

Supporting Information

The Fe–V Cofactor of Vanadium Nitrogenase Contains an Interstitial Carbon Atom

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Contents

Geometry-optimized coordinates of 225 atom models of FeMoco and FeVco.

FeMoco

Fe	10.114690	-7.703790	55.997150
Fe	12.592775	-8.339455	55.593136
Fe	11.356470	-7.022600	53.763435
Fe	11.989671	-5.848783	55.995784
Fe	14.842328	-7.594401	54.593006
Fe	13.612667	-6.211558	52.817352
Fe	14.234095	-5.136327	54.988659
Mo	16.077071	-5.653495	53.244568
C	13.102740	-6.709656	54.635949
S	11.807082	-7.458315	57.529824
S	16.171063	-6.063151	55.523514
S	9.960555	-5.706635	54.999953
S	13.080692	-4.002049	56.434792
S	14.474498	-9.492158	55.653370
S	14.345906	-4.097768	53.045264
S	10.859698	-9.137724	54.335204
S	15.240920	-7.632743	52.391762
S	11.782288	-6.521044	51.634265
S	8.472275	-8.499543	57.326499
C	13.316384	-2.413022	49.965591
N	12.425824	-3.225190	50.780743
C	11.214124	-2.866263	51.225022
N	10.617098	-1.750139	50.745069
N	10.601417	-3.600968	52.165990
C	15.063349	-1.104757	59.472637
C	16.188172	-0.874018	58.459017
C	17.508370	-1.552718	58.851301
O	17.846567	-1.662403	60.041149
N	18.260644	-1.971887	57.810564
C	8.309011	-1.265150	60.668388
C	9.374563	-2.061132	59.971486
N	9.875068	-3.240159	60.503655
C	9.991673	-1.799698	58.749682
C	10.769159	-3.680906	59.620493
N	10.872615	-2.844130	58.547194
C	8.218378	-4.722853	49.893699
C	7.616688	-4.456436	51.253789
C	6.932230	-3.258140	51.549364
C	7.714039	-5.417041	52.289939
C	6.363728	-3.027760	52.816367
C	7.145403	-5.207436	53.550653
C	6.462765	-4.004559	53.826707
O	5.935693	-3.849413	55.071069
N	5.189974	-10.309180	55.594579
C	6.173738	-9.891618	56.595389
C	5.372065	-9.531258	57.863129
O	4.442077	-8.724396	57.807398
C	7.068687	-8.715081	56.169104
N	5.716086	-10.192512	59.005750
C	18.209415	-9.757026	57.686986
O	19.094079	-9.519956	58.511731
N	17.022321	-9.107395	57.576854
C	16.598814	-8.045138	58.475762
C	15.682461	-8.583320	59.581185
O	16.125776	-9.030411	60.643646
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C	12.513295	-10.226553	59.894688

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C	12.246939	-12.884970	57.402563
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N	13.244929	-12.587316	56.525002
C	13.844459	-13.595855	55.652239
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C	13.298223	-12.256689	53.530919
C	13.906853	-11.237475	52.565863
N	12.863176	-10.515558	51.830452
C	13.085663	-9.875832	50.675674
N	14.352179	-9.731156	50.219331
N	12.048040	-9.448131	49.915097
O	22.411739	-6.803003	47.266653
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C	18.655893	-7.288474	51.993059
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C	18.924365	-6.615980	54.069419
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C	17.605447	-1.196886	54.030510
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O	16.609054	-4.901531	51.303459
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O	17.404062	-3.972800	53.533269
O	15.606667	-5.093831	47.074467
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O	18.255575	-4.325647	47.685024
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O	20.524911	-4.348752	55.182937
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H	11.140540	-12.084535	59.042750
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H	17.303605	-8.180622	50.566094
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H	21.375800	-6.743019	50.065050
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H	19.135600	-4.673373	47.939202
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H	18.071230	-1.626023	49.696796
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H	20.609893	0.870359	55.368459
H	19.201791	0.248679	55.392978
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H	19.720233	1.683846	50.542538
H	20.409897	0.153968	52.186029
H	18.950918	0.359428	52.702384
H	20.888560	-7.383400	54.327013
H	9.833968	-1.368058	51.257433
H	11.130253	-9.531265	50.337970
C	23.423591	-8.025902	52.090595
C	24.594596	-7.467753	51.291413
O	25.669951	-8.083136	51.178192
N	24.384662	-6.235359	50.751332
C	25.386619	-5.627016	49.892543
C	24.767845	-4.525655	49.023980
O	22.298862	-7.556026	55.236596
H	17.346543	-3.350389	54.345803
H	23.080988	-7.317130	52.842857
H	23.739240	-8.957282	52.567397
H	22.607203	-8.212979	51.383416
H	23.453909	-5.788887	50.794369
H	26.204923	-5.207831	50.498231
H	25.838195	-6.411758	49.270537
H	24.340503	-3.729918	49.643640
H	23.952123	-4.935911	48.419877
H	25.522670	-4.092421	48.358913
H	22.888649	-6.825622	54.914125
H	22.782379	-8.370279	55.048978

FeVco

Fe	10.06665618106691	-7.72920787434537	56.08067386623114
Fe	12.58277956978973	-8.37900718752773	55.65506007634426
Fe	11.30538416389474	-7.06686187740933	53.78562181287211
Fe	11.97717881867746	-5.84751057013968	56.07621774479177
Fe	14.86266080982731	-7.62893603064411	54.65543456008214
Fe	13.59522126237661	-6.24259950347247	52.82373090422340
Fe	14.22689199744966	-5.10597386906711	55.01891501243668

