Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:36 AM EST

PDB ID	:	7T30
EMDB ID	:	EMD-25647
Title	:	Structure of electron bifurcating Ni-Fe hydrogenase complex HydABCSL in FMN/NAD(H) bound state
Authors	:	Feng, X.; Li, H.
Deposited on	:	2021-12-06
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

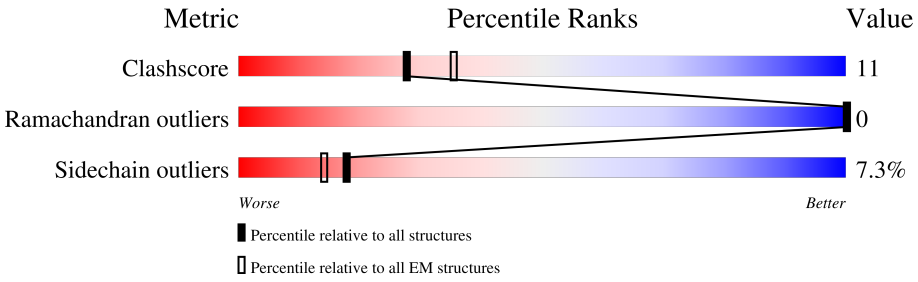
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	692	70% 23%
1	F	692	70% 23%
2	B	597	52% 17% 29%
2	G	597	51% 18% 29%
3	C	156	31% 13% 54%
3	H	156	31% 13% 54%
4	D	475	70% 23% 6%
4	I	475	71% 22% 6%

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Mol	Chain	Length	Quality of chain
5	E	179	
5	J	179	

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
11	FCO	D	502	-	-	X	-
11	FCO	I	502	-	-	X	-
6	FES	A	701	-	-	X	-
6	FES	F	701	-	-	X	-
7	SF4	A	702	-	-	X	-
7	SF4	A	703	-	-	X	-
7	SF4	A	704	-	-	X	-
7	SF4	B	702	-	-	X	-
7	SF4	F	702	-	-	X	-
7	SF4	F	703	-	-	X	-
7	SF4	F	704	-	-	X	-
7	SF4	G	702	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28126 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NiFe hydrogenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	666	Total	C	N	O	S	0	0
			5183	3273	906	961	43		
1	F	666	Total	C	N	O	S	0	0
			5183	3273	906	961	43		

- Molecule 2 is a protein called NiFe hydrogenase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	425	Total	C	N	O	S	0	0
			3236	2046	551	609	30		
2	G	425	Total	C	N	O	S	0	0
			3236	2046	551	609	30		

- Molecule 3 is a protein called NiFe hydrogenase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			570	373	95	101	1		
3	H	72	Total	C	N	O	S	0	0
			570	373	95	101	1		

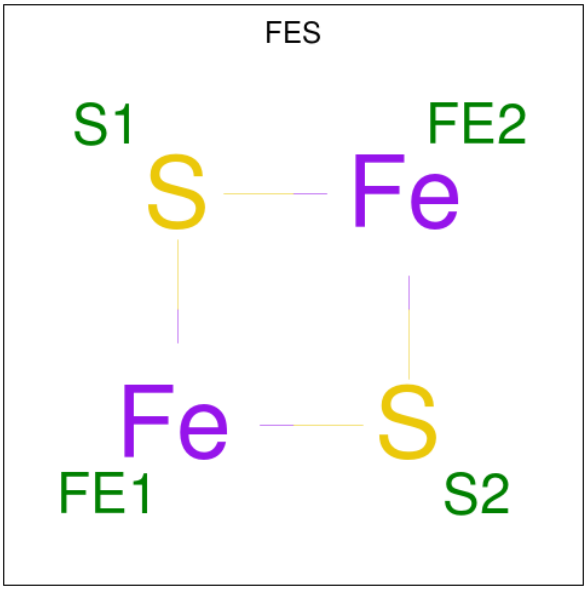
- Molecule 4 is a protein called NiFe hydrogenase large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	447	Total	C	N	O	S	0	0
			3537	2264	615	642	16		
4	I	447	Total	C	N	O	S	0	0
			3537	2264	615	642	16		

- Molecule 5 is a protein called NiFe hydrogenase small subunit.

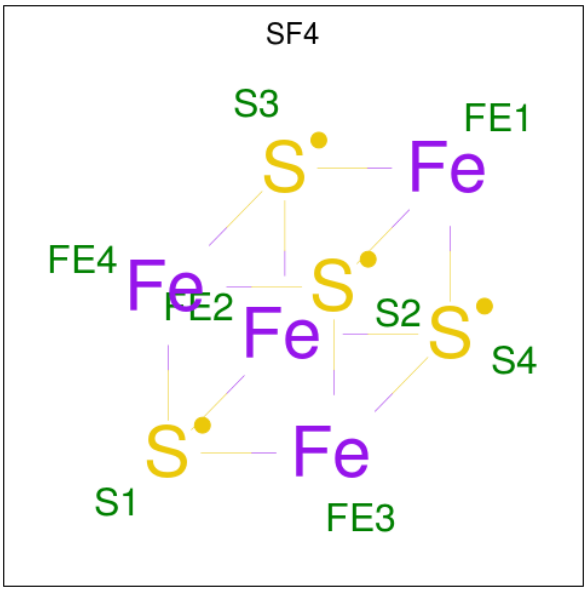
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	179	Total	C	N	O	S	0	0
			1398	900	225	261	12		
5	J	179	Total	C	N	O	S	0	0
			1398	900	225	261	12		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



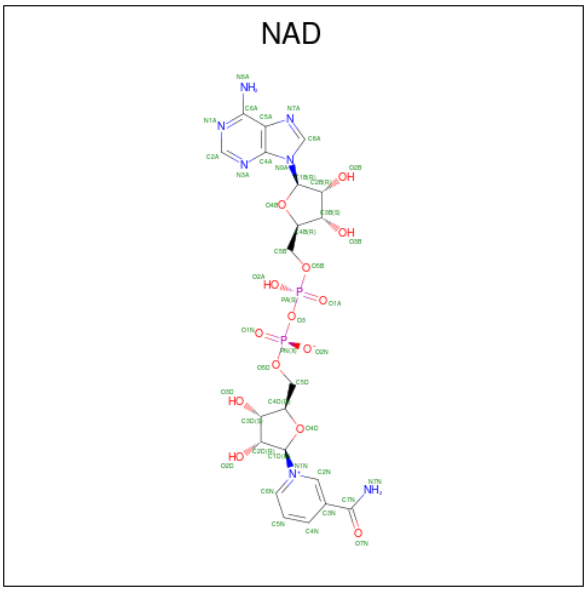
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	Fe	S		0
			4	2	2		
6	B	1	Total	Fe	S		0
			4	2	2		
6	F	1	Total	Fe	S		0
			4	2	2		
6	G	1	Total	Fe	S		0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



