	-	-	5/7/17/17	-
11	ADP	G	3291	8	-	3/12/32/32	0/3/3/3
10	SF4	M	5090	3	-	-	0/6/5/5
11	ADP	H	3391	8	-	0/12/32/32	0/3/3/3
10	SF4	G	3290	3	-	-	0/6/5/5
11	ADP	N	5191	8	-	0/12/32/32	0/3/3/3
4	HCA	I	4094	-	1/1/4/4	6/7/17/17	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	4094	HCA	C2-C3	4.34	1.61	1.54
4	A	2094	HCA	C2-C3	4.30	1.61	1.54
4	K	4294	HCA	O7-C3	3.89	1.49	1.43
11	H	3391	ADP	C8-N7	-3.49	1.28	1.34
11	E	3091	ADP	C8-N7	-3.11	1.29	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2094	HCA	O7-C3-C4	-10.10	82.41	107.15
4	I	4094	HCA	O7-C3-C4	-10.10	82.41	107.15
4	A	2094	HCA	C3-C2-C1	9.80	130.67	114.98
4	I	4094	HCA	C3-C2-C1	9.78	130.64	114.98
4	K	4294	HCA	O7-C3-C4	-9.71	83.34	107.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2094	HCA	C3
4	I	4094	HCA	C3

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2094	HCA	C1-C2-C3-C7
4	A	2094	HCA	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2094	HCA	C7-C3-C4-C5
4	A	2094	HCA	O7-C3-C4-C5
4	I	4094	HCA	C1-C2-C3-C7

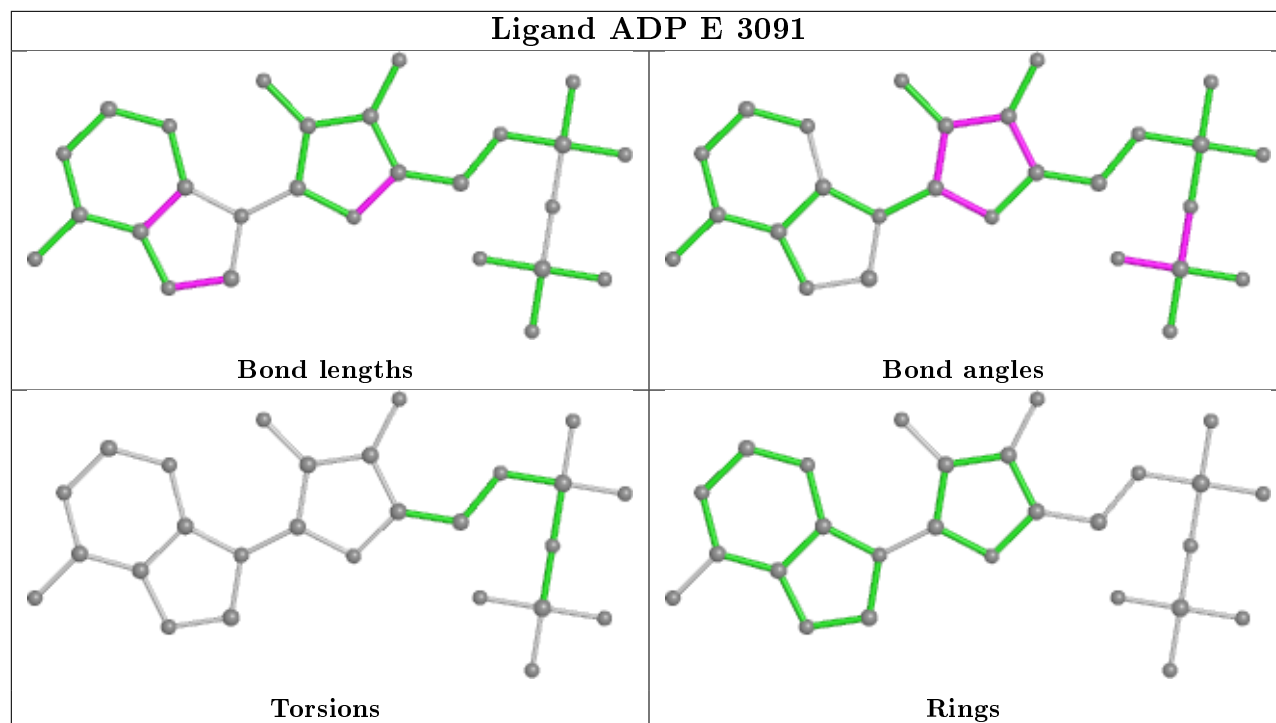
There are no ring outliers.

