wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:29 AM GMT

PDB ID	:	2AFI
Title	:	Crystal Structure of MgADP bound Av2-Av1 Complex
Authors	:	Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.
Deposited on	:	2005-07-25
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

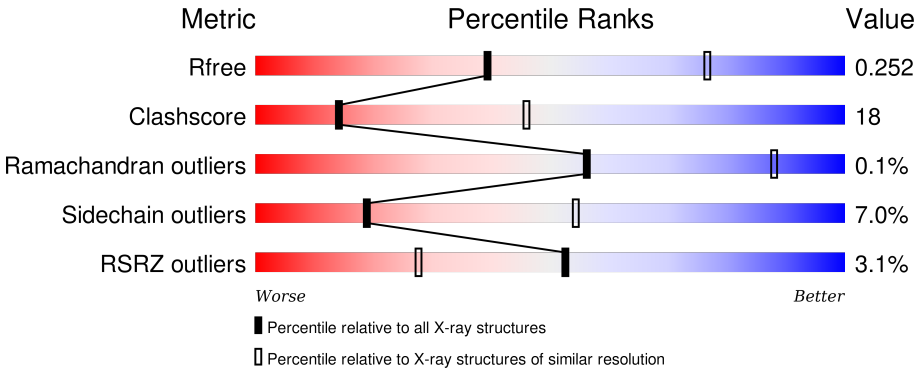
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	60% 34%
1	C	491	59% 36%
1	I	491	57% 37%
1	K	491	60% 34%
2	B	522	68% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	522	69% 29%
2	J	522	66% 32%
2	L	522	67% 31%
3	E	289	10% 58% 30% 5% 6%
3	F	289	4% 49% 41% 5%
3	G	289	% 49% 39% 9%
3	H	289	6% 67% 22% 7%
3	M	289	6% 55% 36% 7%
3	N	289	18% 72% 19% 7%
3	O	289	4% 49% 39% 9%
3	P	289	11% 65% 24% 8%

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
6	HCA	C	494	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 48501 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	31	0	0
			3782	2405	645	708	24			
1	C	476	Total	C	N	O	S	28	0	0
			3782	2405	645	708	24			
1	I	476	Total	C	N	O	S	0	0	0
			3782	2405	645	708	24			
1	K	476	Total	C	N	O	S	17	0	0
			3782	2405	645	708	24			

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	39	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	10	0	0
			4174	2666	705	775	28			
2	J	522	Total	C	N	O	S	5	0	0
			4174	2666	705	775	28			
2	L	522	Total	C	N	O	S	5	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	271	Total	C	N	O	S	453	0	0
			2053	1283	350	400	20			
3	F	275	Total	C	N	O	S	242	0	0
			2082	1301	354	406	21			
3	G	263	Total	C	N	O	S	280	0	0
			1983	1236	342	386	19			
3	H	269	Total	C	N	O	S	1031	0	0
			2037	1271	348	398	20			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	268	Total	C	N	O	S	458	0	0
			2029	1269	344	397	19			
3	N	270	Total	C	N	O	S	1220	0	0
			2041	1277	346	399	19			
3	O	262	Total	C	N	O	S	302	0	0
			1978	1233	341	385	19			
3	P	267	Total	C	N	O	S	868	0	0
			2018	1263	342	395	18			

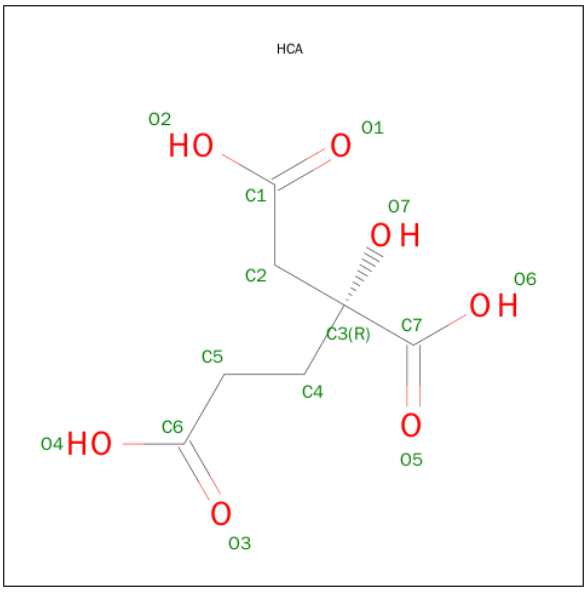
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		
4	L	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

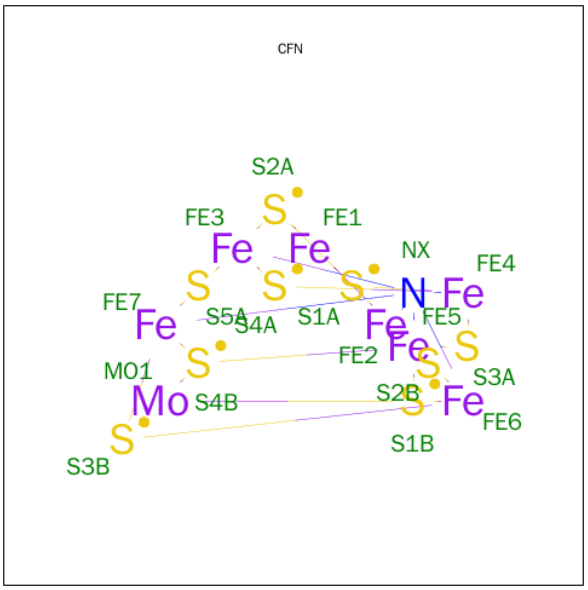
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		
5	O	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: $C_7H_{10}O_7$).



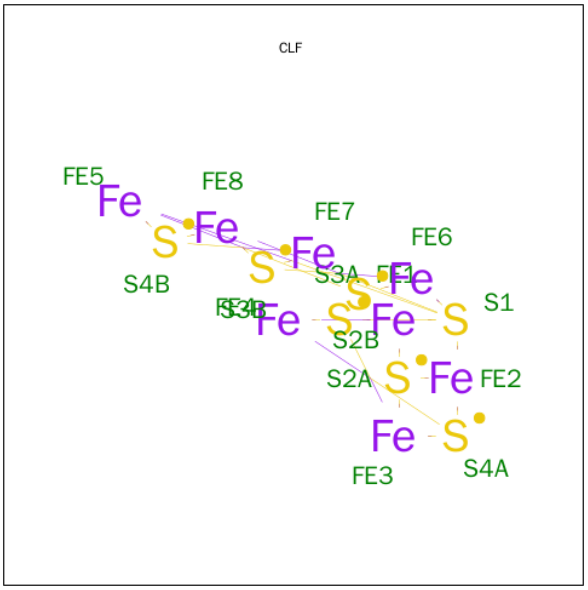
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 14 7 7	0	0
6	C	1	Total C O 14 7 7	0	0
6	I	1	Total C O 14 7 7	0	0
6	K	1	Total C O 14 7 7	0	0

- Molecule 7 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe_7MoNS_9).