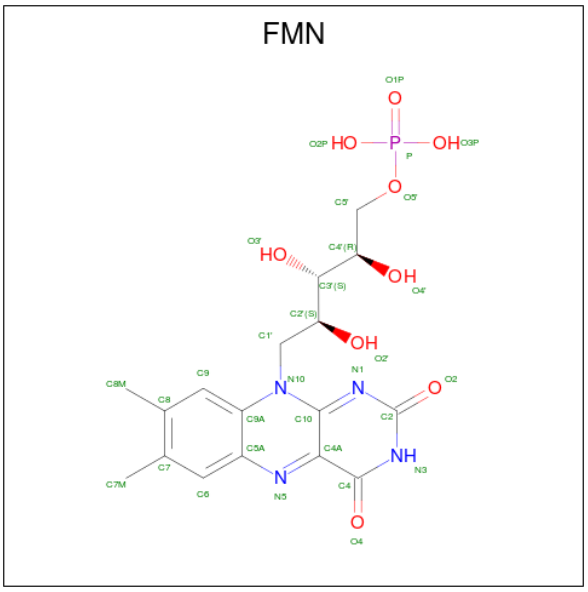
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Fe S 32 16 16	0
7	A	1	Total Fe S 32 16 16	0
7	A	1	Total Fe S 32 16 16	0
7	A	1	Total Fe S 32 16 16	0
7	B	1	Total Fe S 8 4 4	0
7	E	1	Total Fe S 8 4 4	0
7	F	1	Total Fe S 32 16 16	0
7	F	1	Total Fe S 32 16 16	0
7	F	1	Total Fe S 32 16 16	0
7	F	1	Total Fe S 32 16 16	0
7	G	1	Total Fe S 8 4 4	0
7	J	1	Total Fe S 8 4 4	0

- Molecule 8 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
8	G	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

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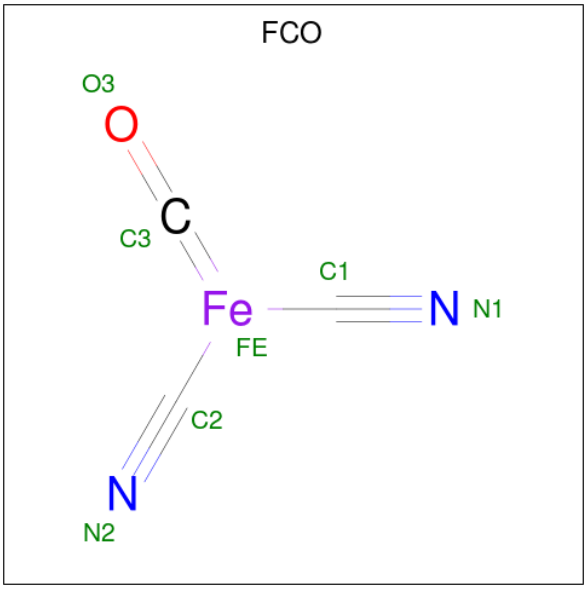
Mol	Chain	Residues	Atoms					AltConf
9	G	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 10 is NICKEL (III) ION (three-letter code: 3NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Ni	0
			1	1	
10	I	1	Total	Ni	0
			1	1	

- Molecule 11 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).



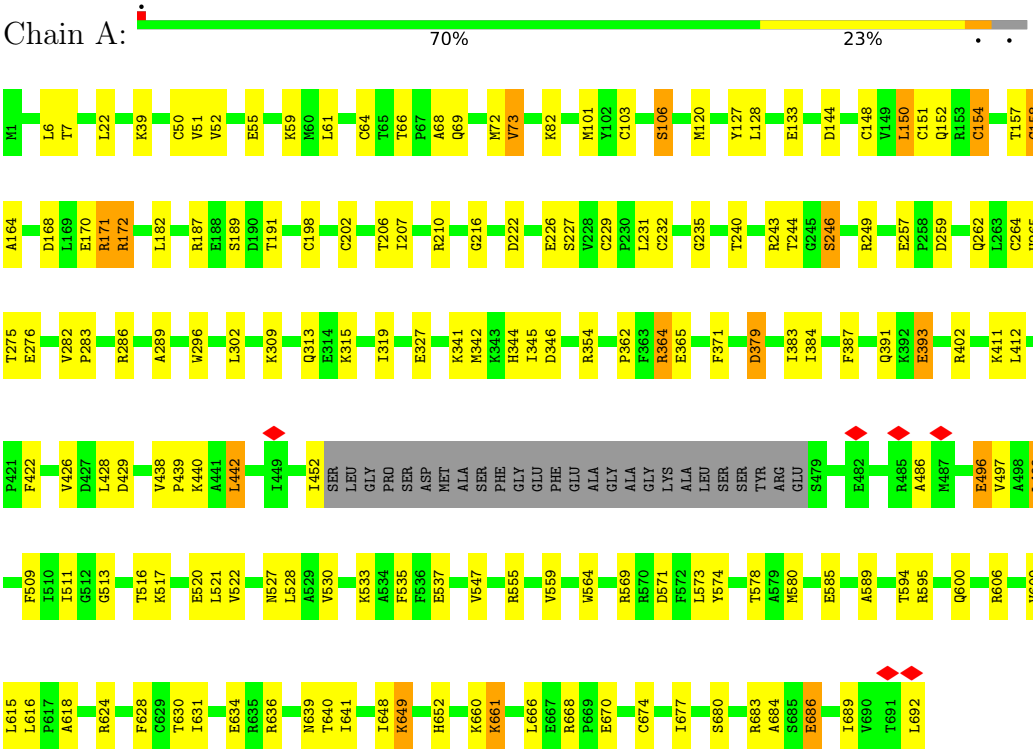
Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	Fe	N	O	0
			7	3	1	2	1	
11	I	1	Total	C	Fe	N	O	0
			7	3	1	2	1	

