wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 08:27 AM EDT

PDB ID	:	1M34 / pdb_00001m34
Title	:	Nitrogenase Complex From Azotobacter Vinelandii Stabilized By ADP-Tetra fluoroaluminate
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 (i) 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 (1)) were used in the production of this report:

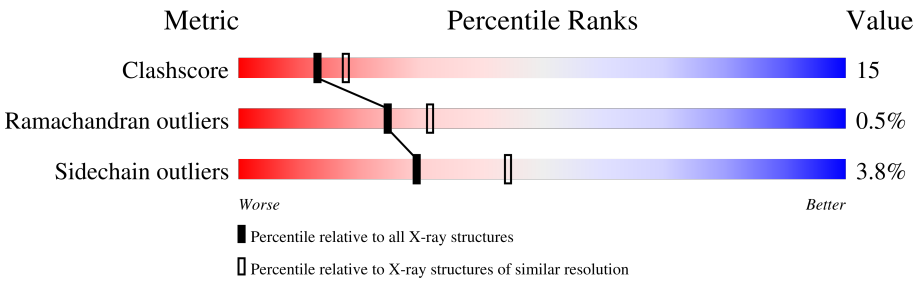
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	491	65% 29% • •
1	C	491	66% 28% • •
1	I	491	63% 30% • •
1	K	491	64% 30% • •
2	B	522	74% 23% •
2	D	522	69% 30% •
2	J	522	76% 22% •
2	L	522	75% 22% •

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Mol	Chain	Length	Quality of chain
3	E	289	61% 30% • 5%
3	F	289	60% 32% • 5%
3	G	289	61% 31% • 5%
3	H	289	63% 29% • 5%
3	M	289	66% 27% • 5%
3	N	289	62% 29% • 5%
3	O	289	62% 30% • 5%
3	P	289	62% 30% • 5%

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	X	-	-
4	HCA	C	2294	-	X	-	-
4	HCA	I	4094	X	X	-	-
4	HCA	K	4294	-	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
			Total	C	N	O	S			
1	A	478	3795	2413	647	710	25	0	0	0
1	C	478	3795	2413	647	710	25	0	0	0
1	I	478	3795	2413	647	710	25	0	0	0
1	K	478	3795	2413	647	710	25	0	0	0

- Molecule 2 is a protein called Nitrogenase Molybdenum-Iron Protein beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4174	2666	705	775	28	0	0	0
2	D	522	4174	2666	705	775	28	0	0	0
2	J	522	4174	2666	705	775	28	0	0	0
2	L	522	4174	2666	705	775	28	0	0	0

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

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

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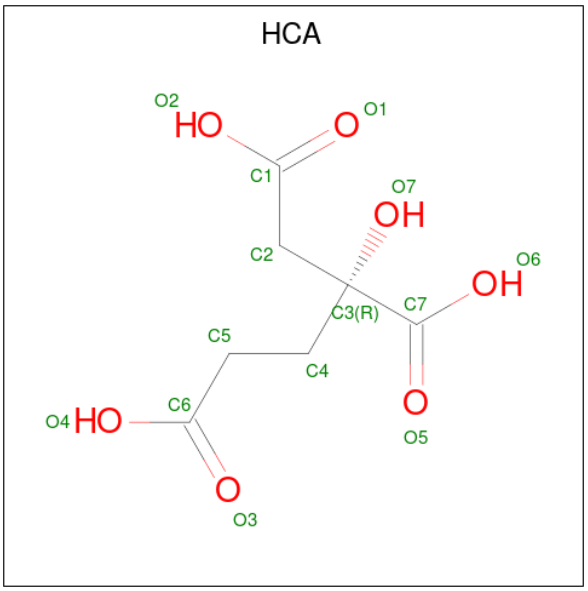
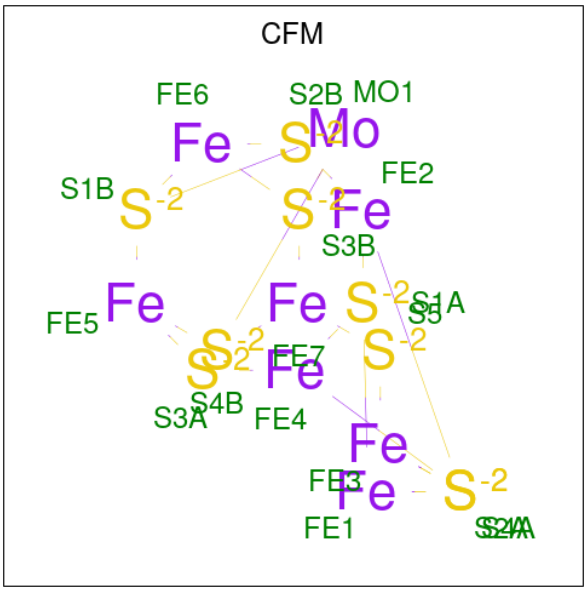
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	274	2073	1296	353	403	21	0	0	0
3	N	274	2073	1296	353	403	21	0	0	0
3	O	274	2073	1296	353	403	21	0	0	0
3	P	274	2073	1296	353	403	21	0	0	0

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



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

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

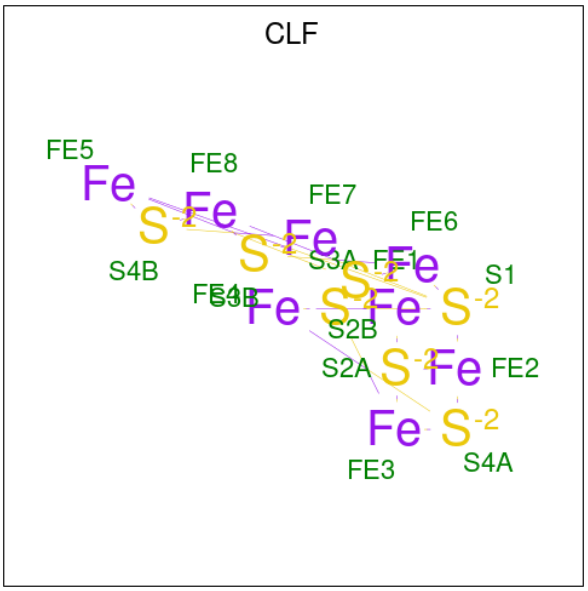


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Mo	S		
5	A	1	17	7	1	9	0	0
5	C	1	17	7	1	9	0	0
5	I	1	17	7	1	9	0	0
5	K	1	17	7	1	9	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 7 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).

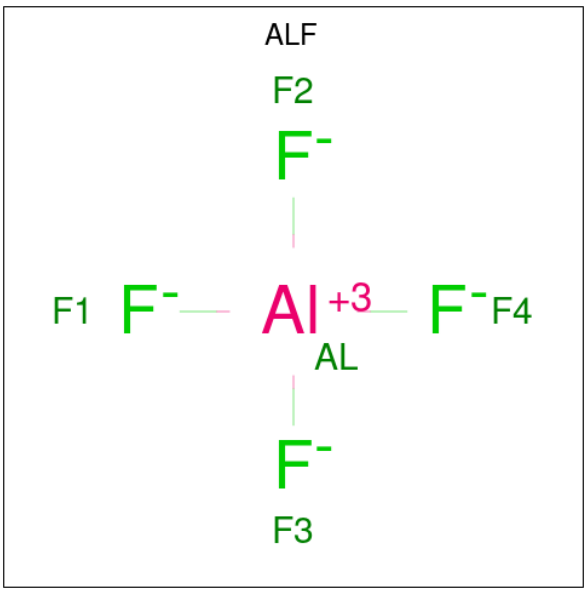


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 15 8 7	0	0
7	D	1	Total Fe S 15 8 7	0	0
7	J	1	Total Fe S 15 8 7	0	0
7	L	1	Total Fe S 15 8 7	0	0