9 monomers are involved in 13 short contacts:

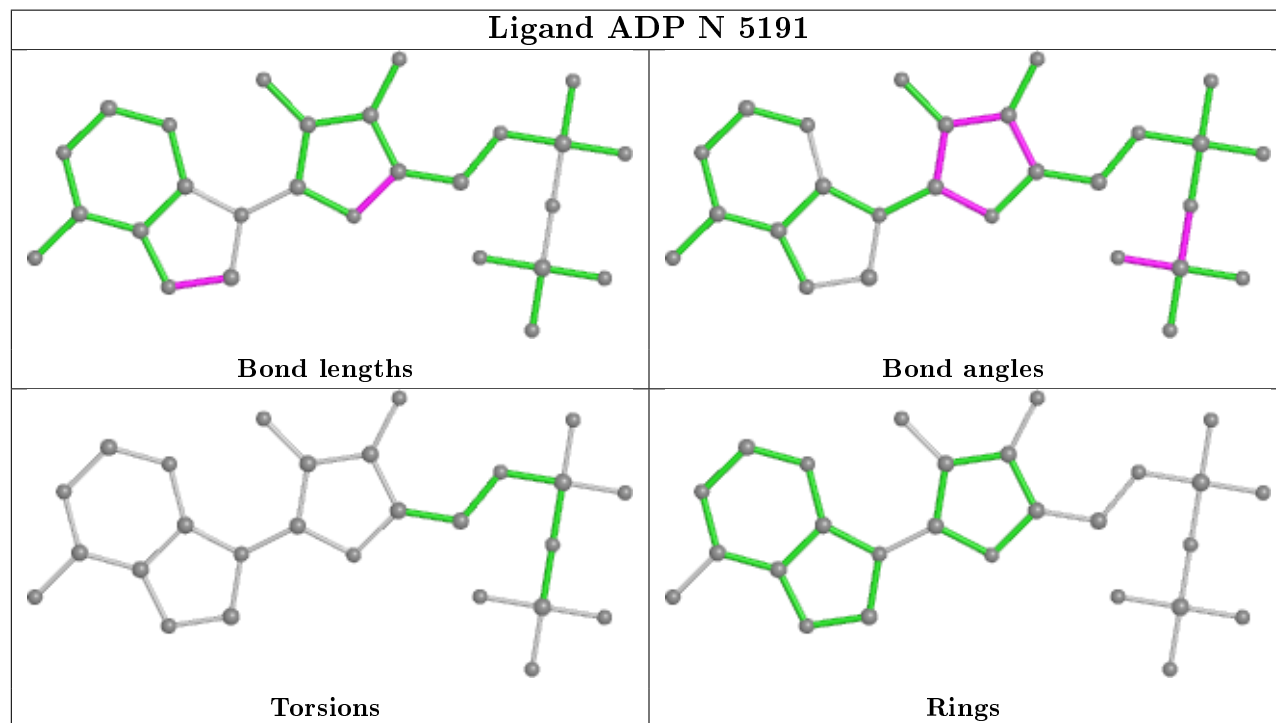
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	3091	ADP	2	0
11	O	5291	ADP	2	0
5	I	4096	CFM	1	0
5	A	2096	CFM	1	0
7	J	4098	CLF	1	0
11	G	3291	ADP	2	0
11	M	5091	ADP	1	0
11	P	5391	ADP	1	0
11	H	3391	ADP	2	0

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.