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

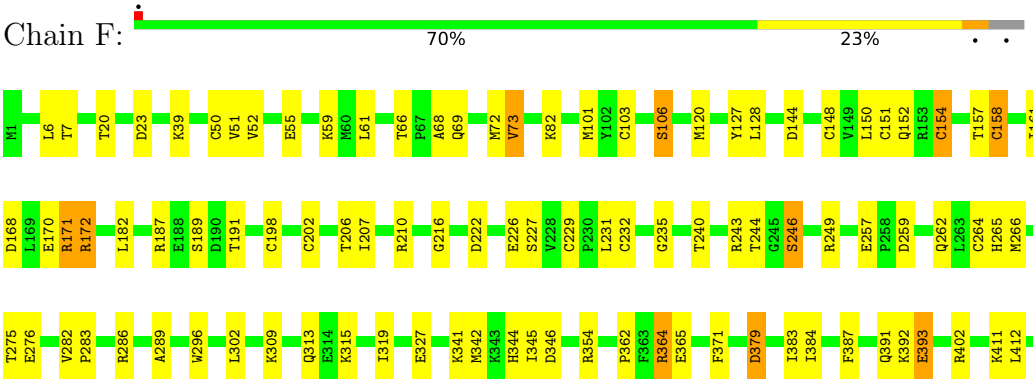
• Molecule 1: NiFe hydrogenase subunit A

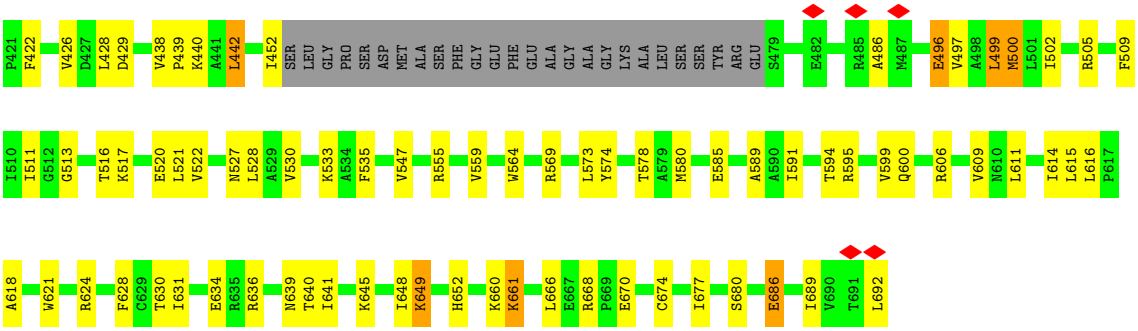
Chain A:



• Molecule 1: NiFe hydrogenase subunit A

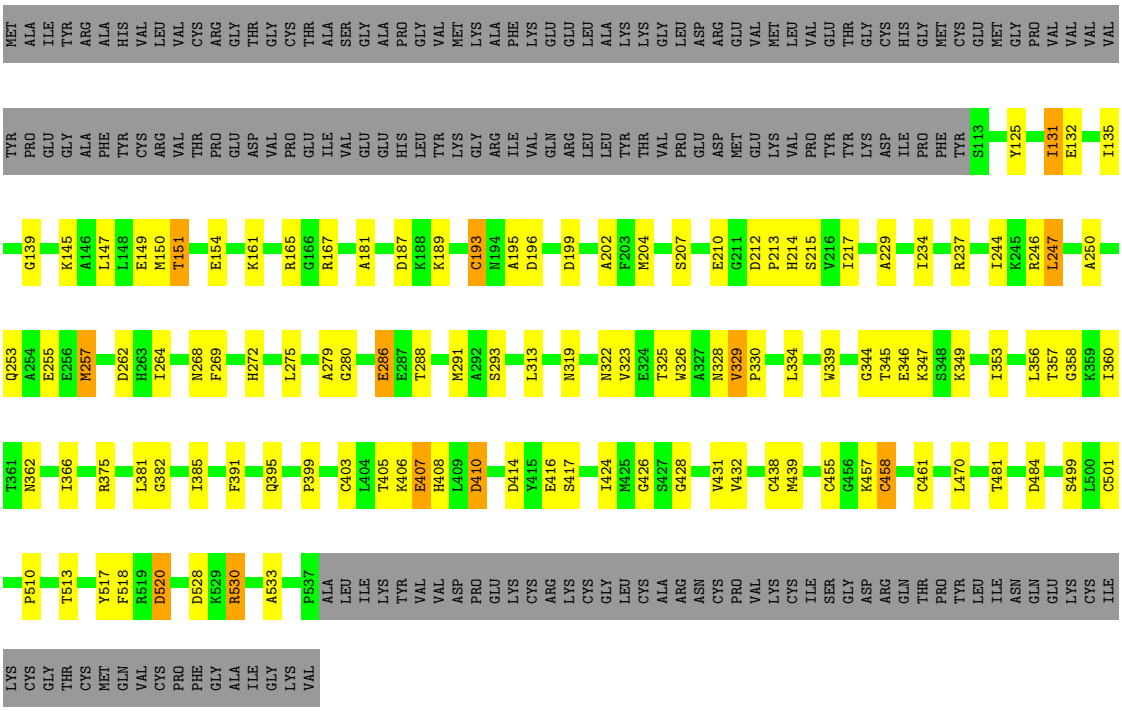
Chain F:





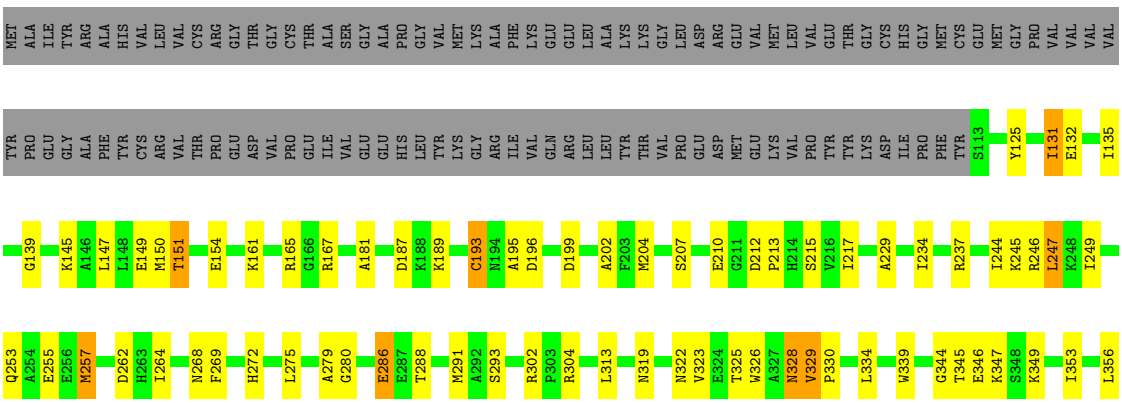
• Molecule 2: NiFe hydrogenase subunit B