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

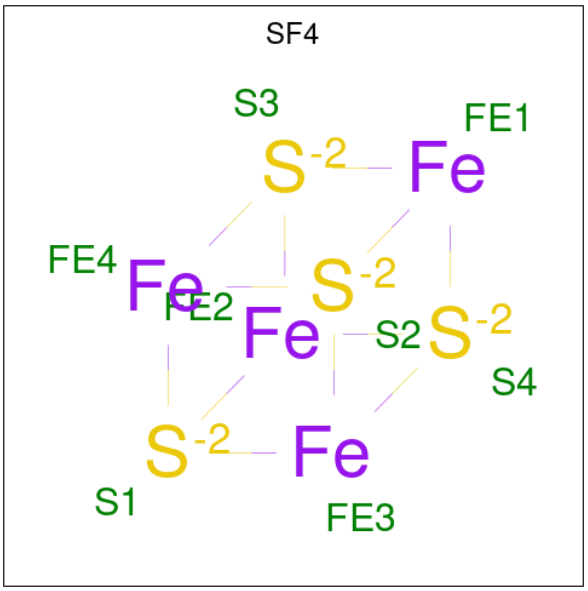
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Mg 1 1	0	0
8	F	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	M	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0
8	O	1	Total Mg 1 1	0	0
8	P	1	Total Mg 1 1	0	0

- Molecule 9 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



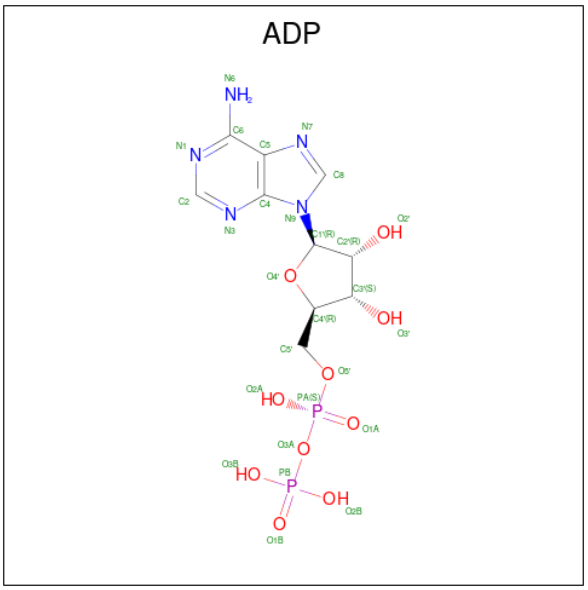
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
9	E	1	5	1	4	0	0
9	F	1	5	1	4	0	0
9	G	1	5	1	4	0	0
9	H	1	5	1	4	0	0
9	M	1	5	1	4	0	0
9	N	1	5	1	4	0	0
9	O	1	5	1	4	0	0
9	P	1	5	1	4	0	0

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



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

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 12 is water.

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

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

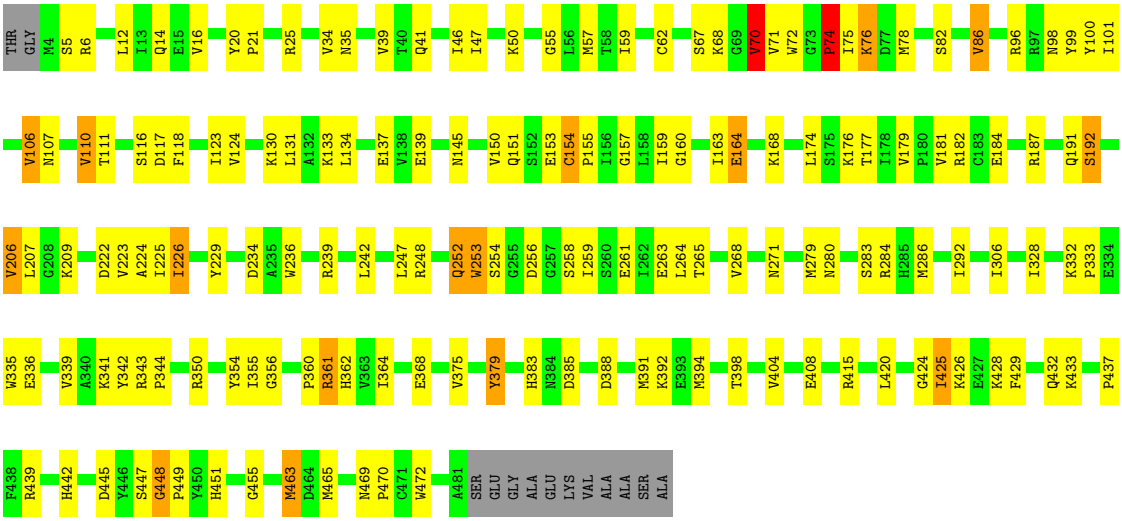
3 Residue-property plots (i)

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.

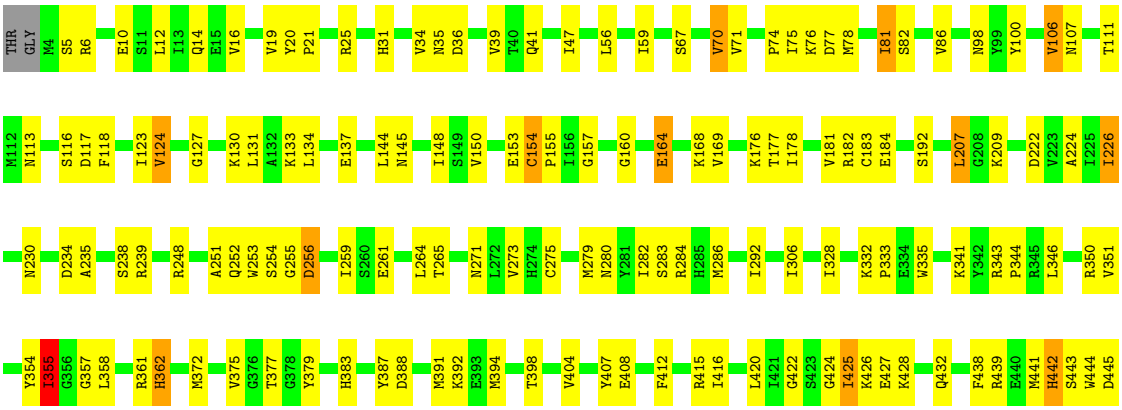
• Molecule 1: Nitrogenase Molybdenum-Iron Protein alpha chain

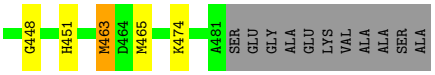
Chain A:



• Molecule 1: Nitrogenase Molybdenum-Iron Protein alpha chain

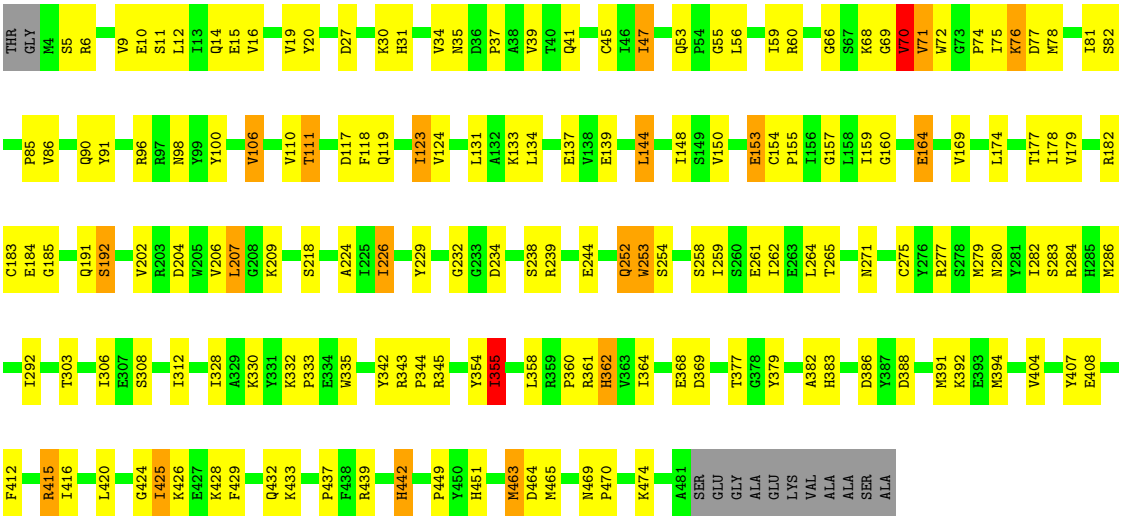
Chain C:





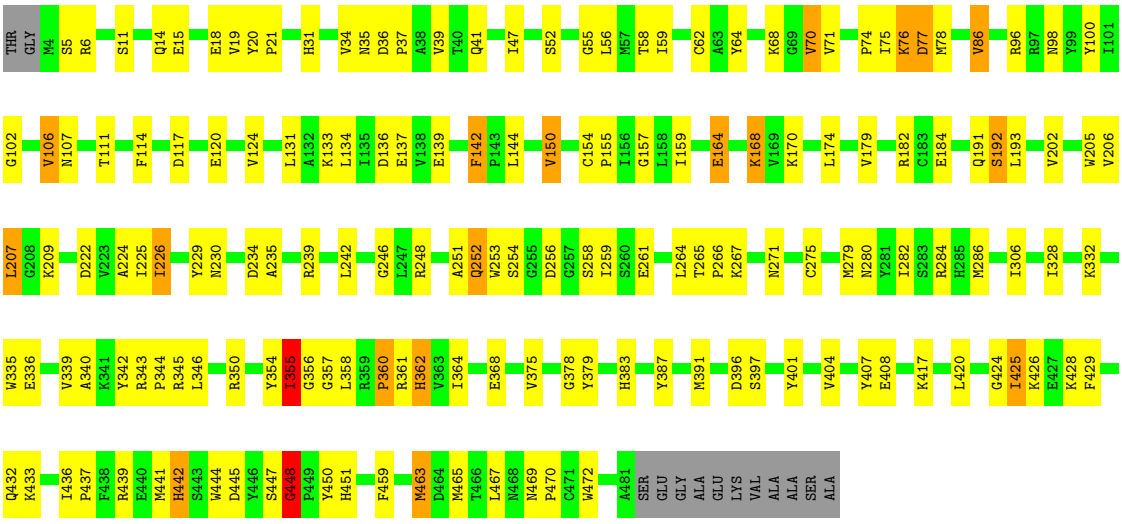
• Molecule 1: Nitrogenase Molybdenum-Iron Protein alpha chain

Chain I:



• Molecule 1: Nitrogenase Molybdenum-Iron Protein alpha chain

Chain K:



• Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain B:

P144 V149 S150 T151 T152 C153 M154 G159 D160 D161 L162 I166 K171 E178 V181 T186 P187 S188 D198 N199 E202 R206 T209 D214 D215 K216 N221 P228 E231 N236 M247 G248 V249 L254 S255 D256 P257 E258 E259 V260 M281

P285 L293 Q294 P295 W296 H297 L298 E299 F304 V305 W309 V313 P314 P319 L322 D323 W324 K331 P341 K346 R350 L351 V352 T356 D357 S358 H359 H363 R366 F367 A368 L369 W370 V376 M377 V380 K381 F382 L383 L384 E385 P390 V391

H392 I393 L394 N397 G398 N399 K400 R401 W402 K403 A419 T420 V421 H429 K438 N445 R453 R468 P472 D475 R476 H477 L485 G486 Y487 M491 L494 V498 N499 S500 R504 L505 T509 M512 Q513 D516 Y517 N518 R523

- Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain D: 69% 30%

S2 Q3 Q4 V5 Y12 P13 L14 F15 L16 K21 K27 E32 Q37 I40 D41 E51 P66 A67 K68 Q71 F82 E83 K84 T85 M86 P87 Y88 V89 H90 G91 S92 C95 V96 F103 N104 R108 E109 P110 V111 V114 S115 D116 S117 M118 T119 E120

V124 F125 Q128 K132 N137 C138 K139 P144 V149 S150 T151 T152 C153 M154 G159 D160 D161 L162 F165 K170 F174 D177 E178 F179 P180 T186 D198 N199 E202 A205 R206 Y207 F208 T209 M213 D214 D215 K216 G219 E231 T232

N236 F237 R238 V239 M243 M247 L254 S255 E258 E259 V260 L261 D262 M281 P285 L288 Q294 P295 W296 H297 K300 F304 V305 T308 W309 P314 I318 P319 M320 T325 K331 P341 K346 R350 L351 V352 M355 T356 D357 S358 H359

H363 G364 K365 R366 F367 A368 L369 W370 F375 V376 M377 V380 K381 F382 L383 L384 E385 L386 E389 P390 V391 L394 N397 A419 K438 F441 M442 I443 G444 N445 I451 Q452 R453 D454 V464 R468 I469 G470 F471 P472 I473 F474 D475 R476 H477 H478 R481

E488 M491 L494 V498 N499 S500 I501 R504 L505 E508 T509 M512 Q513 D516 Y517 N518 R523

- Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain J: 76% 22%

S2 Q3 Q4 A10 S11 Y12 P13 L14 Y35 I40 V43 T47 E51 K68 A69 C70 Q71 F82 E83 K84 T85 M86 P87 Y88 G91 F103 N104 V111 V114 S115 D116 S117 M118 T119 E120 F125 Q128 K132 C138 D145 V149 S150

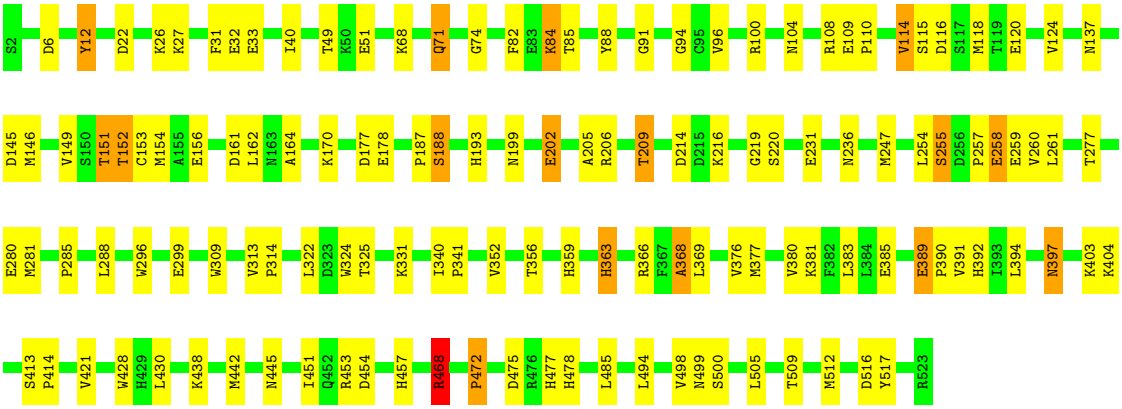
T151 T152 C153 M154 G159 L162 K170 I175 S188 D198 N199 E202 A205 R206 T209 D214 D215 K216 E231 N236 F237 L254 S255 E258 E259 V260 M281 P285 W296 H297 F304 V305 W309 P314 K331 V352 T356

H359 H363 G364 K365 R366 F367 A368 L369 D372 P373 D374 F375 V376 M377 K381 F382 L383 L384 E385 E389 P390 V391 H392 I393 L394 C395 H396 N397 K400 S413 P414 I423 L430 F435 K438 P439 M442 N445 I451 Q452 R453 D454 T455 L456 H457

R468 I469 P472 D475 R476 H477 H478 Y487 E488 M491 L494 V498 N499 S500 I501 R504 L505 T509 M512 Q513 D516 Y517 N518 R523

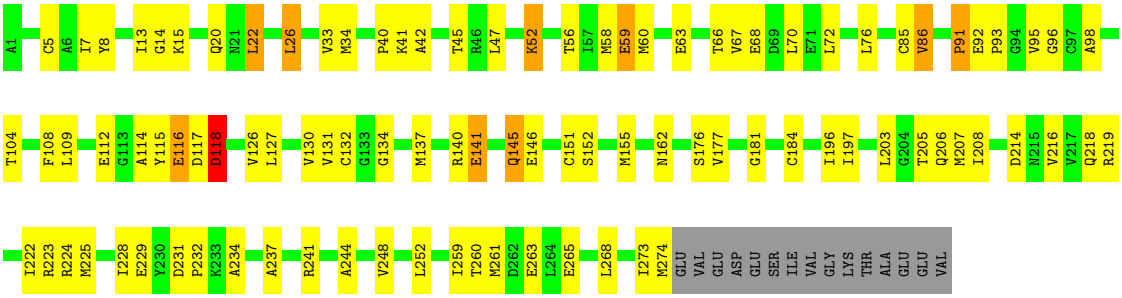
- Molecule 2: Nitrogenase Molybdenum-Iron Protein beta chain