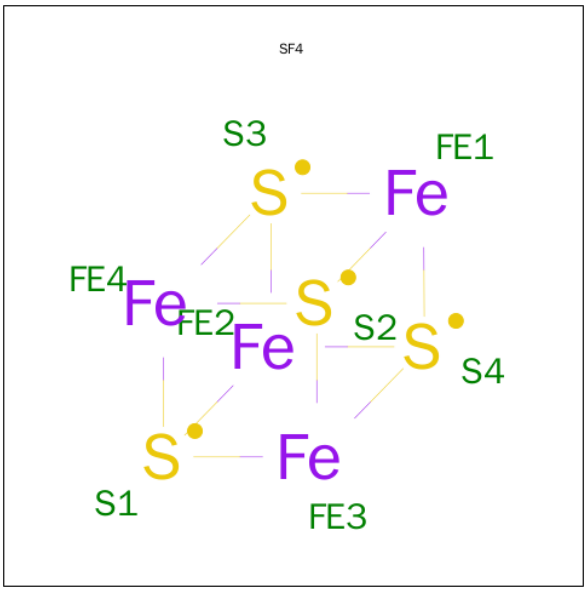
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Fe Mo N S 18 7 1 1 9	0	0
7	C	1	Total Fe Mo N S 18 7 1 1 9	0	0
7	I	1	Total Fe Mo N S 18 7 1 1 9	0	0
7	K	1	Total Fe Mo N S 18 7 1 1 9	0	0

- Molecule 8 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



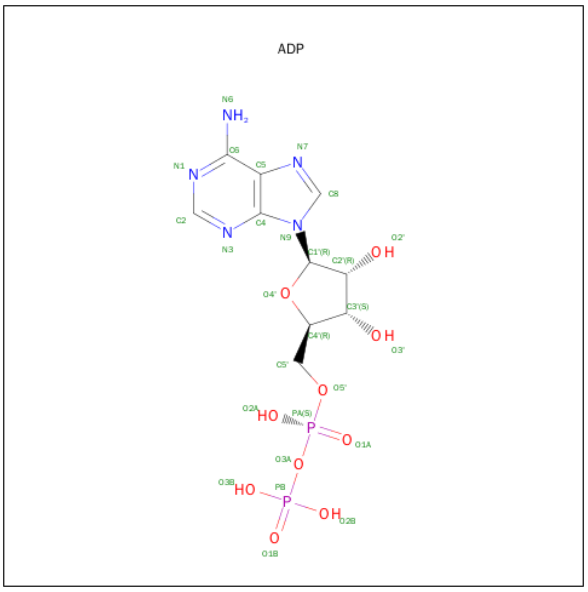
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 15 8 7	0	0
8	D	1	Total Fe S 15 8 7	0	0
8	J	1	Total Fe S 15 8 7	0	0
8	L	1	Total Fe S 15 8 7	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	N	1	Total Fe S 8 4 4	0	0
9	P	1	Total Fe S 8 4 4	0	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 11 is water.

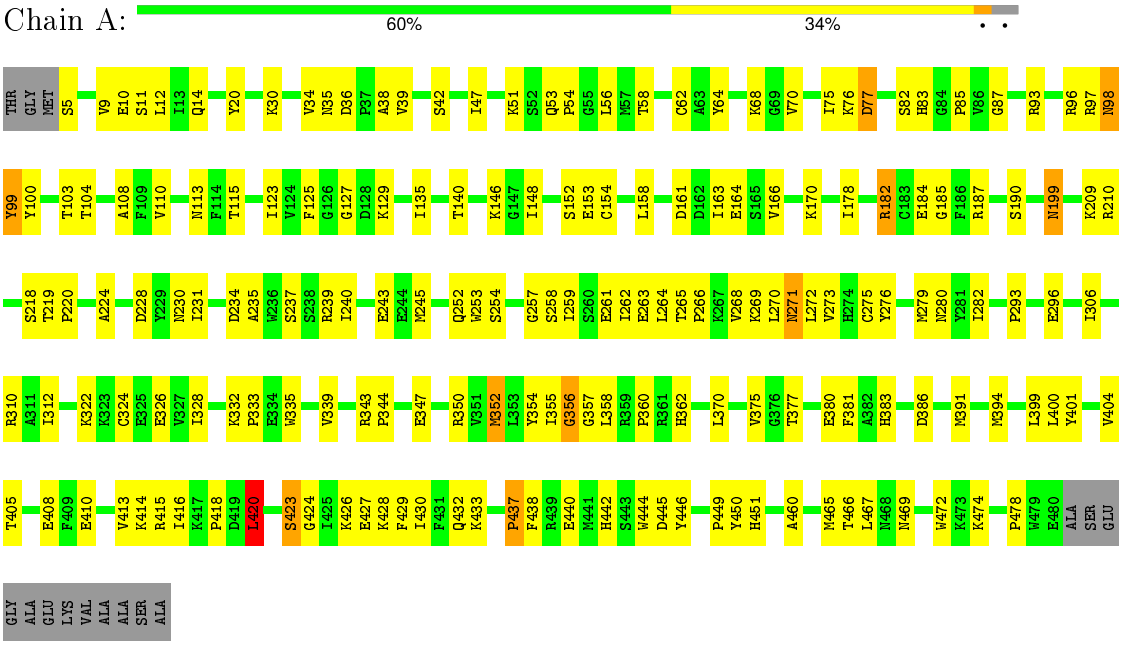
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	2	Total	O	0	0
			2	2		
11	D	2	Total	O	0	0
			2	2		
11	J	2	Total	O	0	0
			2	2		
11	L	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

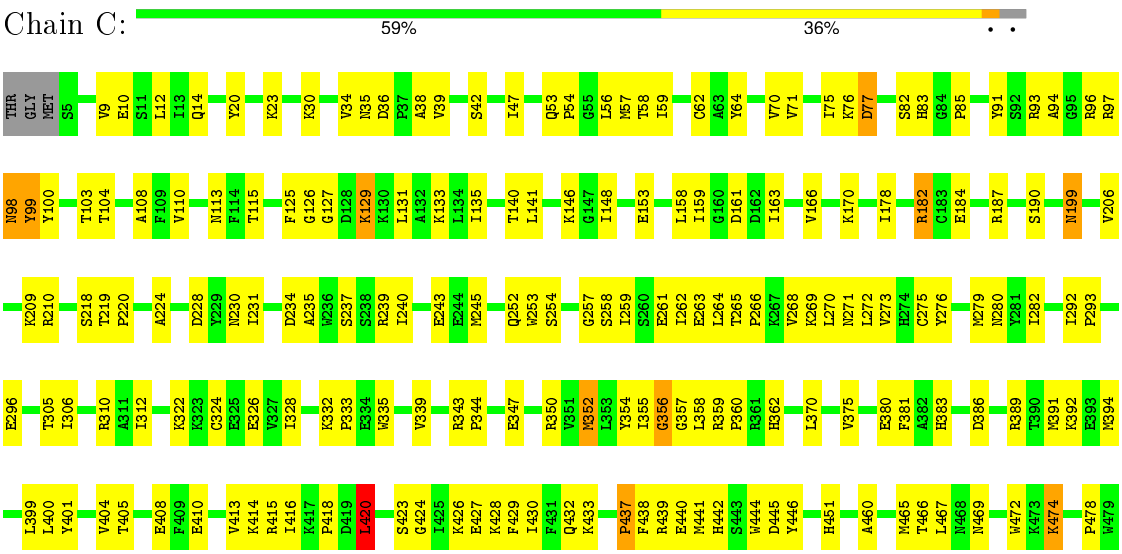
- Molecule 1: Nitrogenase molybdenum-iron protein