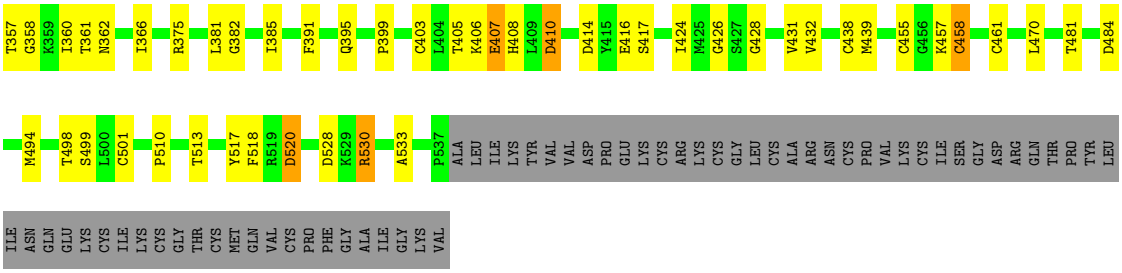
Chain B:



• Molecule 2: NiFe hydrogenase subunit B

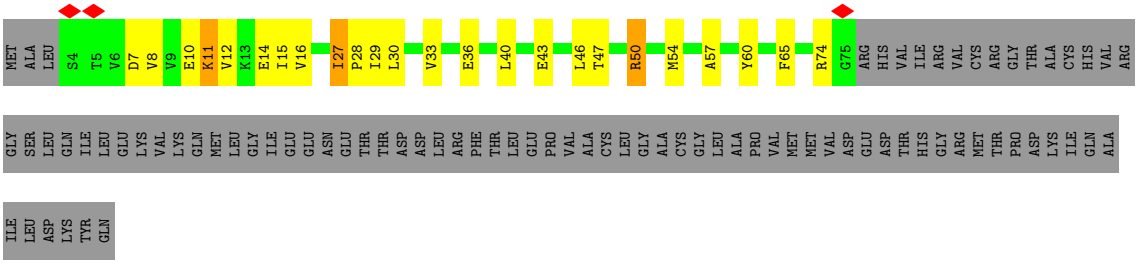
Chain G:





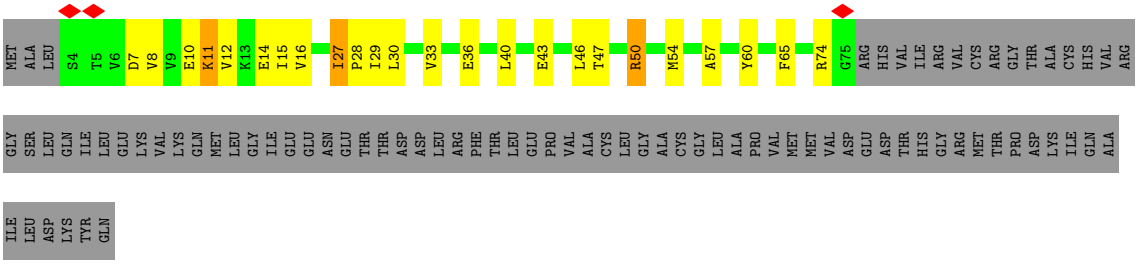
• Molecule 3: NiFe hydrogenase subunit C

Chain C:



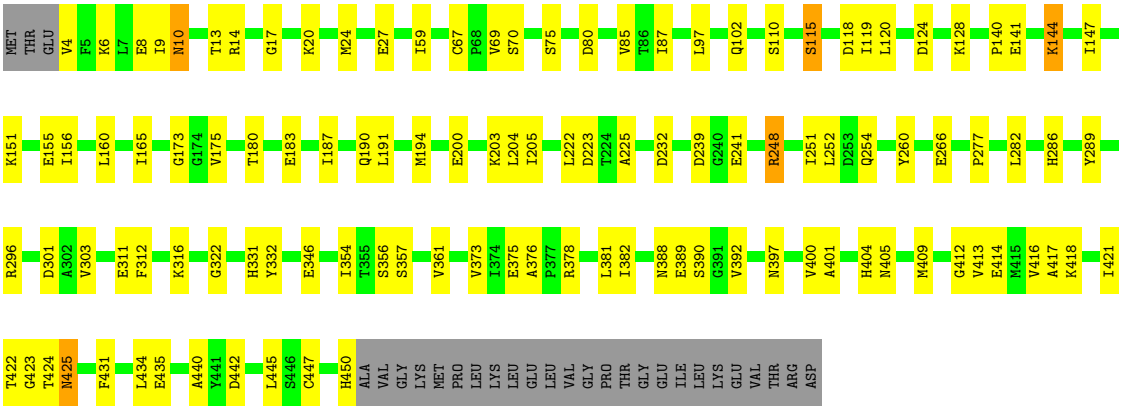
• Molecule 3: NiFe hydrogenase subunit C

Chain H:



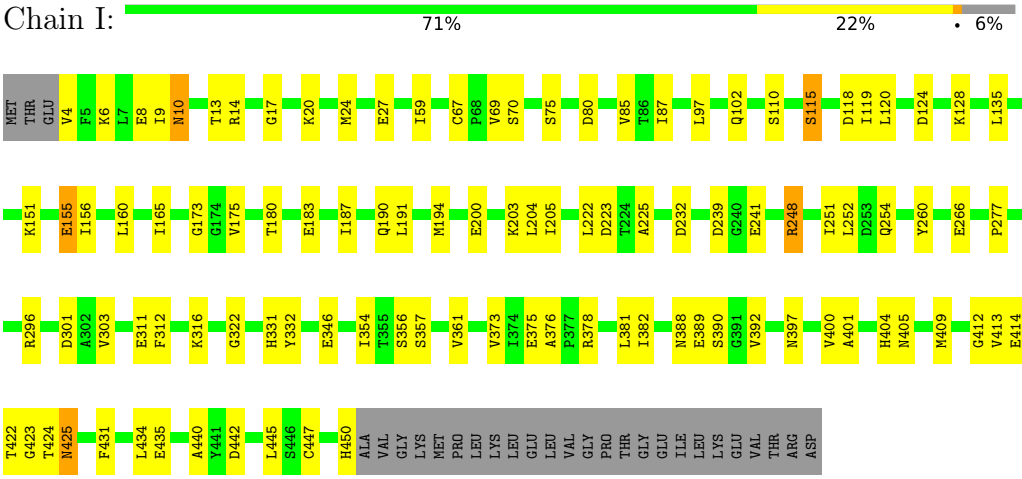
• Molecule 4: NiFe hydrogenase large subunit

Chain D:



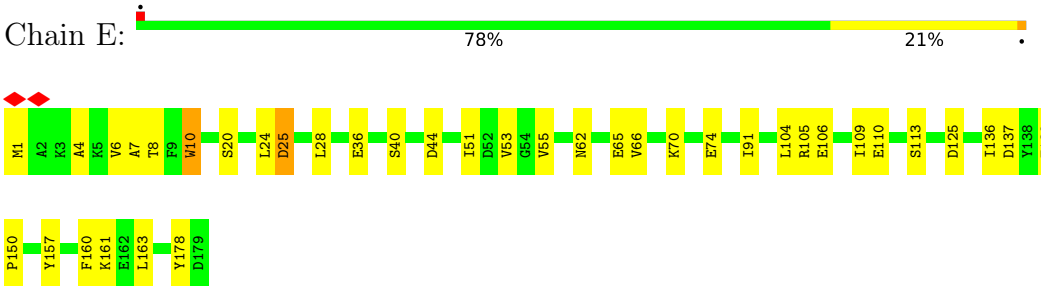
• Molecule 4: NiFe hydrogenase large subunit

Chain I:



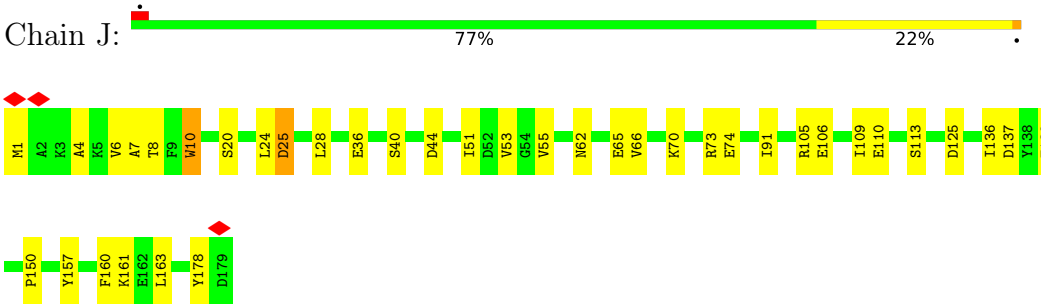
• Molecule 5: NiFe hydrogenase small subunit

Chain E:



• Molecule 5: NiFe hydrogenase small subunit

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217361	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.252	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	231.84, 231.84, 231.84	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 3NI, FES, FCO, FMN, 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	0.36	0/5280	0.51	0/7143
1	F	0.36	0/5280	0.51	0/7143
2	B	0.32	0/3299	0.50	0/4445
2	G	0.32	0/3299	0.50	0/4445
3	C	0.27	0/582	0.44	0/787
3	H	0.27	0/582	0.44	0/787
4	D	0.30	0/3624	0.44	0/4908
4	I	0.30	0/3624	0.44	0/4908
5	E	0.31	0/1429	0.46	0/1941
5	J	0.31	0/1429	0.46	0/1941
All	All	0.33	0/28428	0.48	0/38448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5183	0	5228	117	0
1	F	5183	0	5228	118	0
2	B	3236	0	3239	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3236	0	3239	82	0
3	C	570	0	594	15	0
3	H	570	0	594	15	0
4	D	3537	0	3534	83	0
4	I	3537	0	3534	81	0
5	E	1398	0	1399	28	0
5	J	1398	0	1399	28	0
6	A	4	0	0	2	0
6	B	4	0	0	0	0
6	F	4	0	0	2	0
6	G	4	0	0	0	0
7	A	32	0	0	17	0
7	B	8	0	0	13	0
7	E	8	0	0	0	0
7	F	32	0	0	17	0
7	G	8	0	0	13	0
7	J	8	0	0	0	0
8	B	44	0	26	1	0
8	G	44	0	26	1	0
9	B	31	0	19	0	0
9	G	31	0	19	0	0
10	D	1	0	0	0	0
10	I	1	0	0	0	0
11	D	7	0	0	4	0
11	I	7	0	0	4	0
All	All	28126	0	28078	600	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 11.