Chain L: 75% 22%



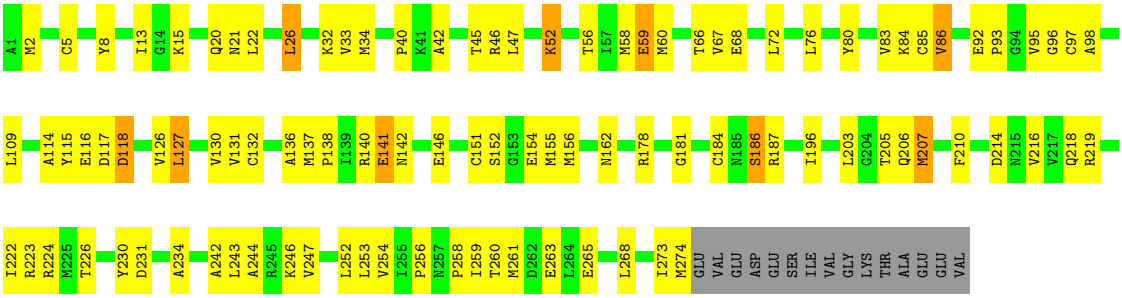
- Molecule 3: Nitrogenase Iron Protein 1

Chain E:



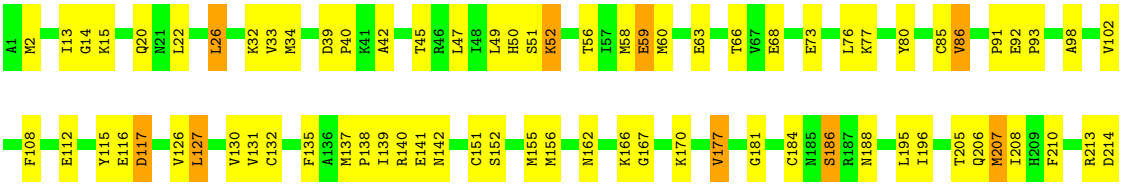
- Molecule 3: Nitrogenase Iron Protein 1

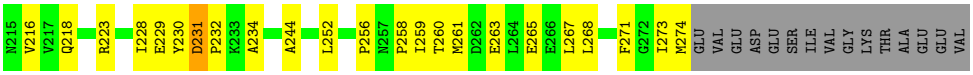
Chain F:



- Molecule 3: Nitrogenase Iron Protein 1

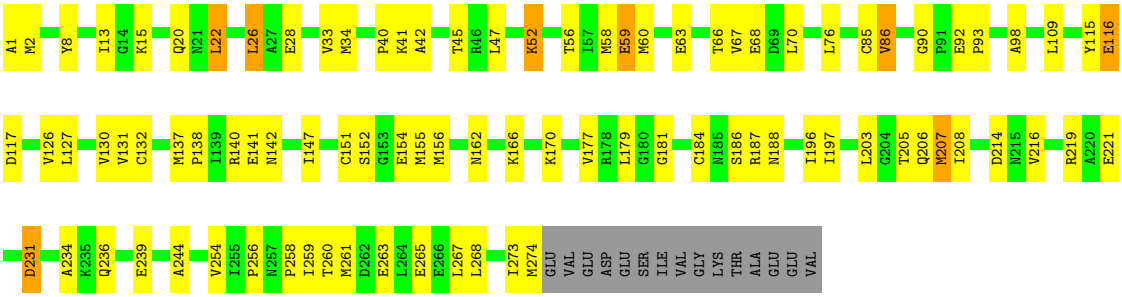
Chain G:





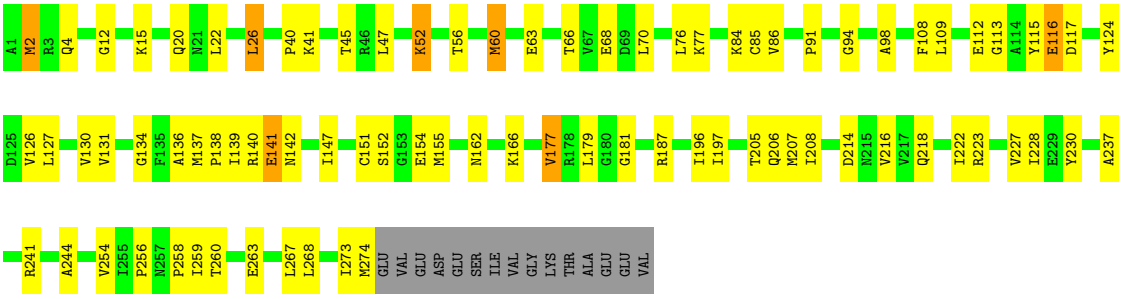
• Molecule 3: Nitrogenase Iron Protein 1

Chain H:



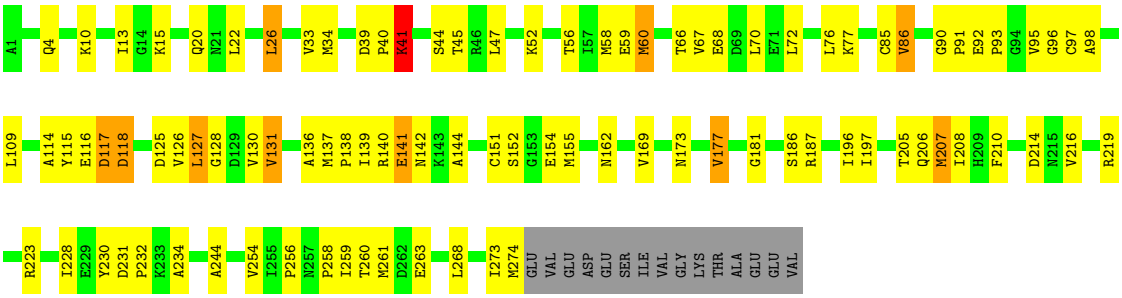
• Molecule 3: Nitrogenase Iron Protein 1

Chain M:



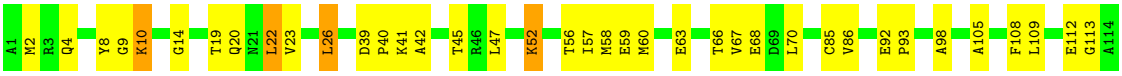
• Molecule 3: Nitrogenase Iron Protein 1

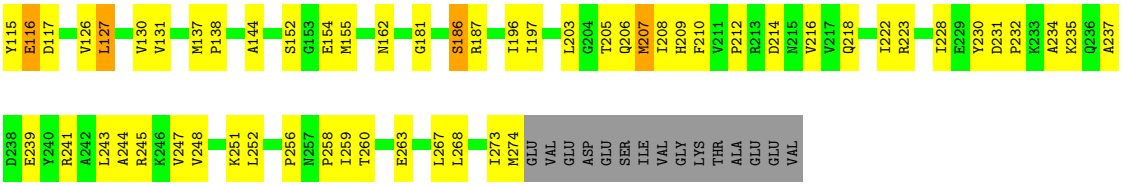
Chain N:



• Molecule 3: Nitrogenase Iron Protein 1

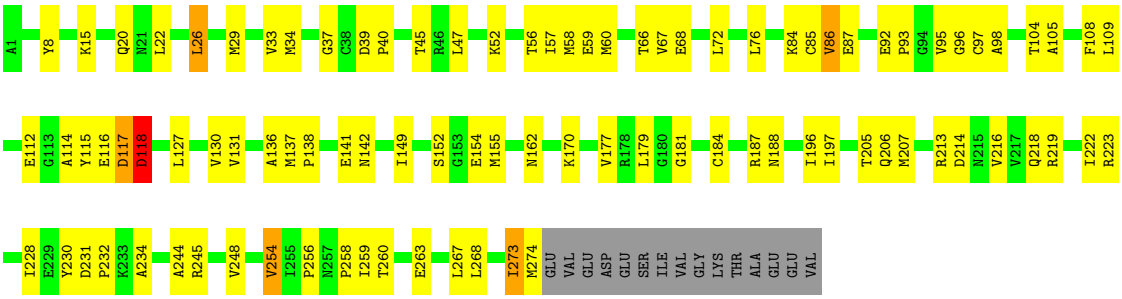
Chain O:





- Molecule 3: Nitrogenase Iron Protein 1

Chain P: 62% 30% • 5%



4 Data and refinement statistics (i)

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	326.10Å 75.80Å 312.20Å 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, ADP, CLF, CFM, HCA, MG, ALF