Chain A:



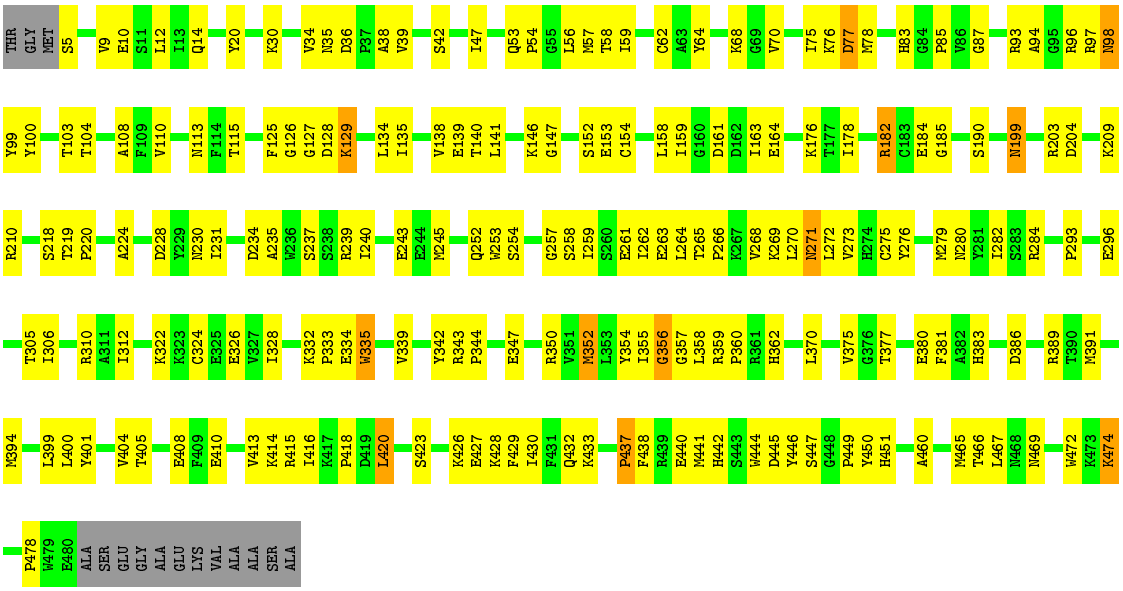
- Molecule 1: Nitrogenase molybdenum-iron protein

Chain C:



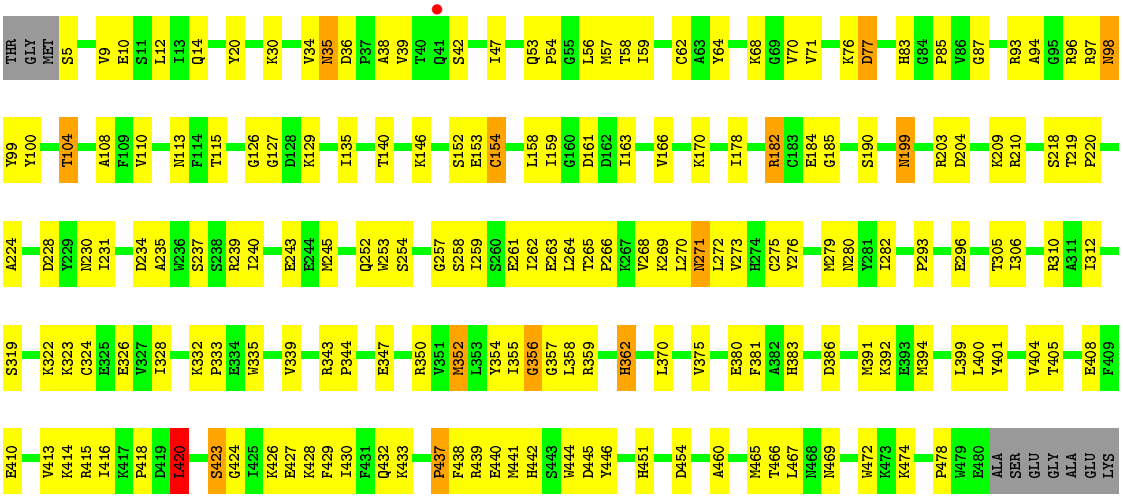
- Molecule 1: Nitrogenase molybdenum-iron protein

Chain I:



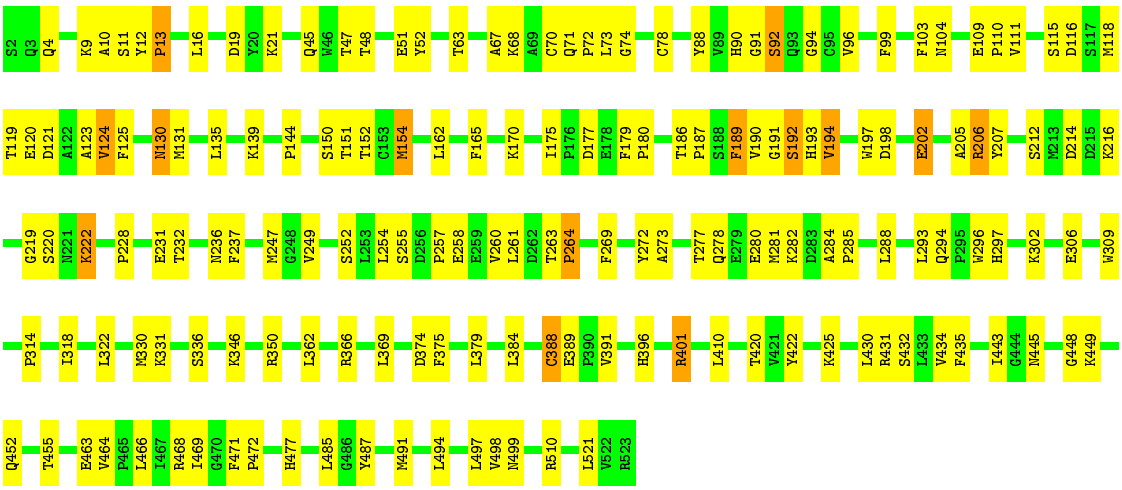
- Molecule 1: Nitrogenase molybdenum-iron protein

Chain K:



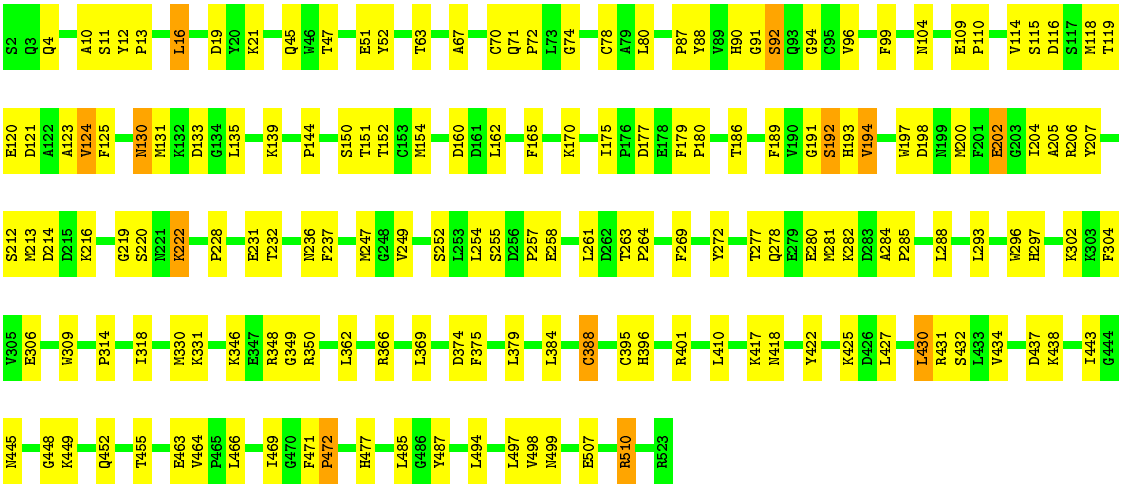
- Molecule 2: Nitrogenase molybdenum-iron protein

Chain B:



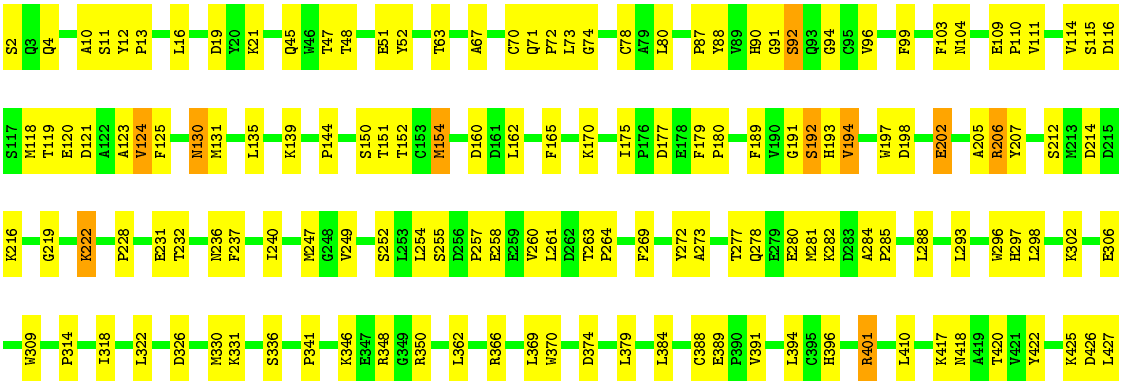
• Molecule 2: Nitrogenase molybdenum-iron protein

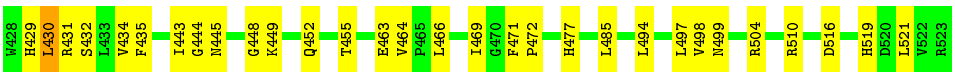
Chain D:



• Molecule 2: Nitrogenase molybdenum-iron protein

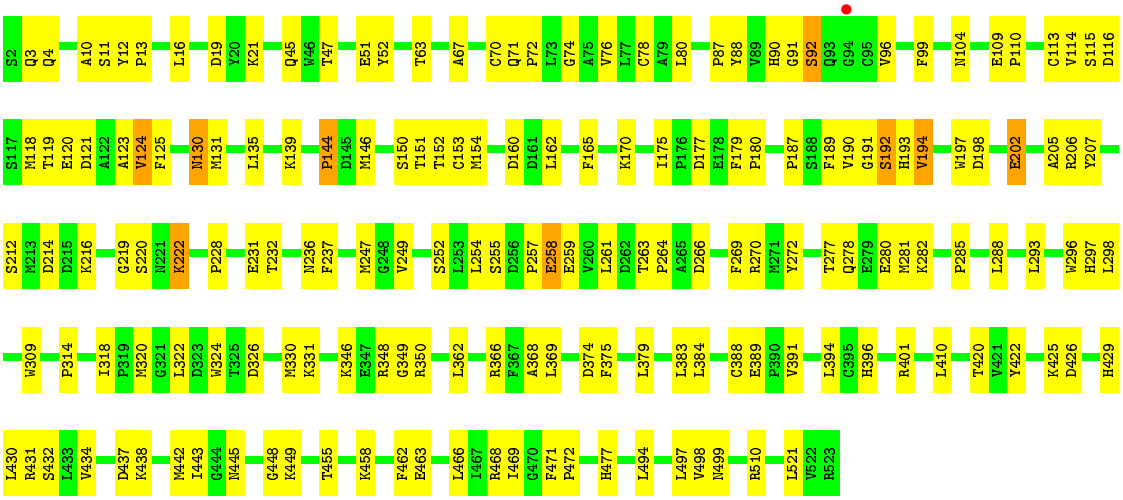
Chain J:





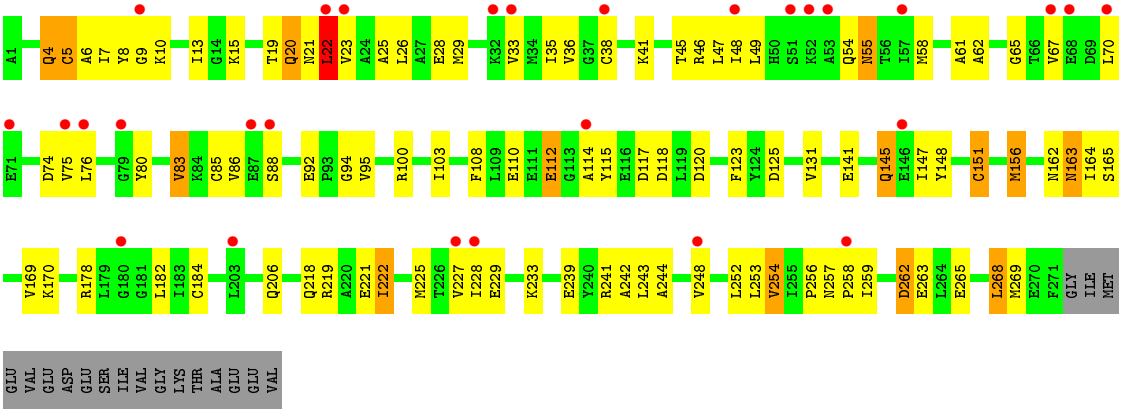
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain L:



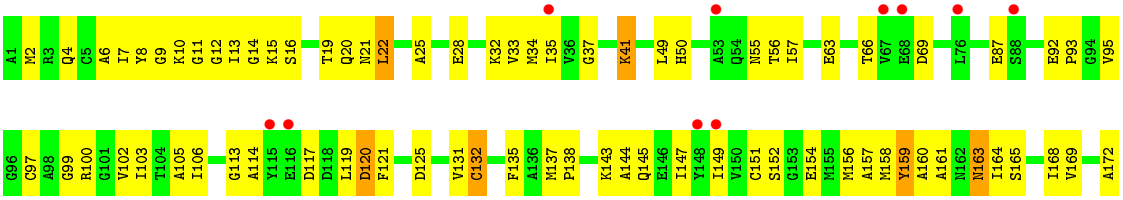
• Molecule 3: Nitrogenase iron protein 1

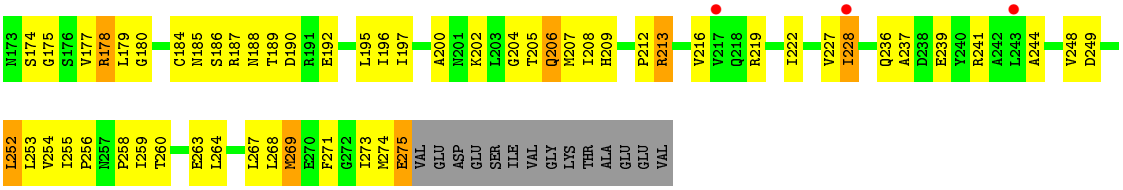
Chain E:



• Molecule 3: Nitrogenase iron protein 1

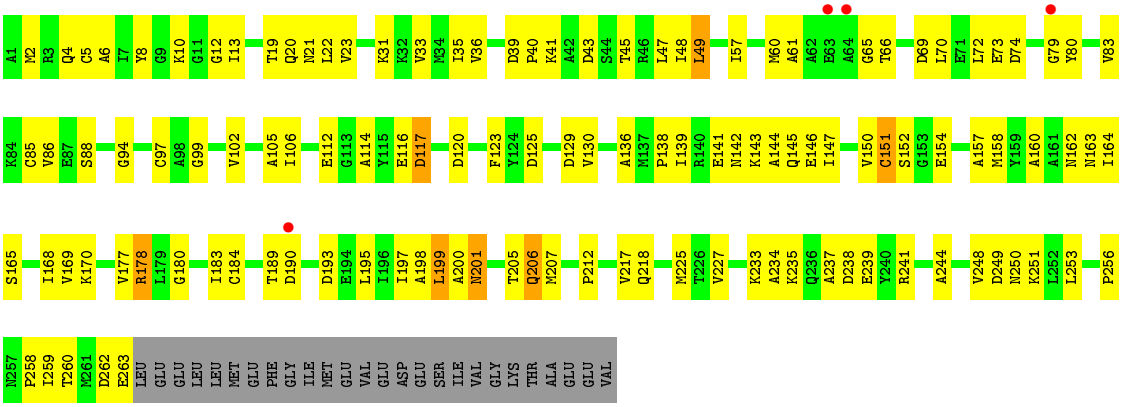
Chain F:





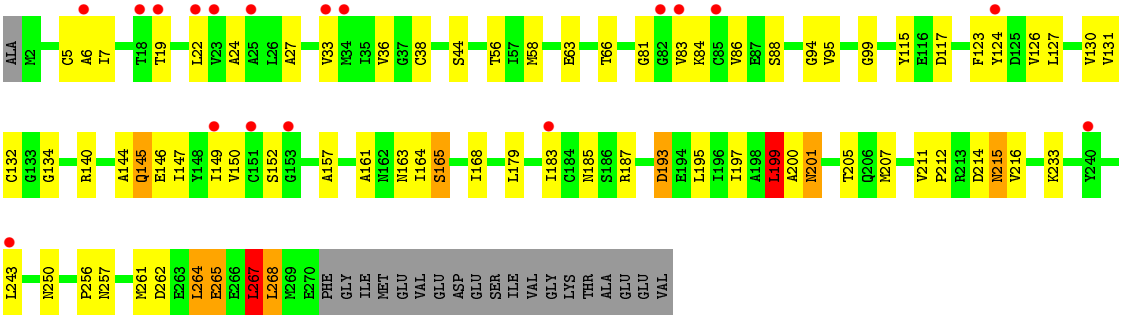
• Molecule 3: Nitrogenase iron protein 1

Chain G:



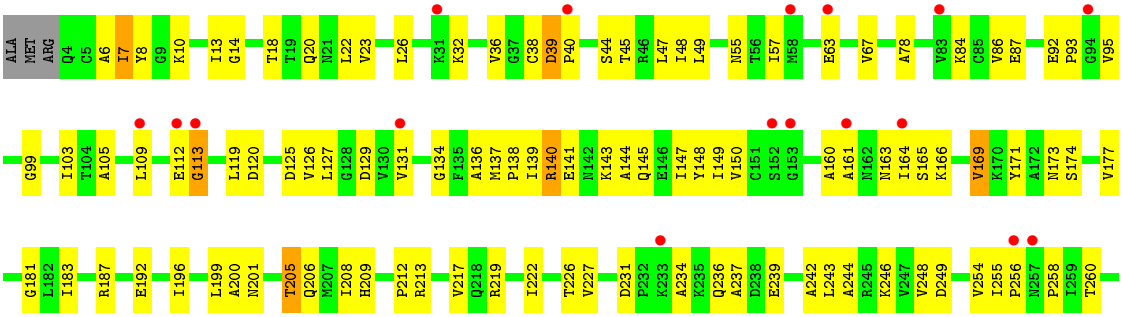
• Molecule 3: Nitrogenase iron protein 1

Chain H:



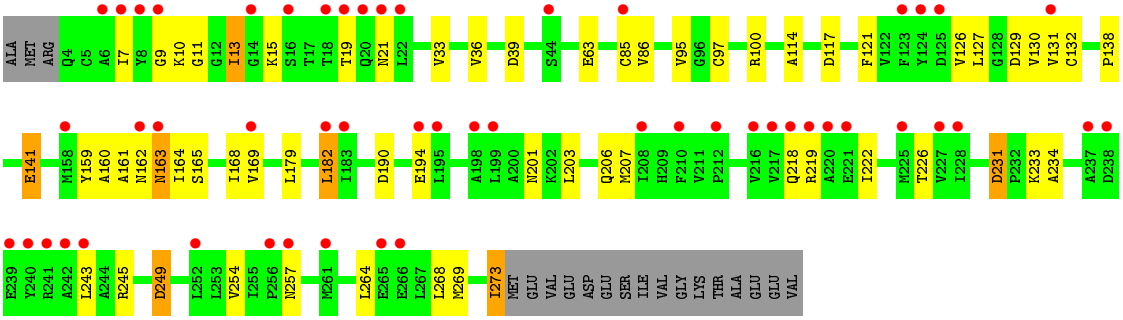
• Molecule 3: Nitrogenase iron protein 1

Chain M:



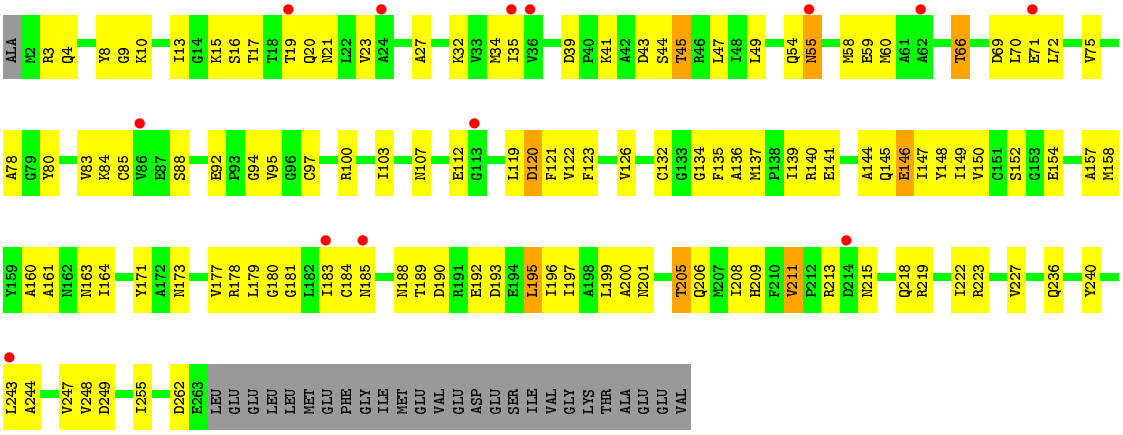
- Molecule 3: Nitrogenase iron protein 1

Chain N:



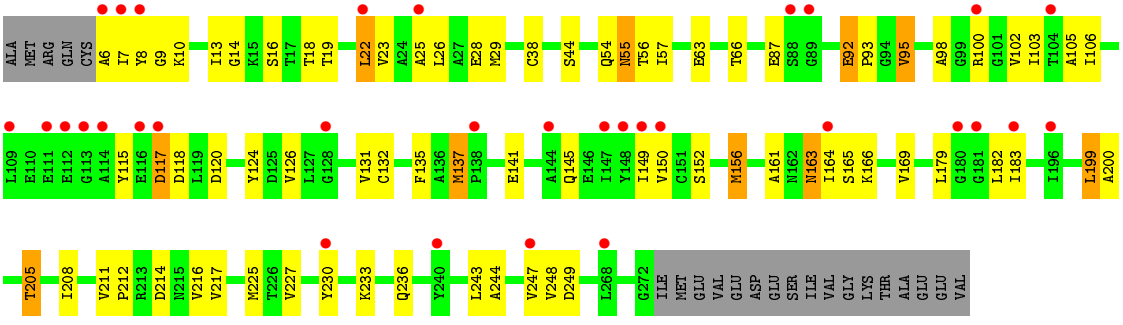
- Molecule 3: Nitrogenase iron protein 1

Chain O:



- Molecule 3: Nitrogenase iron protein 1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.92Å 141.43Å 165.55Å 73.69° 79.37° 76.58°	Depositor
Resolution (Å)	49.43 – 3.10 49.43 – 3.10	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.43-3.10) 80.8 (49.43-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.270 0.214 , 0.252	Depositor DCC
R_{free} test set	10115 reflections (11.55%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.4	EDS
Estimated twinning fraction	0.048 for h,h-k,h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 101183 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	48501	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFN, MG, ADP, 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	0.67	0/3870	0.97	12/5219 (0.2%)
1	C	0.71	0/3870	0.97	11/5219 (0.2%)
1	I	0.67	1/3870 (0.0%)	0.98	12/5219 (0.2%)
1	K	0.68	1/3870 (0.0%)	1.11	10/5219 (0.2%)
2	B	0.78	1/4280 (0.0%)	0.97	6/5786 (0.1%)
2	D	0.76	2/4280 (0.0%)	0.96	7/5786 (0.1%)
2	J	0.77	0/4280	0.96	7/5786 (0.1%)
2	L	0.74	2/4280 (0.0%)	0.98	7/5786 (0.1%)
3	E	0.60	0/2077	1.00	5/2798 (0.2%)
3	F	0.62	0/2106	1.00	3/2836 (0.1%)
3	G	0.66	1/2006 (0.0%)	1.02	4/2703 (0.1%)
3	H	0.55	0/2060	0.98	5/2775 (0.2%)
3	M	0.59	0/2053	0.98	3/2767 (0.1%)
3	N	0.54	0/2065	0.99	8/2783 (0.3%)
3	O	0.62	0/2001	1.01	4/2696 (0.1%)
3	P	0.56	0/2042	0.98	3/2752 (0.1%)
All	All	0.68	8/49010 (0.0%)	0.99	107/66130 (0.2%)

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	2
1	C	0	3
1	I	0	1
1	K	0	1
2	B	0	1
2	D	0	1
2	J	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
3	F	0	1
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	388	CYS	CB-SG	-7.12	1.70	1.82
2	L	113	CYS	CB-SG	-6.13	1.71	1.82
3	G	151	CYS	CB-SG	-5.63	1.72	1.81
2	L	153	CYS	CB-SG	-5.61	1.72	1.81
2	D	388	CYS	CB-SG	-5.35	1.73	1.81

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	182	ARG	NE-CZ-NH1	-27.96	106.32	120.30
1	K	182	ARG	NE-CZ-NH2	26.72	133.66	120.30
2	B	510	ARG	NE-CZ-NH1	-15.74	112.43	120.30
2	L	510	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	K	182	ARG	CD-NE-CZ	14.03	143.24	123.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	A	99	TYR	Sidechain
2	B	12	TYR	Sidechain
1	C	91	TYR	Sidechain
1	C	99	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	3782	0	3720	133	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3782	0	3720	150	0
1	I	3782	0	3720	159	0
1	K	3782	0	3720	148	0
2	B	4174	0	4088	125	0
2	D	4174	0	4088	113	0
2	J	4174	0	4088	129	0
2	L	4174	0	4088	127	0
3	E	2053	0	2069	83	0
3	F	2082	0	2097	117	0
3	G	1983	0	2000	79	0
3	H	2037	0	2052	45	0
3	M	2029	0	2039	86	0
3	N	2041	0	2053	27	0
3	O	1978	0	1991	98	0
3	P	2018	0	2029	48	0
4	B	2	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
6	A	14	0	6	1	0
6	C	14	0	6	1	0
6	I	14	0	6	1	0
6	K	14	0	6	1	0
7	A	18	0	0	2	0
7	C	18	0	0	3	0
7	I	18	0	0	2	0
7	K	18	0	0	3	0
8	B	15	0	0	2	0
8	D	15	0	0	2	0
8	J	15	0	0	2	0
8	L	15	0	0	2	0
9	F	8	0	0	1	0
9	G	8	0	0	0	0
9	N	8	0	0	0	0
9	P	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	27	0	12	0	0
10	F	27	0	12	4	0
10	G	27	0	12	1	0
10	H	27	0	12	0	0
10	M	27	0	12	2	0
10	N	27	0	12	0	0
10	O	27	0	12	0	0
10	P	27	0	12	1	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
11	J	2	0	0	0	0
11	L	2	0	0	0	0
All	All	48501	0	47682	1542	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 18.