All (600) 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)
2:B:501:CYS:SG	7:B:702:SF4:FE2	1.02	1.49
2:G:501:CYS:SG	7:G:702:SF4:FE2	1.02	1.48
2:G:455:CYS:SG	7:G:702:SF4:FE4	1.07	1.46
2:B:455:CYS:SG	7:B:702:SF4:FE4	1.07	1.45
2:B:458:CYS:SG	7:B:702:SF4:FE1	1.18	1.35
2:G:458:CYS:SG	7:G:702:SF4:FE1	1.18	1.33
1:A:264:CYS:SG	7:A:704:SF4:FE1	1.37	1.15
1:F:264:CYS:SG	7:F:704:SF4:FE1	1.37	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:10:ASN:HB3	4:I:20:LYS:HG3	1.26	1.10
4:D:10:ASN:HB3	4:D:20:LYS:HG3	1.26	1.08
1:A:232:CYS:HG	7:A:704:SF4:FE2	0.66	0.97
1:F:50:CYS:HG	6:F:701:FES:FE2	0.66	0.96
2:G:438:CYS:HB2	2:G:533:ALA:HB2	1.48	0.95
1:A:264:CYS:HG	7:A:704:SF4:FE1	0.76	0.93
1:F:229:CYS:SG	7:F:704:SF4:FE3	1.59	0.93
2:B:438:CYS:HB2	2:B:533:ALA:HB2	1.48	0.93
1:A:229:CYS:SG	7:A:704:SF4:FE3	1.59	0.93
1:F:154:CYS:HG	7:F:702:SF4:FE3	0.81	0.93
1:F:232:CYS:HG	7:F:704:SF4:FE2	0.63	0.92
1:F:264:CYS:HG	7:F:704:SF4:FE1	0.78	0.92
1:A:202:CYS:HG	7:A:702:SF4:FE1	0.88	0.90
1:A:151:CYS:SG	7:A:702:SF4:FE4	1.64	0.90
1:A:50:CYS:HG	6:A:701:FES:FE2	0.66	0.89
1:A:154:CYS:HG	7:A:702:SF4:FE3	0.68	0.89
1:A:438:VAL:HG11	1:A:520:GLU:HB3	1.53	0.88
1:F:151:CYS:SG	7:F:702:SF4:FE4	1.64	0.88
1:F:438:VAL:HG11	1:F:520:GLU:HB3	1.53	0.88
1:F:158:CYS:SG	7:F:703:SF4:FE2	1.66	0.88
1:F:202:CYS:HG	7:F:702:SF4:FE1	0.85	0.86
1:A:158:CYS:SG	7:A:703:SF4:FE2	1.66	0.86
4:I:10:ASN:CB	4:I:20:LYS:HG3	2.06	0.85
4:D:10:ASN:CB	4:D:20:LYS:HG3	2.06	0.85
1:A:232:CYS:SG	7:A:704:SF4:FE2	1.73	0.79
2:B:501:CYS:SG	7:B:702:SF4:S3	2.80	0.79
1:F:232:CYS:SG	7:F:704:SF4:FE2	1.73	0.78
1:A:286:ARG:NH1	4:I:251:ILE:O	2.16	0.78
4:D:251:ILE:O	1:F:286:ARG:NH1	2.16	0.78
2:G:501:CYS:SG	7:G:702:SF4:S3	2.80	0.78
4:I:400:VAL:HG11	4:I:447:CYS:HB3	1.66	0.77
4:D:400:VAL:HG11	4:D:447:CYS:HB3	1.66	0.77
2:B:455:CYS:SG	7:B:702:SF4:S1	2.83	0.76
1:F:154:CYS:SG	7:F:702:SF4:FE3	1.78	0.76
2:B:455:CYS:SG	7:B:702:SF4:S3	2.85	0.74
1:A:202:CYS:SG	7:A:702:SF4:FE1	1.80	0.74
2:G:455:CYS:SG	7:G:702:SF4:S1	2.83	0.74
5:E:24:LEU:O	5:E:28:LEU:N	2.20	0.74
5:J:24:LEU:O	5:J:28:LEU:N	2.20	0.74
1:F:202:CYS:SG	7:F:702:SF4:FE1	1.80	0.74
2:G:455:CYS:SG	7:G:702:SF4:S3	2.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:CYS:SG	7:B:702:SF4:S4	2.86	0.73
1:A:154:CYS:SG	7:A:702:SF4:FE3	1.78	0.73
2:B:132:GLU:HA	2:B:135:ILE:HG12	1.71	0.72
1:F:362:PRO:HB3	1:F:689:ILE:HG21	1.72	0.72
2:G:458:CYS:SG	7:G:702:SF4:S4	2.86	0.72
1:A:362:PRO:HB3	1:A:689:ILE:HG21	1.72	0.72
2:G:132:GLU:HA	2:G:135:ILE:HG12	1.71	0.71
2:B:501:CYS:SG	7:B:702:SF4:S1	2.89	0.70
2:G:501:CYS:SG	7:G:702:SF4:S1	2.89	0.70
4:I:401:ALA:HB3	11:I:502:FCO:N1	2.07	0.70
1:F:265:HIS:O	1:F:269:TRP:HB2	1.92	0.69
1:A:265:HIS:O	1:A:269:TRP:HB2	1.92	0.69
4:D:17:GLY:HA3	4:D:445:LEU:HB2	1.74	0.69
4:I:17:GLY:HA3	4:I:445:LEU:HB2	1.74	0.69
2:G:345:THR:OG1	2:G:346:GLU:N	2.26	0.68
4:D:401:ALA:HB3	11:D:502:FCO:N1	2.07	0.68
1:F:600:GLN:HG2	1:F:618:ALA:HB2	1.75	0.68
1:F:158:CYS:HG	7:F:703:SF4:FE2	1.08	0.68
4:D:400:VAL:HG12	4:D:401:ALA:H	1.58	0.67
1:A:600:GLN:HG2	1:A:618:ALA:HB2	1.75	0.67
1:F:574:TYR:OH	1:F:600:GLN:OE1	2.12	0.67
4:I:400:VAL:HG12	4:I:401:ALA:H	1.58	0.67
1:A:530:VAL:HB	1:A:686:GLU:HB2	1.77	0.67
1:A:158:CYS:HG	7:A:703:SF4:FE2	1.10	0.66
2:G:375:ARG:NH1	2:G:410:ASP:OD1	2.28	0.66
4:I:69:VAL:HB	4:I:102:GLN:HG3	1.78	0.66
2:B:375:ARG:NH1	2:B:410:ASP:OD1	2.28	0.66
4:D:69:VAL:HB	4:D:102:GLN:HG3	1.78	0.66
2:B:345:THR:OG1	2:B:346:GLU:N	2.26	0.65
2:B:501:CYS:SG	7:B:702:SF4:S4	2.95	0.65
1:F:530:VAL:HB	1:F:686:GLU:HB2	1.77	0.65
4:D:120:LEU:HD21	4:D:204:LEU:HD11	1.79	0.65
1:F:50:CYS:SG	6:F:701:FES:FE2	1.82	0.65
1:A:50:CYS:SG	6:A:701:FES:FE2	1.82	0.64
1:A:648:ILE:O	1:A:649:LYS:NZ	2.22	0.64
2:G:501:CYS:SG	7:G:702:SF4:S4	2.95	0.64
4:I:316:LYS:NZ	4:I:322:GLY:O	2.28	0.63
4:D:316:LYS:NZ	4:D:322:GLY:O	2.28	0.63
5:E:106:GLU:HA	5:E:110:GLU:HB2	1.80	0.63
1:F:442:LEU:HD13	1:F:692:LEU:HG	1.80	0.63