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	0.56	1/3883 (0.0%)	1.09	24/5236 (0.5%)
1	C	0.50	0/3883	1.03	18/5236 (0.3%)
1	I	0.50	0/3883	1.09	30/5236 (0.6%)
1	K	0.50	0/3883	1.05	25/5236 (0.5%)
2	B	0.60	3/4280 (0.1%)	0.99	22/5786 (0.4%)
2	D	0.49	0/4280	1.00	23/5786 (0.4%)
2	J	0.58	1/4280 (0.0%)	1.02	25/5786 (0.4%)
2	L	0.51	1/4280 (0.0%)	0.99	22/5786 (0.4%)
3	E	0.49	0/2097	1.00	8/2824 (0.3%)
3	F	0.45	0/2097	0.96	4/2824 (0.1%)
3	G	0.47	0/2097	0.95	5/2824 (0.2%)
3	H	0.43	0/2097	0.99	10/2824 (0.4%)
3	M	0.45	0/2097	0.93	3/2824 (0.1%)
3	N	0.46	0/2097	0.99	10/2824 (0.4%)
3	O	0.40	0/2097	0.93	2/2824 (0.1%)
3	P	0.41	0/2097	0.96	6/2824 (0.2%)
All	All	0.51	6/49428 (0.0%)	1.01	237/66680 (0.4%)

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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	439	PRO	N-CD	-18.05	1.22	1.47
2	B	66	PRO	N-CD	-18.00	1.22	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	186	THR	C-N	7.06	1.41	1.33
1	A	46	ILE	C-N	6.85	1.43	1.33
2	L	390	PRO	C-N	-6.05	1.26	1.33

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	188	SER	CA-CB-OG	12.70	136.50	111.10
2	L	188	SER	CA-CB-OG	10.93	132.97	111.10
1	A	179	VAL	N-CA-C	10.51	117.95	107.55
1	K	191	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	I	191	GLN	OE1-CD-NE2	-10.29	112.31	122.60

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 (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	3795	0	3734	124	0
1	C	3795	0	3734	117	0
1	I	3795	0	3734	132	0
1	K	3795	0	3734	130	0
2	B	4174	0	4088	112	0
2	D	4174	0	4088	123	0
2	J	4174	0	4087	95	0
2	L	4174	0	4087	104	0
3	E	2073	0	2092	88	0
3	F	2073	0	2089	81	0
3	G	2073	0	2092	86	0
3	H	2073	0	2092	87	1
3	M	2073	0	2091	76	0
3	N	2073	0	2091	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2073	0	2091	87	1
3	P	2073	0	2092	78	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

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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	1456	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 15.

The worst 5 of 1456 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 (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	476/491 (97%)	450 (94%)	24 (5%)	2 (0%)	30	38
1	C	476/491 (97%)	448 (94%)	25 (5%)	3 (1%)	21	27
1	I	476/491 (97%)	450 (94%)	24 (5%)	2 (0%)	30	38
1	K	476/491 (97%)	447 (94%)	25 (5%)	4 (1%)	16	20
2	B	520/522 (100%)	500 (96%)	19 (4%)	1 (0%)	43	55
2	D	520/522 (100%)	503 (97%)	16 (3%)	1 (0%)	43	55
2	J	520/522 (100%)	499 (96%)	19 (4%)	2 (0%)	30	38
2	L	520/522 (100%)	496 (95%)	23 (4%)	1 (0%)	43	55
3	E	272/289 (94%)	254 (93%)	18 (7%)	0	100	100
3	F	272/289 (94%)	256 (94%)	14 (5%)	2 (1%)	18	23
3	G	272/289 (94%)	256 (94%)	13 (5%)	3 (1%)	11	13
3	H	272/289 (94%)	251 (92%)	20 (7%)	1 (0%)	30	38
3	M	272/289 (94%)	258 (95%)	12 (4%)	2 (1%)	18	23
3	N	272/289 (94%)	258 (95%)	12 (4%)	2 (1%)	18	23
3	O	272/289 (94%)	254 (93%)	14 (5%)	4 (2%)	8	8
3	P	272/289 (94%)	253 (93%)	18 (7%)	1 (0%)	30	38
All	All	6160/6364 (97%)	5833 (95%)	296 (5%)	31 (0%)	24	31

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 (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	407/414 (98%)	391 (96%)	16 (4%)	28	43
1	C	407/414 (98%)	390 (96%)	17 (4%)	26	40
1	I	407/414 (98%)	387 (95%)	20 (5%)	22	34
1	K	407/414 (98%)	388 (95%)	19 (5%)	23	35
2	B	454/454 (100%)	441 (97%)	13 (3%)	37	55
2	D	454/454 (100%)	443 (98%)	11 (2%)	43	62
2	J	454/454 (100%)	444 (98%)	10 (2%)	45	65
2	L	454/454 (100%)	438 (96%)	16 (4%)	32	48
3	E	220/233 (94%)	208 (94%)	12 (6%)	19	28
3	F	220/233 (94%)	211 (96%)	9 (4%)	27	41
3	G	220/233 (94%)	209 (95%)	11 (5%)	22	33
3	H	220/233 (94%)	212 (96%)	8 (4%)	31	47
3	M	220/233 (94%)	213 (97%)	7 (3%)	34	51
3	N	220/233 (94%)	208 (94%)	12 (6%)	19	28
3	O	220/233 (94%)	214 (97%)	6 (3%)	39	58
3	P	220/233 (94%)	211 (96%)	9 (4%)	27	41
All	All	5204/5336 (98%)	5008 (96%)	196 (4%)	29	44

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	437	PRO
1	K	444	TRP
2	J	152	THR
1	K	106	VAL
2	L	120	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	442	HIS
3	N	20	GLN
2	L	58	GLN
2	L	478	HIS
3	O	4	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 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	$\#\|Z\| > 2$
9	ALF	H	3393	12	4,4,4	1.26	0	-		
5	CFM	I	4096	1	0,24,24	-	-	-		
5	CFM	K	4296	1	0,24,24	-	-	-		
11	ADP	F	3191	8	28,29,29	1.48	6 (21%)	43,45,45	1.22	3 (6%)
10	SF4	G	3290	3	0,12,12	-	-	-		
7	CLF	B	2098	1,2	0,24,24	-	-	-		
9	ALF	F	3193	12	4,4,4	1.25	0	-		
9	ALF	G	3293	12	4,4,4	1.19	0	-		
11	ADP	M	5091	8	28,29,29	1.41	5 (17%)	43,45,45	1.29	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	ADP	G	3291	8	28,29,29	1.53	5 (17%)	43,45,45	1.38	4 (9%)
4	HCA	K	4294	-	13,13,13	3.72	6 (46%)	15,18,18	6.13	10 (66%)
7	CLF	J	4098	1,2	0,24,24	-	-	-		
10	SF4	O	5290	3	0,12,12	-	-	-		
11	ADP	P	5391	8	28,29,29	1.42	5 (17%)	43,45,45	1.22	3 (6%)
7	CLF	D	2298	1,2	0,24,24	-	-	-		
10	SF4	E	3090	3	0,12,12	-	-	-		
7	CLF	L	4298	1,2	0,24,24	-	-	-		
11	ADP	O	5291	8	28,29,29	1.47	6 (21%)	43,45,45	1.35	5 (11%)
9	ALF	O	5293	12	4,4,4	1.23	0	-		
4	HCA	C	2294	-	13,13,13	2.68	5 (38%)	15,18,18	3.03	7 (46%)
10	SF4	M	5090	3	0,12,12	-	-	-		
4	HCA	A	2094	-	13,13,13	4.44	7 (53%)	15,18,18	6.48	9 (60%)
9	ALF	P	5393	12	4,4,4	1.27	0	-		
11	ADP	E	3091	8	28,29,29	1.35	5 (17%)	43,45,45	1.30	4 (9%)
11	ADP	N	5191	8	28,29,29	1.36	4 (14%)	43,45,45	1.28	5 (11%)
4	HCA	I	4094	-	13,13,13	4.45	7 (53%)	15,18,18	6.48	9 (60%)
11	ADP	H	3391	8	28,29,29	1.42	5 (17%)	43,45,45	1.26	3 (6%)
9	ALF	M	5093	12	4,4,4	1.20	0	-		
9	ALF	N	5193	12	4,4,4	1.17	0	-		
9	ALF	E	3093	12	4,4,4	1.20	0	-		
5	CFM	A	2096	1	0,24,24	-	-	-		
5	CFM	C	2296	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
11	ADP	F	3191	8	-	5/16/32/32	0/3/3/3
10	SF4	G	3290	3	-	-	0/6/5/5
7	CLF	B	2098	1,2	-	-	0/12/10/10
11	ADP	M	5091	8	-	4/16/32/32	0/3/3/3
11	ADP	G	3291	8	-	3/16/32/32	0/3/3/3
4	HCA	K	4294	-	-	9/17/17/17	-
7	CLF	J	4098	1,2	-	-	0/12/10/10
11	ADP	P	5391	8	-	0/16/32/32	0/3/3/3
10	SF4	O	5290	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLF	D	2298	1,2	-	-	0/12/10/10
10	SF4	E	3090	3	-	-	0/6/5/5
7	CLF	L	4298	1,2	-	-	0/12/10/10
11	ADP	O	5291	8	-	0/16/32/32	0/3/3/3
4	HCA	C	2294	-	-	9/17/17/17	-
10	SF4	M	5090	3	-	-	0/6/5/5
4	HCA	A	2094	-	1/1/4/4	12/17/17/17	-
11	ADP	E	3091	8	-	0/16/32/32	0/3/3/3
11	ADP	N	5191	8	-	0/16/32/32	0/3/3/3
4	HCA	I	4094	-	1/1/4/4	12/17/17/17	-
11	ADP	H	3391	8	-	0/16/32/32	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2094	HCA	C3-C7	11.61	1.65	1.53
4	I	4094	HCA	C3-C7	11.60	1.65	1.53
4	K	4294	HCA	C3-C7	9.18	1.63	1.53
4	I	4094	HCA	O5-C7	6.94	1.43	1.22
4	A	2094	HCA	O5-C7	6.94	1.43	1.22