V	16.18064042709096	-5.68218785570081	53.20723801524418
C	13.08219632481630	-6.74124572668077	54.68264077448573
S	11.78052034145107	-7.47848968294182	57.61743260629350
S	16.22019439653405	-6.00271589950703	55.49849779593968
S	9.91821732600423	-5.72115738602787	55.07352310352677
S	13.09907509784662	-4.01963821229400	56.57683787745588
S	14.46114995800933	-9.57093917143504	55.71858123502280
S	14.38455681637458	-4.11084801844825	53.01736435989789
S	10.80746387071428	-9.20502759925486	54.40929358119582
S	15.28743668654594	-7.64941217360487	52.41388267079939
S	11.71019794566769	-6.56387262042048	51.63647010806233
S	8.39481523167303	-8.47684921451968	57.42633741516953
C	13.31638401160193	-2.41302199869100	49.96559102590154
N	12.42582395363956	-3.22519004052874	50.78074290009194
C	11.21412412870424	-2.86626298133521	51.22502212277942
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N	10.60141689996648	-3.60096802991584	52.16598992853930
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C	16.18817193164066	-0.87401804530651	58.45901698746828
C	17.50837016924337	-1.55271789351203	58.85130102938035
O	17.84656695100814	-1.66240303755265	60.04114898284882
N	18.26064391177471	-1.97188705459007	57.81056400788281
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C	9.37456300512751	-2.06113199595091	59.97148599955102
N	9.87506799737523	-3.24015900152209	60.50365499627240
C	9.99167300571269	-1.79969799998963	58.74968200172899
C	10.76915900002499	-3.68090599734465	59.62049300814185
N	10.87261499577986	-2.84413000420620	58.54719398978931
C	8.21837800417380	-4.72285303682557	49.89369906892578
C	7.61668799757506	-4.45643590242411	51.25378886305576
C	6.93223000851967	-3.25814006312559	51.54936407701768
C	7.71403911302380	-5.41704094237655	52.28993906789410
C	6.36372796356810	-3.02776000082182	52.81636697678010
C	7.14540288409979	-5.20743608091442	53.55065296553154
C	6.46276507346937	-4.00455895960756	53.82670701882559
O	5.93569300254142	-3.84941300305243	55.07106899914216
N	5.18997399814692	-10.30918001173405	55.59457899557496
C	6.17373799495537	-9.89161797842726	56.59538900295792
C	5.37114741702238	-9.53183790966148	57.86220833475056
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N	17.02232102156402	-9.10739497435354	57.57685399885823
C	16.59881398956715	-8.04513802877832	58.47576200765151
C	15.68246101108924	-8.58331994962198	59.58118499482923
O	16.12577600117538	-9.03041102107562	60.64364599707933
N	14.34720902476877	-8.55452805102573	59.27808900985899
C	13.34842493871262	-8.98273094575736	60.22950396839815
C	12.51329521720782	-10.22655314697091	59.89468809598946
O	11.82046194450553	-10.75461296518024	60.77344198745303
N	12.56663778407901	-10.67093380484409	58.60339186370370
C	11.63872808539059	-11.69232310874084	58.15400208249857
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N	14.35217902712681	-9.73115599939598	50.21933100171135
N	12.04804001580772	-9.44813100842709	49.91509700290752
O	22.41173899243418	-6.80300299309927	47.26665300812319
C	18.10543000033571	-7.43245299992693	50.61133099711081
C	18.66327439597313	-7.35174810086762	51.99321740959866
N	18.07348560869041	-6.67806479558616	53.05745137573169
C	19.88539600218375	-7.82580320105410	52.41858571089556
C	18.93678470394589	-6.72812609224335	54.07134049889316
N	20.03512630249169	-7.42273445131863	53.72735561070878
C	17.62106100239840	-1.21475216294637	54.04539129022421
C	17.11606132195027	-1.75315055494611	52.70716843969404
C	17.75884393329219	-3.12412888042451	52.41462984544750
C	19.29452480894392	-3.01640924212517	52.25053232905003
C	19.85727154965518	-4.22188733338566	51.50451562619888
C	21.34709606794287	-4.47902787371764	51.60067865573090
C	17.15654953529355	-3.75421408194395	51.15065606101057
O	17.46082637635497	-1.95998498897880	55.04523269882966
O	18.18257356906622	-0.07211786629718	54.07537997806329
O	21.90861132758066	-4.94334124418498	50.54553604419028
O	21.94082961409434	-4.29709482703218	52.69110941242423
O	16.63818238782730	-4.90758579537934	51.30256652768080
O	17.25040659911778	-3.15957273962754	50.05486638062890
O	17.47218355597652	-4.01896472957091	53.49184795090382
O	15.60666700268119	-5.09383100223536	47.07446698838238
O	20.55280799281125	-3.04682199764652	45.68019899405552
O	20.97262002343478	-2.04537498649150	56.44251799448381
O	14.51280698463428	-5.46942597238272	49.69713003462189
O	21.34351100400783	-7.62745700172003	49.65665099999433
O	20.91616402089468	-4.71119101094311	48.06139600202062
O	18.25557499206339	-4.32564699145745	47.68502400080805
O	23.74274400213028	-5.61366600574374	54.16831999277097
O	18.53391599429017	-0.79243401476921	49.48314899245386
O	20.52491099239986	-4.34875200105820	55.18293700237192
O	20.00008799720579	0.41245099848886	55.96222000507066
O	19.85130200417328	2.01969601196704	49.63645499606432
O	19.53955700458074	0.46174699835395	51.90121700756075
H	14.09892554173047	-3.07937621034477	49.59518366113348
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