4:I:378:ARG:HB2	11:I:502:FCO:N2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HE2	1:A:486:ALA:H	1.63	0.63
4:I:120:LEU:HD21	4:I:204:LEU:HD11	1.79	0.63
4:D:378:ARG:HB2	11:D:502:FCO:N2	2.13	0.63
4:D:282:LEU:O	1:F:585:GLU:HB3	1.99	0.62
1:F:229:CYS:HG	7:F:704:SF4:FE3	0.44	0.62
5:J:106:GLU:HA	5:J:110:GLU:HB2	1.80	0.62
1:A:442:LEU:HD13	1:A:692:LEU:HG	1.80	0.62
1:A:574:TYR:OH	1:A:600:GLN:OE1	2.12	0.62
1:F:609:VAL:HG12	1:F:615:LEU:HD21	1.82	0.62
1:A:513:GLY:O	1:A:516:THR:OG1	2.17	0.62
1:F:513:GLY:O	1:F:516:THR:OG1	2.17	0.62
2:B:344:GLY:HA3	2:B:349:LYS:HA	1.80	0.62
2:G:344:GLY:HA3	2:G:349:LYS:HA	1.80	0.61
1:F:535:PHE:HZ	1:F:686:GLU:HB3	1.65	0.61
1:A:535:PHE:HZ	1:A:686:GLU:HB3	1.65	0.61
1:F:440:LYS:HE2	1:F:486:ALA:H	1.63	0.61
4:D:10:ASN:O	4:D:10:ASN:ND2	2.34	0.61
4:I:10:ASN:O	4:I:10:ASN:ND2	2.34	0.61
4:D:416:VAL:HG23	4:D:434:LEU:HD23	1.83	0.60
4:I:416:VAL:HG23	4:I:434:LEU:HD23	1.83	0.60
4:D:381:LEU:HD13	4:D:400:VAL:HG13	1.83	0.60
1:F:648:ILE:O	1:F:649:LYS:NZ	2.22	0.60
1:F:161:ILE:O	1:F:262:GLN:NE2	2.35	0.60
1:A:609:VAL:HG12	1:A:615:LEU:HD21	1.82	0.60
1:A:346:ASP:OD1	1:A:354:ARG:NH1	2.34	0.60
1:F:168:ASP:HB2	3:H:57:ALA:HB1	1.84	0.60
1:F:226:GLU:O	1:F:639:ASN:ND2	2.35	0.60
4:I:376:ALA:CB	11:I:502:FCO:O3	2.50	0.60
1:A:168:ASP:HB2	3:C:57:ALA:HB1	1.84	0.59
4:D:376:ALA:CB	11:D:502:FCO:O3	2.50	0.59
1:A:226:GLU:O	1:A:639:ASN:ND2	2.35	0.59
1:A:264:CYS:SG	7:A:704:SF4:S4	3.01	0.59
1:A:585:GLU:HB3	4:I:282:LEU:O	2.02	0.59
1:A:161:ILE:O	1:A:262:GLN:NE2	2.35	0.59
2:B:356:LEU:HD11	2:B:360:ILE:HD13	1.85	0.59
1:A:511:ILE:HD11	1:A:522:VAL:HG22	1.84	0.59
1:F:264:CYS:SG	7:F:704:SF4:S4	3.01	0.59
2:G:193:CYS:HB3	2:G:234:ILE:HG12	1.85	0.59
4:I:277:PRO:HG2	4:I:404:HIS:HA	1.83	0.59
2:B:193:CYS:HB3	2:B:234:ILE:HG12	1.85	0.59
1:F:511:ILE:HD11	1:F:522:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:356:LEU:HD11	2:G:360:ILE:HD13	1.85	0.59
4:I:381:LEU:HD13	4:I:400:VAL:HG13	1.83	0.59
4:D:277:PRO:HG2	4:D:404:HIS:HA	1.83	0.58
4:D:266:GLU:N	5:E:113:SER:O	2.33	0.58
1:A:342:MET:HB3	1:A:345:ILE:HD11	1.86	0.58
4:D:70:SER:OG	4:D:102:GLN:OE1	2.21	0.58
1:F:346:ASP:OD1	1:F:354:ARG:NH1	2.34	0.58
4:I:9:ILE:O	4:I:9:ILE:HG22	2.03	0.58
1:A:573:LEU:HD22	1:A:594:THR:HG21	1.84	0.57
2:G:131:ILE:HG22	2:G:253:GLN:HE21	1.69	0.57
4:D:9:ILE:O	4:D:9:ILE:HG22	2.03	0.57
1:F:573:LEU:HD22	1:F:594:THR:HG21	1.84	0.57
1:F:342:MET:HB3	1:F:345:ILE:HD11	1.86	0.57
1:F:428:LEU:HD21	1:F:497:VAL:HG22	1.86	0.57
2:B:131:ILE:HG22	2:B:253:GLN:HE21	1.69	0.57
2:G:286:GLU:OE1	2:G:288:THR:OG1	2.21	0.57
2:G:458:CYS:SG	7:G:702:SF4:S3	3.03	0.57
1:A:428:LEU:HD21	1:A:497:VAL:HG22	1.86	0.57
4:I:10:ASN:HB3	4:I:20:LYS:CG	2.19	0.57
1:F:496:GLU:HA	1:F:499:LEU:HB3	1.87	0.56
5:J:7:ALA:HB3	5:J:51:ILE:HD13	1.86	0.56
2:B:455:CYS:SG	7:B:702:SF4:S2	3.02	0.56
4:I:70:SER:OG	4:I:102:GLN:OE1	2.21	0.56
1:A:170:GLU:HG2	1:A:171:ARG:H	1.70	0.56
2:B:458:CYS:SG	7:B:702:SF4:S3	3.03	0.56
2:G:455:CYS:SG	7:G:702:SF4:S2	3.02	0.56
5:E:7:ALA:HB3	5:E:51:ILE:HD13	1.86	0.56
1:F:393:GLU:OE2	1:F:547:VAL:HA	2.06	0.56
1:F:438:VAL:HB	1:F:439:PRO:HD3	1.88	0.56
1:A:216:GLY:O	1:A:249:ARG:NH1	2.39	0.56
1:A:6:LEU:HD11	1:A:68:ALA:HB1	1.88	0.56
1:A:438:VAL:HB	1:A:439:PRO:HD3	1.88	0.56
1:F:170:GLU:HG2	1:F:171:ARG:H	1.70	0.56
3:C:27:ILE:HG12	3:C:28:PRO:HD3	1.88	0.55
3:C:29:ILE:O	3:C:33:VAL:HG23	2.06	0.55
4:D:10:ASN:HB3	4:D:20:LYS:CG	2.19	0.55
3:H:11:LYS:HE2	3:H:36:GLU:HB3	1.89	0.55
4:I:266:GLU:N	5:J:113:SER:O	2.33	0.55
1:F:216:GLY:O	1:F:249:ARG:NH1	2.39	0.55
3:H:29:ILE:O	3:H:33:VAL:HG23	2.06	0.55
2:G:247:LEU:HD22	2:G:275:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLU:HA	1:A:499:LEU:HB3	1.87	0.55
3:C:11:LYS:HE2	3:C:36:GLU:HB3	1.89	0.55
1:F:364:ARG:NH1	1:F:677:ILE:O	2.39	0.55
1:A:229:CYS:HG	7:A:704:SF4:FE3	0.41	0.55
1:F:652:HIS:CE1	1:F:668:ARG:HD3	2.42	0.55
1:A:393:GLU:OE2	1:A:547:VAL:HA	2.06	0.55
2:B:405:THR:OG1	2:B:406:LYS:N	2.40	0.55