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2094	HCA	O7-C3-C4	-16.55	82.41	108.88
4	I	4094	HCA	O7-C3-C4	-16.55	82.41	108.88
4	K	4294	HCA	O7-C3-C4	-15.97	83.34	108.88
4	A	2094	HCA	O7-C3-C2	-11.85	82.36	109.38
4	I	4094	HCA	O7-C3-C2	-11.84	82.37	109.38

All (2) chirality outliers are listed below:

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

5 of 54 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

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Mol	Chain	Res	Type	Atoms
4	A	2094	HCA	C7-C3-C4-C5
4	A	2094	HCA	O7-C3-C4-C5
4	A	2094	HCA	O7-C3-C7-O5

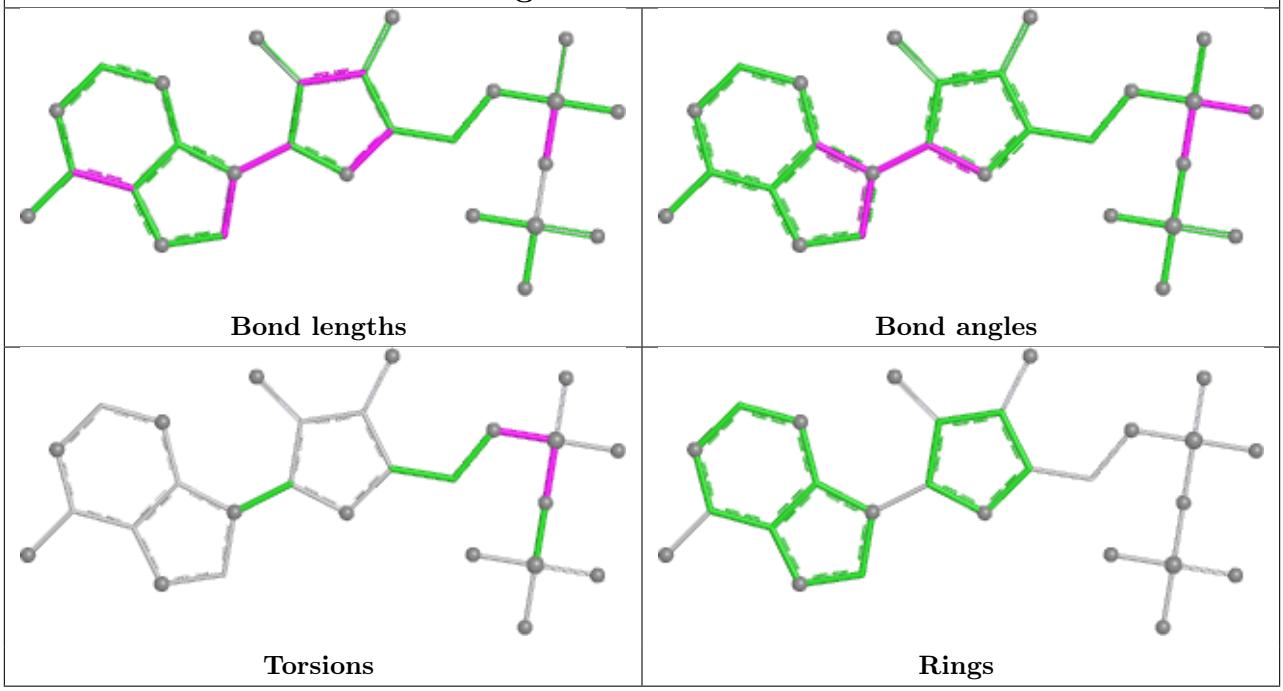
There are no ring outliers.

9 monomers are involved in 13 short contacts:

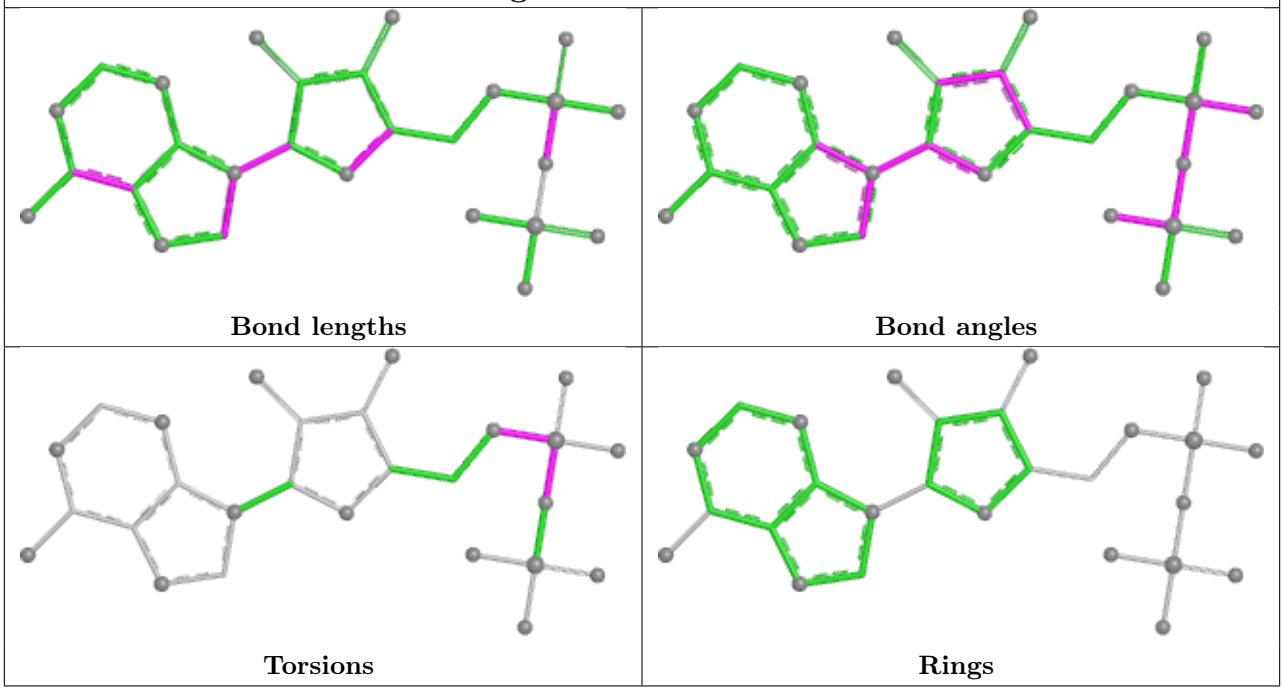
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	4096	CFM	1	0
11	M	5091	ADP	1	0
11	G	3291	ADP	2	0
7	J	4098	CLF	1	0
11	P	5391	ADP	1	0
11	O	5291	ADP	2	0
11	E	3091	ADP	2	0
11	H	3391	ADP	2	0
5	A	2096	CFM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