The worst 5 of 1542 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:356:GLY:HA2	1:I:380:GLU:HB2	1.42	1.02
1:C:356:GLY:HA2	1:C:380:GLU:HB2	1.36	1.00
1:K:356:GLY:HA2	1:K:380:GLU:HB2	1.40	1.00
1:I:129:LYS:H	1:I:129:LYS:HD2	1.27	0.97
2:B:499:ASN:HD21	2:D:477:HIS:H	1.09	0.95

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	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	52 84
1	C	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	52 84
1	I	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	52 84
1	K	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	52 84
2	B	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	D	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	J	520/522 (100%)	514 (99%)	6 (1%)	0	100 100
2	L	520/522 (100%)	513 (99%)	7 (1%)	0	100 100
3	E	269/289 (93%)	268 (100%)	1 (0%)	0	100 100
3	F	273/289 (94%)	270 (99%)	3 (1%)	0	100 100
3	G	261/289 (90%)	259 (99%)	2 (1%)	0	100 100
3	H	267/289 (92%)	265 (99%)	2 (1%)	0	100 100
3	M	266/289 (92%)	264 (99%)	2 (1%)	0	100 100
3	N	268/289 (93%)	267 (100%)	1 (0%)	0	100 100
3	O	260/289 (90%)	259 (100%)	1 (0%)	0	100 100
3	P	265/289 (92%)	264 (100%)	1 (0%)	0	100 100
All	All	6105/6364 (96%)	6039 (99%)	62 (1%)	4 (0%)	56 88

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	357	GLY
1	A	357	GLY
1	K	357	GLY
1	I	357	GLY

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	406/414 (98%)	386 (95%)	20 (5%)	31 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	406/414 (98%)	389 (96%)	17 (4%)	36 73
1	I	406/414 (98%)	389 (96%)	17 (4%)	36 73
1	K	406/414 (98%)	386 (95%)	20 (5%)	31 68
2	B	454/454 (100%)	428 (94%)	26 (6%)	25 62
2	D	454/454 (100%)	429 (94%)	25 (6%)	27 63
2	J	454/454 (100%)	429 (94%)	25 (6%)	27 63
2	L	454/454 (100%)	430 (95%)	24 (5%)	28 64
3	E	218/233 (94%)	192 (88%)	26 (12%)	6 25
3	F	221/233 (95%)	202 (91%)	19 (9%)	13 45
3	G	210/233 (90%)	187 (89%)	23 (11%)	8 30
3	H	217/233 (93%)	192 (88%)	25 (12%)	7 27
3	M	216/233 (93%)	194 (90%)	22 (10%)	9 33
3	N	217/233 (93%)	193 (89%)	24 (11%)	8 29
3	O	210/233 (90%)	188 (90%)	22 (10%)	8 31
3	P	214/233 (92%)	189 (88%)	25 (12%)	7 26
All	All	5163/5336 (97%)	4803 (93%)	360 (7%)	19 54

5 of 360 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	115	TYR
2	J	45	GLN
3	O	236	GLN
3	H	163	ASN
1	I	77	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	107	ASN
1	I	432	GLN
3	O	163	ASN
3	G	163	ASN
3	H	215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
6	HCA	A	494	7	4,13,13	4.55	3 (75%)	3,18,18	0.46	0
7	CFN	A	496	1,6	6,30,30	0.53	0	0,78,78	0.00	-
8	CLF	B	1498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
6	HCA	C	494	7	4,13,13	4.66	3 (75%)	3,18,18	0.58	0
7	CFN	C	496	1,6	6,30,30	1.14	0	0,78,78	0.00	-
8	CLF	D	3498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
10	ADP	E	1292	-	22,29,29	1.08	1 (4%)	27,45,45	2.06	4 (14%)
9	SF4	F	1290	3	0,12,12	0.00	-	0,24,24	0.00	-
10	ADP	F	2292	5	22,29,29	1.11	2 (9%)	27,45,45	1.74	3 (11%)
9	SF4	G	3290	3	0,12,12	0.00	-	0,24,24	0.00	-
10	ADP	G	3292	5	22,29,29	1.51	4 (18%)	27,45,45	1.97	5 (18%)
10	ADP	H	4292	-	22,29,29	1.28	2 (9%)	27,45,45	1.94	5 (18%)
6	HCA	I	494	7	4,13,13	4.36	3 (75%)	3,18,18	0.44	0
7	CFN	I	496	1,6	6,30,30	1.14	1 (16%)	0,78,78	0.00	-
8	CLF	J	5498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
6	HCA	K	494	7	4,13,13	5.65	3 (75%)	3,18,18	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	CFN	K	496	1,6	6,30,30	0.89	0	0,78,78	0.00	-
8	CLF	L	7498	1,2	0,24,24	0.00	-	0,57,57	0.00	-
10	ADP	M	5292	5	22,29,29	1.14	2 (9%)	27,45,45	1.88	6 (22%)
9	SF4	N	5290	3	0,12,12	0.00	-	0,24,24	0.00	-
10	ADP	N	6292	5	22,29,29	1.22	2 (9%)	27,45,45	1.99	5 (18%)
10	ADP	O	7292	5	22,29,29	1.30	2 (9%)	27,45,45	1.79	4 (14%)
9	SF4	P	7290	3	0,12,12	0.00	-	0,24,24	0.00	-
10	ADP	P	8292	5	22,29,29	1.27	3 (13%)	27,45,45	1.99	7 (25%)

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
6	HCA	A	494	7	-	0/7/17/17	0/0/0/0
7	CFN	A	496	1,6	-	0/0/204/204	0/0/13/13
8	CLF	B	1498	1,2	-	0/0/132/132	0/12/10/10
6	HCA	C	494	7	-	0/7/17/17	0/0/0/0
7	CFN	C	496	1,6	-	0/0/204/204	0/0/13/13
8	CLF	D	3498	1,2	-	0/0/132/132	0/12/10/10
10	ADP	E	1292	-	-	0/12/32/32	0/3/3/3
9	SF4	F	1290	3	-	0/0/48/48	0/6/5/5
10	ADP	F	2292	5	-	0/12/32/32	0/3/3/3
9	SF4	G	3290	3	-	0/0/48/48	0/6/5/5
10	ADP	G	3292	5	-	0/12/32/32	0/3/3/3
10	ADP	H	4292	-	-	0/12/32/32	0/3/3/3
6	HCA	I	494	7	-	0/7/17/17	0/0/0/0
7	CFN	I	496	1,6	-	0/0/204/204	0/0/13/13
8	CLF	J	5498	1,2	-	0/0/132/132	0/12/10/10
6	HCA	K	494	7	-	0/7/17/17	0/0/0/0
7	CFN	K	496	1,6	-	0/0/204/204	0/0/13/13
8	CLF	L	7498	1,2	-	0/0/132/132	0/12/10/10
10	ADP	M	5292	5	-	0/12/32/32	0/3/3/3
9	SF4	N	5290	3	-	0/0/48/48	0/6/5/5
10	ADP	N	6292	5	-	0/12/32/32	0/3/3/3
10	ADP	O	7292	5	-	0/12/32/32	0/3/3/3
9	SF4	P	7290	3	-	0/0/48/48	0/6/5/5
10	ADP	P	8292	5	-	0/12/32/32	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	494	HCA	C4-C3	-8.54	1.42	1.53
6	I	494	HCA	C4-C3	-7.42	1.43	1.53
6	C	494	HCA	C4-C3	-6.65	1.44	1.53
6	A	494	HCA	C4-C3	-5.98	1.45	1.53
6	C	494	HCA	C2-C3	-5.64	1.46	1.54