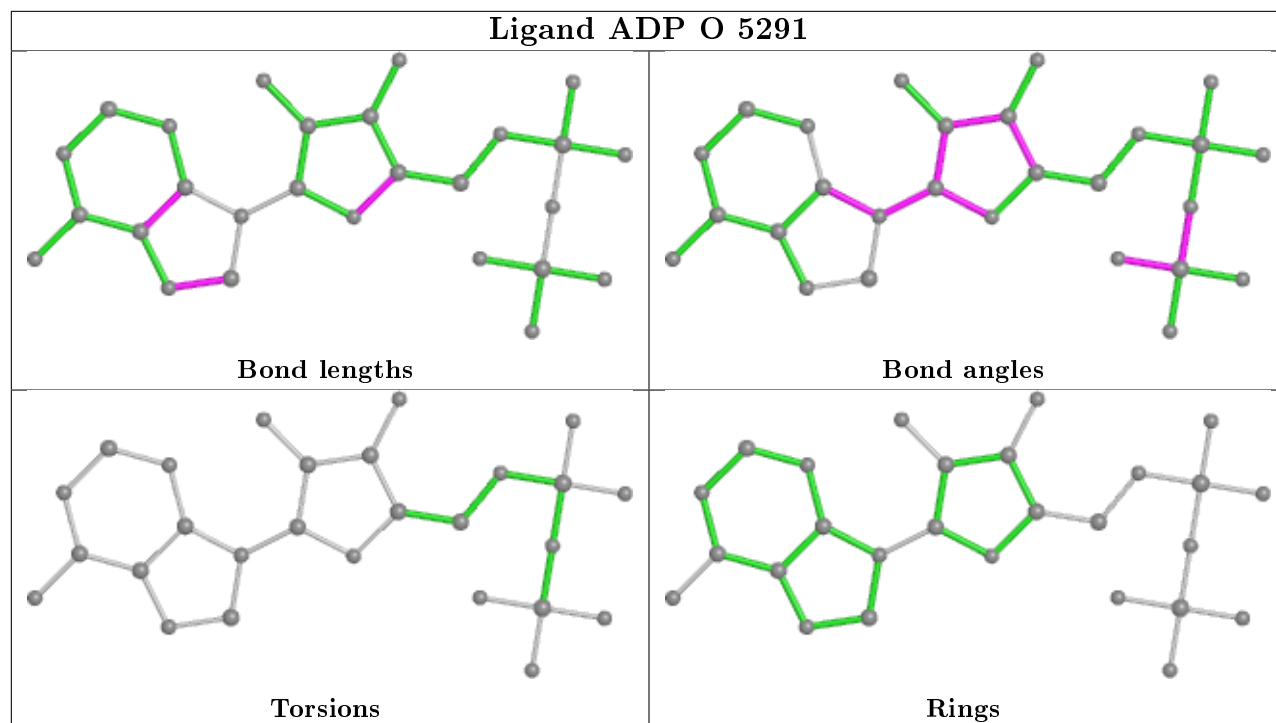
Ligand ADP E 3091



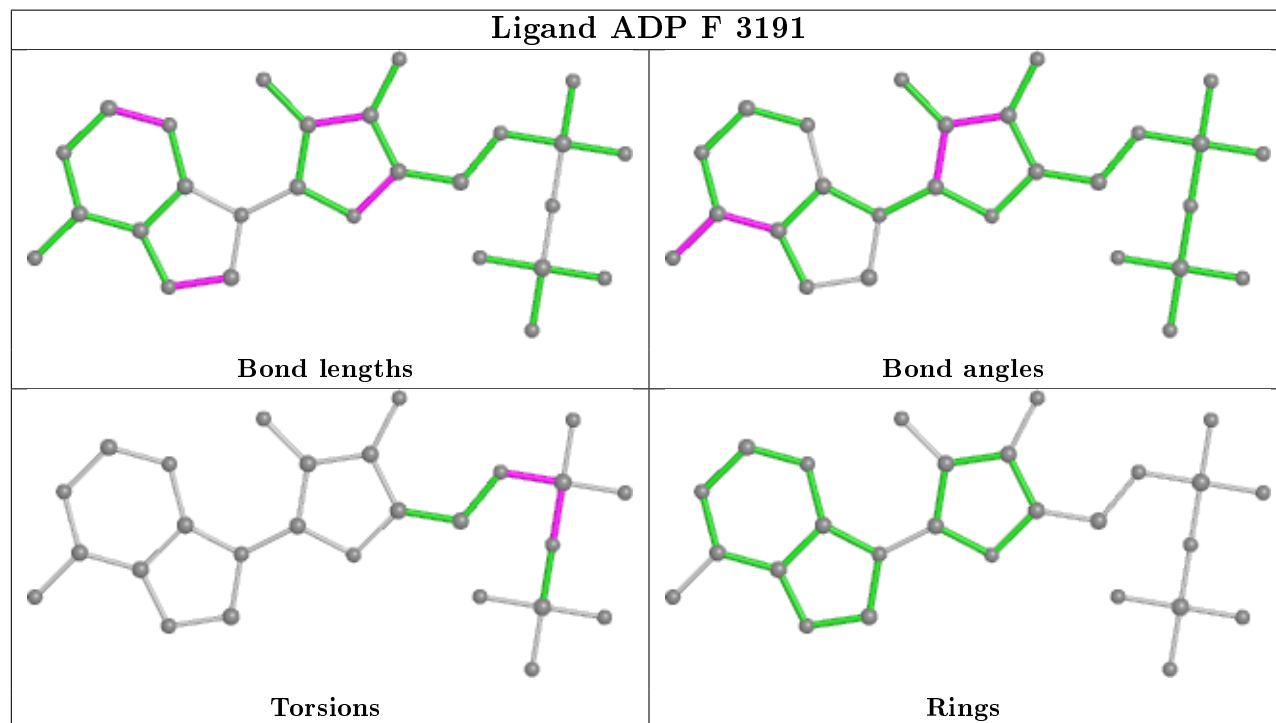