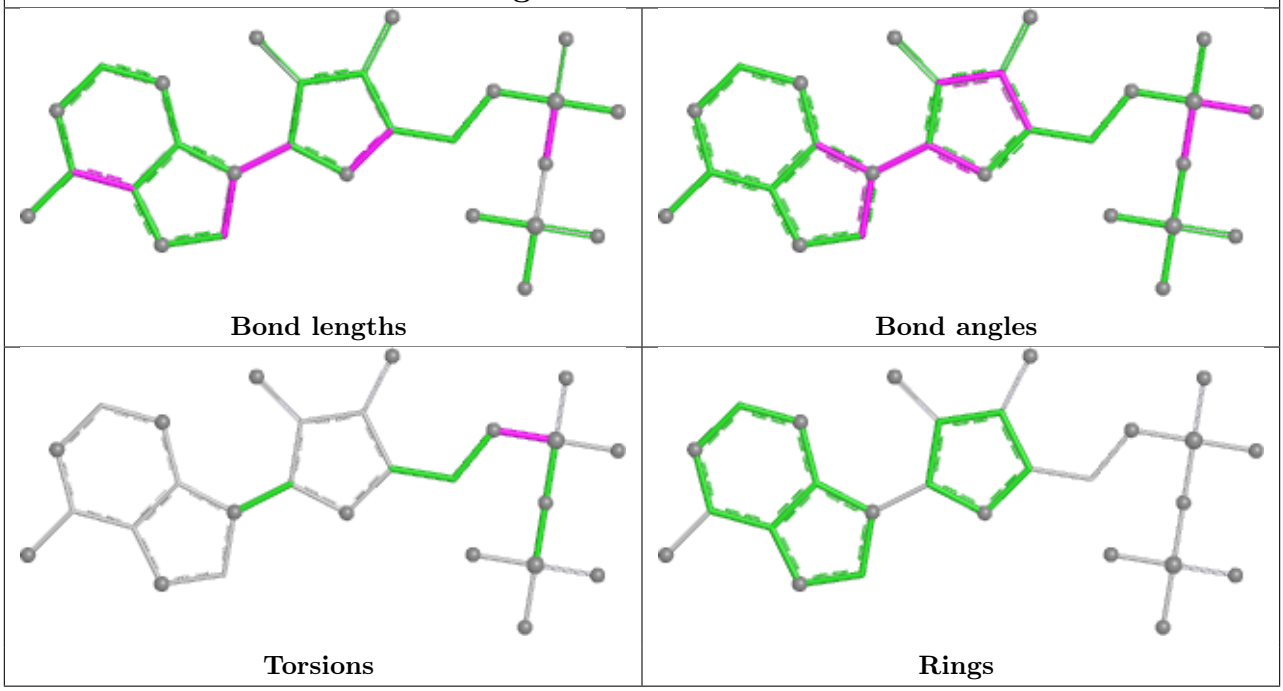
Ligand ADP F 3191



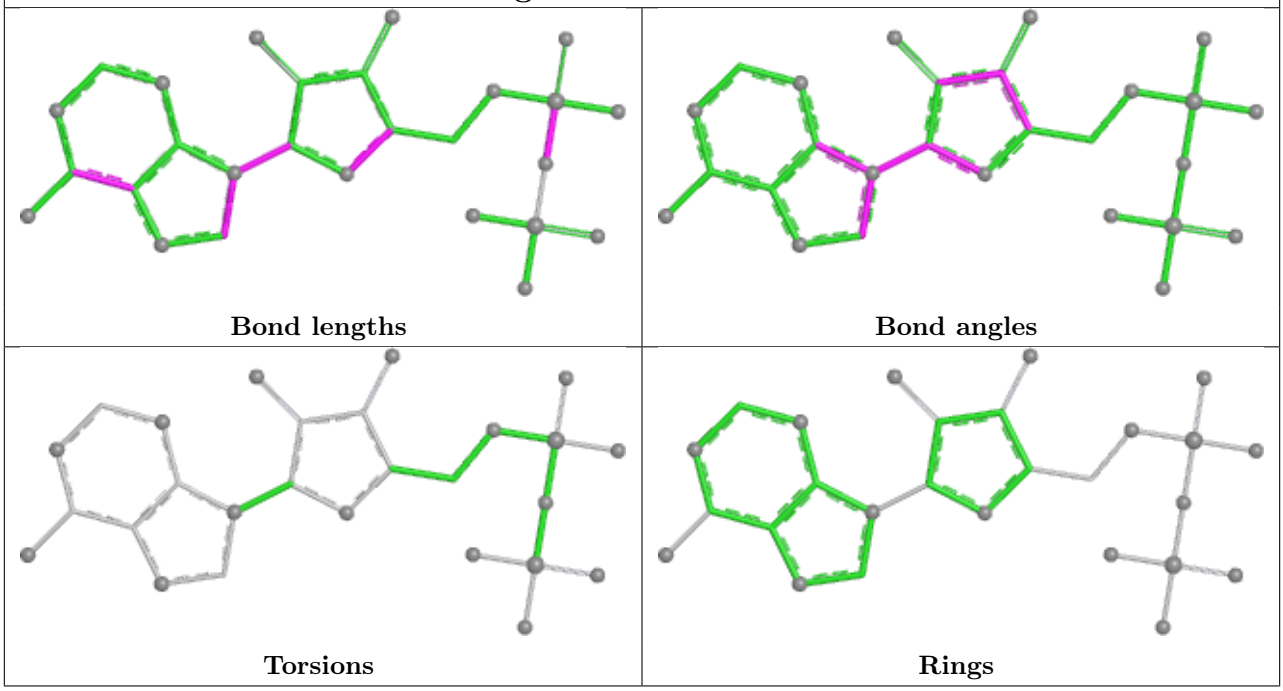
Ligand ADP M 5091



Ligand ADP G 3291



Ligand ADP P 5391



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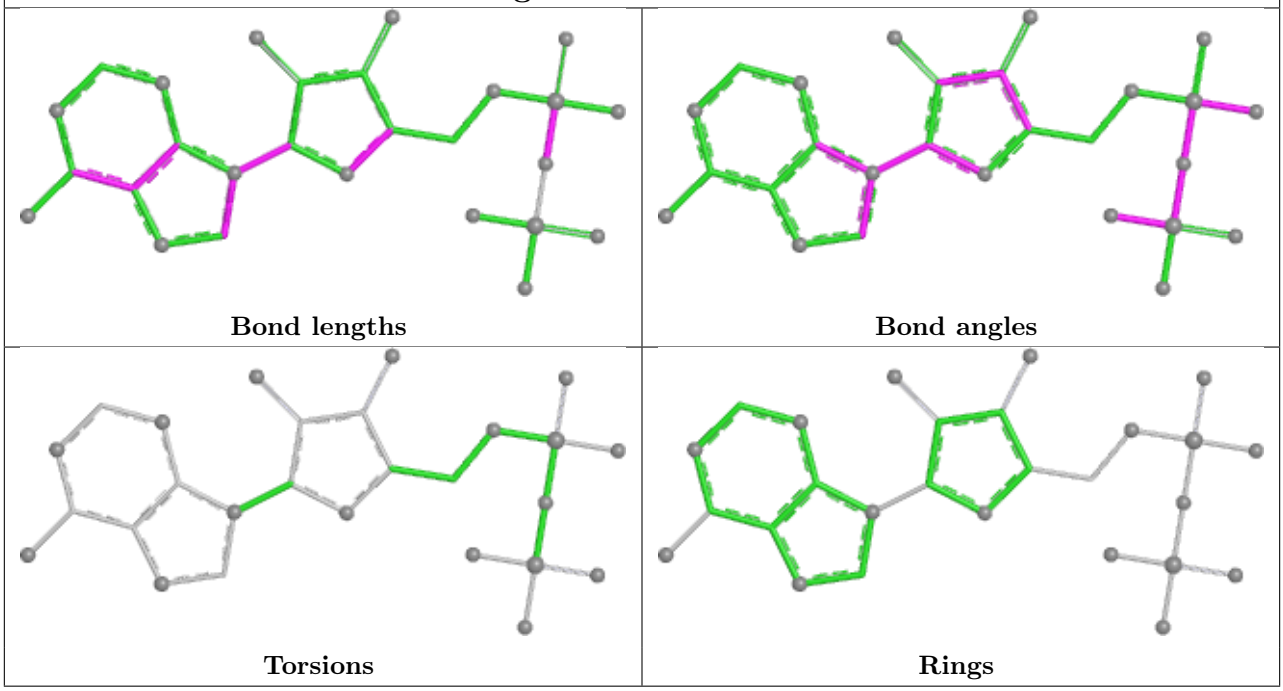