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	1292	ADP	N3-C2-N1	-7.99	122.78	128.89
10	G	3292	ADP	N3-C2-N1	-7.49	123.16	128.89
10	P	8292	ADP	N3-C2-N1	-7.06	123.48	128.89
10	M	5292	ADP	N3-C2-N1	-6.89	123.62	128.89
10	H	4292	ADP	N3-C2-N1	-6.79	123.70	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	494	HCA	1	0
7	A	496	CFN	2	0
8	B	1498	CLF	2	0
6	C	494	HCA	1	0
7	C	496	CFN	3	0
8	D	3498	CLF	2	0
9	F	1290	SF4	1	0
10	F	2292	ADP	4	0
10	G	3292	ADP	1	0
6	I	494	HCA	1	0
7	I	496	CFN	2	0
8	J	5498	CLF	2	0
6	K	494	HCA	1	0
7	K	496	CFN	3	0
8	L	7498	CLF	2	0
10	M	5292	ADP	2	0
10	P	8292	ADP	1	0

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	476/491 (96%)	-0.54	0 100 100	16, 34, 57, 86	7 (1%)
1	C	476/491 (96%)	-0.48	0 100 100	15, 33, 58, 85	6 (1%)
1	I	476/491 (96%)	-0.44	0 100 100	18, 35, 59, 86	0
1	K	476/491 (96%)	-0.47	1 (0%) 95 91	15, 34, 58, 85	3 (0%)
2	B	522/522 (100%)	-0.60	0 100 100	9, 28, 49, 69	8 (1%)
2	D	522/522 (100%)	-0.56	0 100 100	9, 28, 49, 69	2 (0%)
2	J	522/522 (100%)	-0.60	0 100 100	10, 29, 50, 69	1 (0%)
2	L	522/522 (100%)	-0.62	1 (0%) 95 91	9, 29, 51, 70	1 (0%)
3	E	252/289 (87%)	0.33	28 (11%) 7 2	52, 87, 114, 127	65 (25%)
3	F	270/289 (93%)	0.09	13 (4%) 34 15	45, 81, 116, 131	43 (15%)
3	G	257/289 (88%)	-0.13	4 (1%) 74 55	34, 73, 111, 128	49 (19%)
3	H	170/289 (58%)	0.47	18 (10%) 8 3	56, 86, 114, 121	55 (32%)
3	M	253/289 (87%)	0.17	17 (6%) 21 7	55, 93, 126, 134	72 (28%)
3	N	157/289 (54%)	1.46	52 (33%) 0 0	74, 103, 129, 138	77 (49%)
3	O	260/289 (89%)	-0.02	13 (5%) 32 13	54, 82, 115, 131	61 (23%)
3	P	190/289 (65%)	0.81	32 (16%) 2 1	70, 100, 124, 131	54 (28%)
All	All	5801/6364 (91%)	-0.27	179 (3%) 52 28	9, 38, 106, 138	504 (8%)

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	18	THR	10.4
3	N	19	THR	9.4
3	N	22	LEU	8.1
3	E	88	SER	6.7
3	N	256	PRO	6.6

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	HCA	C	494	14/14	0.94	0.34	3.57	18,22,30,32	0
6	HCA	A	494	14/14	0.95	0.25	1.26	21,25,29,30	0
6	HCA	I	494	14/14	0.98	0.29	1.12	19,27,32,37	0
5	MG	M	5291	1/1	0.89	0.24	1.04	47,47,47,47	0
6	HCA	K	494	14/14	0.96	0.25	0.99	17,23,31,33	0
7	CFN	C	496	18/18	0.99	0.23	0.90	9,15,18,18	0
5	MG	O	7291	1/1	0.92	0.25	0.62	39,39,39,39	0
7	CFN	A	496	18/18	0.99	0.21	0.50	14,19,23,28	0
7	CFN	I	496	18/18	0.99	0.21	0.49	17,22,25,27	0
5	MG	F	2291	1/1	0.88	0.21	0.48	23,23,23,23	0
8	CLF	J	5498	15/15	0.99	0.24	0.29	21,27,34,35	0
5	MG	E	1291	1/1	0.97	0.19	0.09	44,44,44,44	0
7	CFN	K	496	18/18	0.99	0.20	0.06	12,21,25,26	0
8	CLF	D	3498	15/15	0.99	0.23	-0.04	15,20,28,29	0
4	CA	J	8492	1/1	0.87	0.17	-0.17	42,42,42,42	0
8	CLF	B	1498	15/15	0.99	0.21	-0.24	17,21,30,33	0
8	CLF	L	7498	15/15	0.99	0.20	-0.28	24,28,34,35	0
10	ADP	P	8292	27/27	0.80	0.21	-0.30	114,122,127,128	0
4	CA	B	4492	1/1	0.97	0.19	-0.44	32,32,32,32	0
10	ADP	O	7292	27/27	0.92	0.18	-0.47	66,81,93,96	0
10	ADP	G	3292	27/27	0.90	0.17	-0.53	50,56,59,60	0
10	ADP	E	1292	27/27	0.92	0.15	-0.58	61,68,71,73	0
5	MG	G	3291	1/1	0.80	0.16	-0.60	41,41,41,41	0
10	ADP	H	4292	27/27	0.90	0.14	-0.79	124,133,136,136	10
10	ADP	F	2292	27/27	0.88	0.16	-0.85	68,75,91,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CA	B	2492	1/1	0.95	0.16	-0.92	34,34,34,34	0
10	ADP	M	5292	27/27	0.91	0.15	-0.96	78,82,85,87	0
10	ADP	N	6292	27/27	0.70	0.20	-1.04	139,148,148,149	10
4	CA	L	6492	1/1	0.98	0.14	-1.36	37,37,37,37	0
9	SF4	N	5290	8/8	0.98	0.09	-1.61	53,57,60,63	0
9	SF4	F	1290	8/8	0.98	0.15	-1.83	55,59,61,62	0
9	SF4	P	7290	8/8	0.97	0.10	-1.99	74,76,80,82	0
9	SF4	G	3290	8/8	0.99	0.09	-2.10	42,46,48,49	0
5	MG	H	4291	1/1	0.90	0.18	-	68,68,68,68	0
5	MG	P	8291	1/1	0.86	0.16	-	66,66,66,66	0
5	MG	N	6291	1/1	0.84	0.09	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.