Ligand ADP N 5191



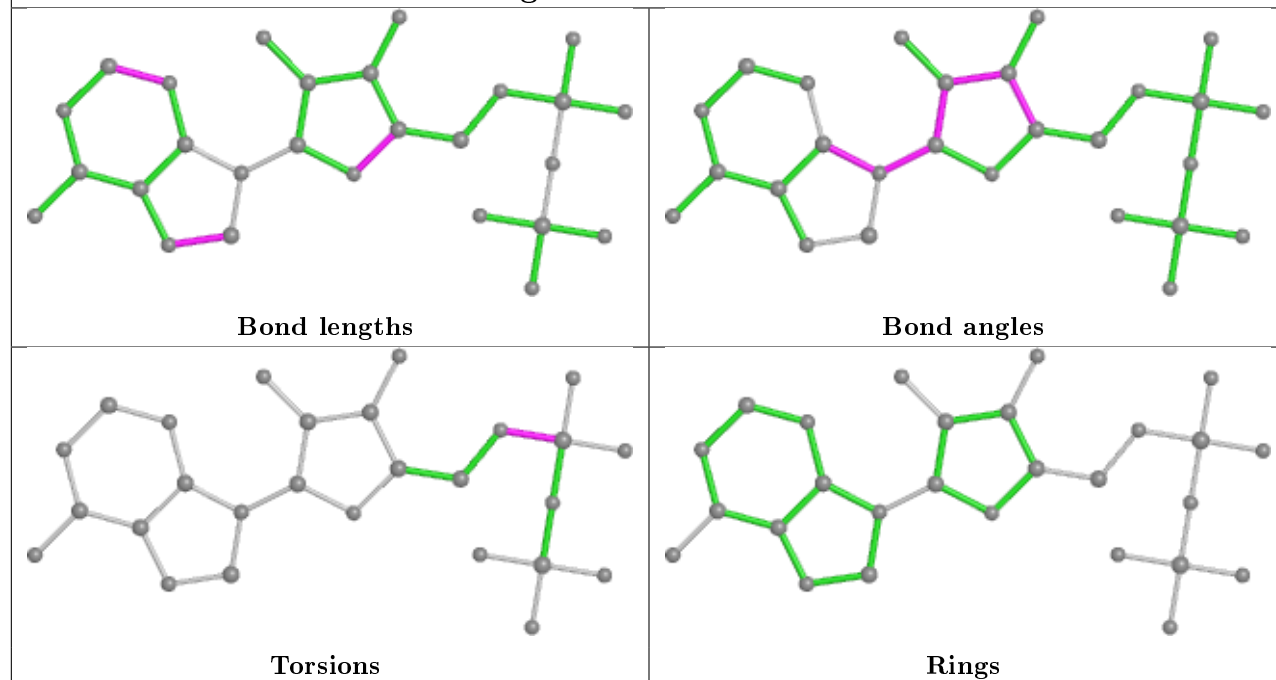
Ligand ADP O 5291



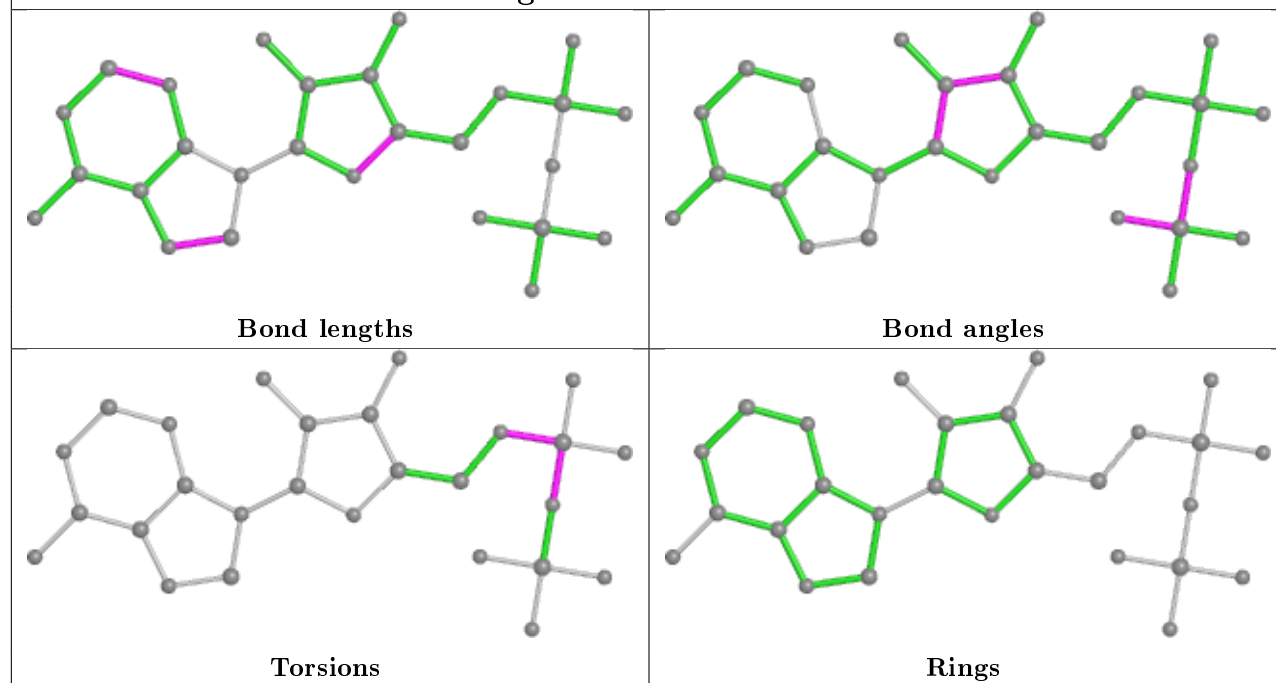