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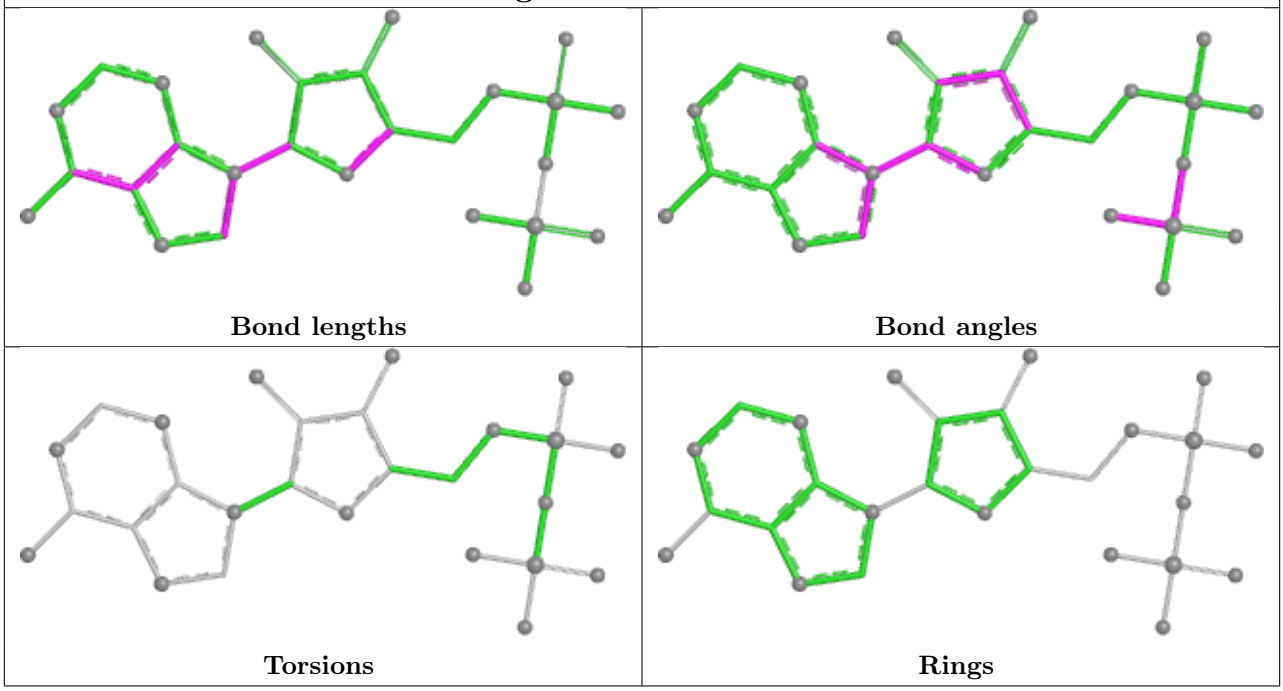
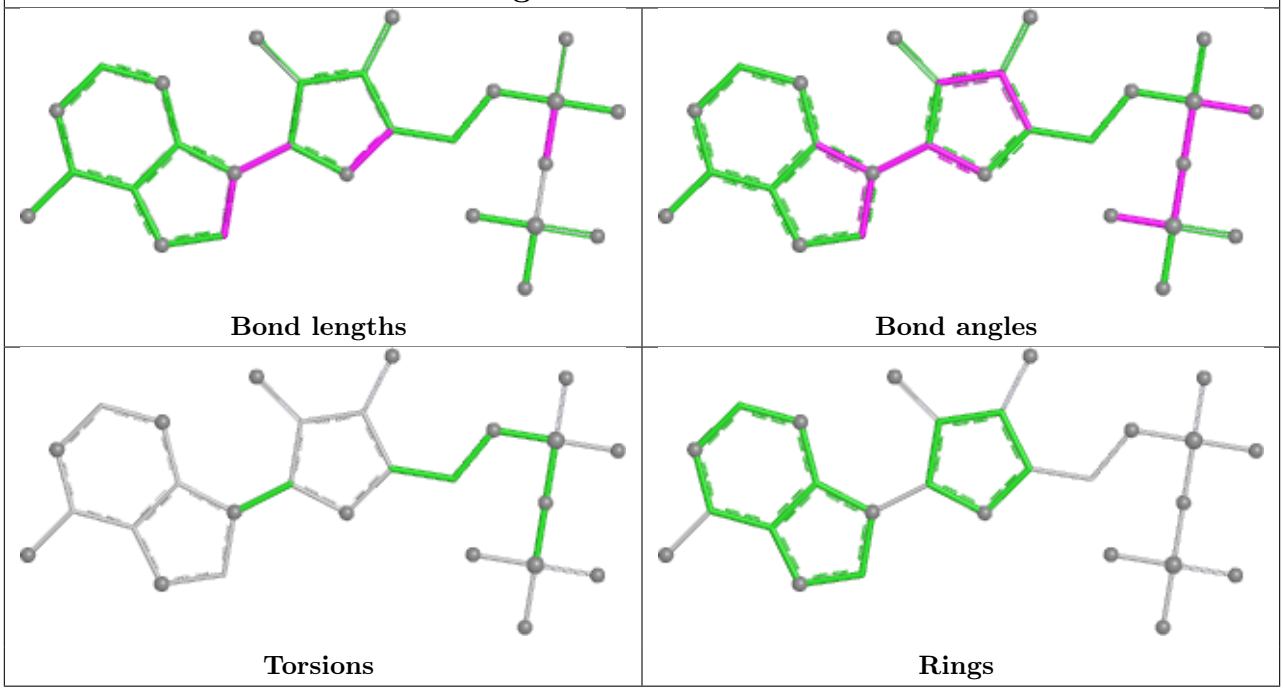
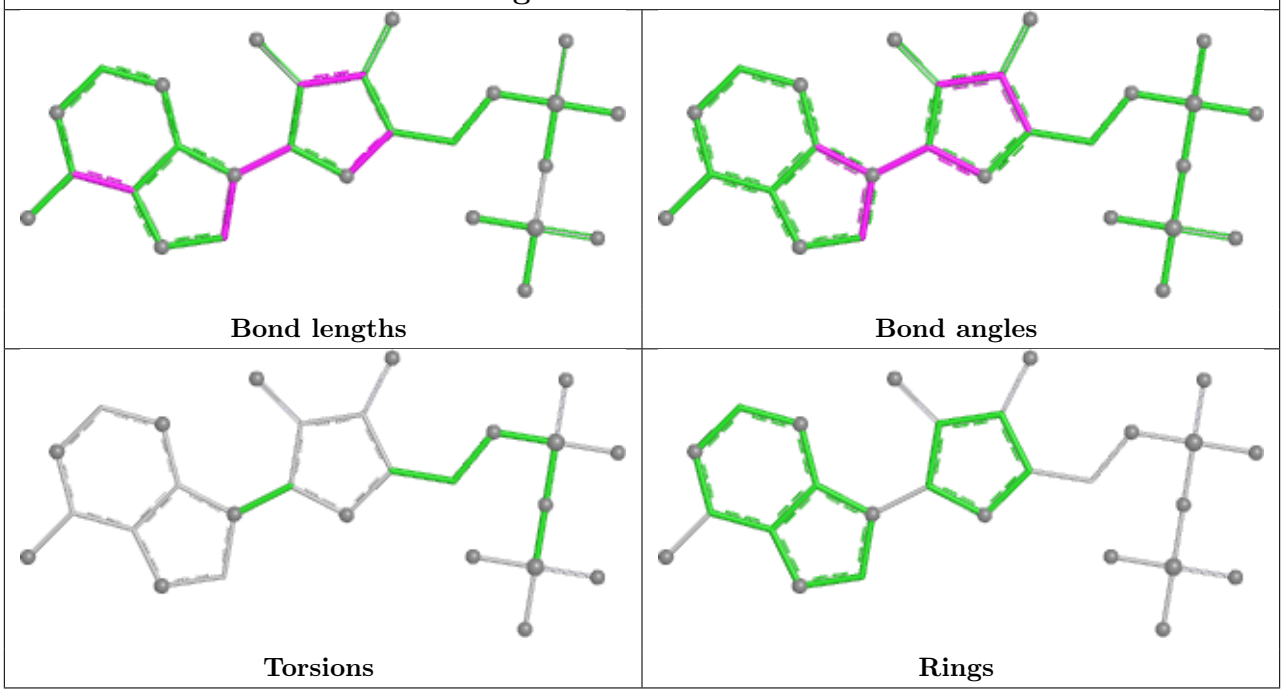


Ligand ADP N 5191



Ligand ADP H 3391



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.