Ligand ADP F 3191

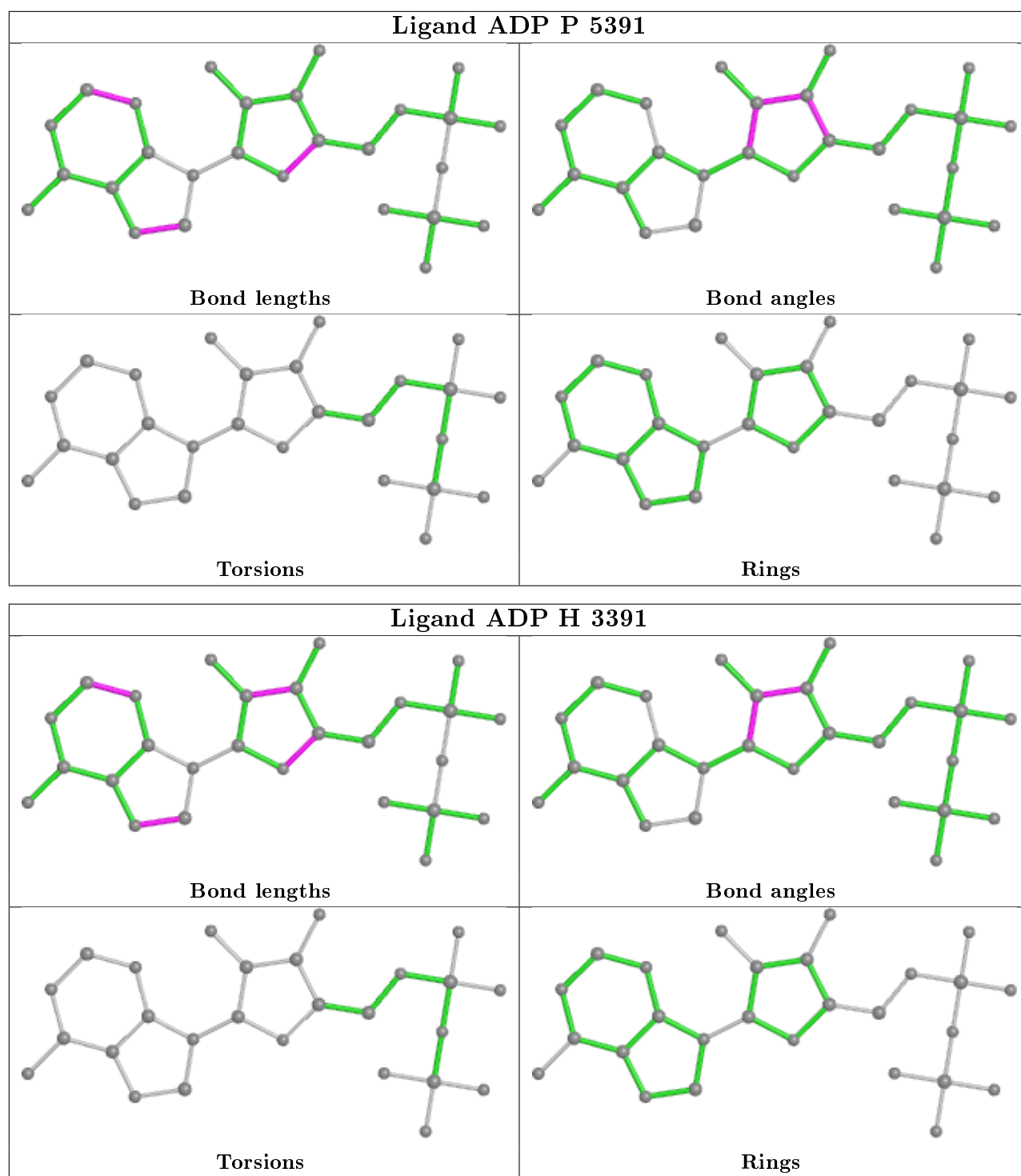


Ligand ADP G 3291



Ligand ADP M 5091





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 ⓘ

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.