1:F:6:LEU:HD11	1:F:68:ALA:HB1	1.88	0.55
1:A:569:ARG:HH11	4:I:248:ARG:HD3	1.72	0.55
1:F:535:PHE:CZ	1:F:686:GLU:HB3	2.43	0.54
3:H:27:ILE:HG12	3:H:28:PRO:HD3	1.88	0.54
4:I:59:ILE:HG23	5:J:91:ILE:HD11	1.88	0.54
1:A:364:ARG:NH1	1:A:677:ILE:O	2.39	0.54
2:G:405:THR:OG1	2:G:406:LYS:N	2.40	0.54
2:B:247:LEU:HD22	2:B:275:LEU:HD13	1.88	0.54
4:D:59:ILE:HG23	5:E:91:ILE:HD11	1.88	0.54
2:G:189:LYS:HB2	2:G:229:ALA:HA	1.90	0.54
1:A:438:VAL:HG22	1:A:521:LEU:HD13	1.88	0.54
4:D:248:ARG:HD3	1:F:569:ARG:HH11	1.72	0.54
1:A:652:HIS:CE1	1:A:668:ARG:HD3	2.42	0.54
2:B:145:LYS:HD3	2:B:334:LEU:HA	1.90	0.54
2:B:189:LYS:HB2	2:B:229:ALA:HA	1.90	0.54
2:G:366:ILE:HG21	2:G:381:LEU:HD11	1.90	0.54
1:A:302:LEU:HD22	1:A:614:ILE:HD11	1.90	0.54
4:D:241:GLU:OE2	4:D:254:GLN:NE2	2.41	0.54
4:I:412:GLY:O	4:I:416:VAL:HG22	2.08	0.53
1:F:302:LEU:HD22	1:F:614:ILE:HD11	1.90	0.53
2:B:322:ASN:HB3	2:B:325:THR:HG22	1.91	0.53
4:D:311:GLU:OE1	4:D:332:TYR:OH	2.18	0.53
1:F:438:VAL:HG22	1:F:521:LEU:HD13	1.88	0.53
1:A:346:ASP:HB2	1:A:564:TRP:NE1	2.23	0.53
4:D:412:GLY:O	4:D:416:VAL:HG22	2.08	0.53
1:F:391:GLN:NE2	1:F:402:ARG:HH12	2.06	0.53
4:I:241:GLU:OE2	4:I:254:GLN:NE2	2.41	0.53
1:A:289:ALA:HB2	4:I:251:ILE:HG21	1.89	0.53
1:A:391:GLN:NE2	1:A:402:ARG:HH12	2.06	0.53
4:D:251:ILE:HG21	1:F:289:ALA:HB2	1.89	0.53
1:F:346:ASP:HB2	1:F:564:TRP:NE1	2.23	0.53
4:I:356:SER:OG	4:I:357:SER:N	2.42	0.53
2:G:145:LYS:HD3	2:G:334:LEU:HA	1.90	0.53
2:G:210:GLU:O	2:G:246:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:GLU:OE1	2:B:288:THR:OG1	2.21	0.53
4:I:85:VAL:HG21	4:I:173:GLY:HA2	1.90	0.53
2:G:458:CYS:SG	7:G:702:SF4:S2	3.04	0.53
1:A:535:PHE:CZ	1:A:686:GLU:HB3	2.43	0.53
5:E:8:THR:HG22	5:E:55:VAL:HB	1.91	0.53
2:B:395:GLN:HB3	2:B:431:VAL:HG13	1.90	0.52
2:B:366:ILE:HG21	2:B:381:LEU:HD11	1.90	0.52
4:D:232:ASP:OD1	4:D:232:ASP:N	2.42	0.52
4:D:356:SER:OG	4:D:357:SER:N	2.42	0.52
2:G:395:GLN:HB3	2:G:431:VAL:HG13	1.90	0.52
2:G:322:ASN:HB3	2:G:325:THR:HG22	1.91	0.52
1:F:128:LEU:HD21	2:G:470:LEU:HD11	1.92	0.52
2:G:279:ALA:HB2	3:H:27:ILE:HD12	1.92	0.52
2:B:135:ILE:HA	2:B:139:GLY:HA3	1.92	0.52
4:D:414:GLU:HG2	4:D:418:LYS:HE2	1.90	0.52
4:D:85:VAL:HG21	4:D:173:GLY:HA2	1.90	0.52
4:I:414:GLU:HG2	4:I:418:LYS:HE2	1.90	0.52
2:G:528:ASP:OD1	2:G:530:ARG:HG3	2.10	0.52
2:G:135:ILE:HA	2:G:139:GLY:HA3	1.92	0.52
1:A:527:ASN:HD21	1:A:689:ILE:H	1.58	0.52
4:D:147:ILE:HG23	5:E:25:ASP:HB3	1.92	0.52
2:G:213:PRO:O	2:G:217:ILE:HG12	2.10	0.51
5:J:8:THR:HG22	5:J:55:VAL:HB	1.91	0.51
1:A:128:LEU:HD21	2:B:470:LEU:HD11	1.92	0.51
1:A:589:ALA:HB2	4:I:286:HIS:HB3	1.92	0.51
2:B:528:ASP:OD1	2:B:530:ARG:HG3	2.10	0.51
2:B:213:PRO:O	2:B:217:ILE:HG12	2.10	0.51
5:J:105:ARG:HG3	5:J:109:ILE:HD12	1.93	0.51
2:B:279:ALA:HB2	3:C:27:ILE:HD12	1.92	0.51
2:G:407:GLU:OE1	2:G:408:HIS:ND1	2.44	0.51
4:I:151:LYS:HB2	5:J:25:ASP:OD2	2.11	0.51
4:I:191:LEU:HD13	4:I:346:GLU:HG2	1.92	0.51
4:I:376:ALA:HB2	11:I:502:FCO:O3	2.11	0.51
1:A:246:SER:HA	1:A:275:THR:HG21	1.93	0.51
2:B:145:LYS:HA	2:B:149:GLU:HG2	1.92	0.51
1:F:120:MET:O	5:J:178:TYR:OH	2.20	0.51
1:F:429:ASP:OD1	1:F:429:ASP:N	2.44	0.51
4:I:147:ILE:HG23	5:J:25:ASP:HB3	1.92	0.51
1:F:246:SER:HA	1:F:275:THR:HG21	1.93	0.51
3:C:10:GLU:O	3:C:14:GLU:HG2	2.11	0.51
2:G:145:LYS:HA	2:G:149:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:CYS:SG	2:B:323:VAL:HG22	2.51	0.50
4:D:191:LEU:HD13	4:D:346:GLU:HG2	1.92	0.50
4:D:424:THR:HG22	4:D:425:ASN:H	1.76	0.50
1:F:527:ASN:HD21	1:F:689:ILE:H	1.58	0.50
4:D:4:VAL:HG13	4:D:27:GLU:HG3	1.94	0.50
4:D:151:LYS:HB2	5:E:25:ASP:OD2	2.11	0.50
4:D:431:PHE:O	4:D:435:GLU:HG3	2.12	0.50
2:G:193:CYS:SG	2:G:323:VAL:HG22	2.51	0.50
2:B:407:GLU:OE1	2:B:408:HIS:ND1	2.44	0.50
4:D:286:HIS:HB3	1:F:589:ALA:HB2	1.92	0.50
4:D:376:ALA:HB2	11:D:502:FCO:O3	2.11	0.50
5:E:105:ARG:HG3	5:E:109:ILE:HD12	1.93	0.50
1:F:411:LYS:NZ	1:F:500:MET:SD	2.85	0.50
4:I:424:THR:HG22	4:I:425:ASN:H	1.76	0.50
3:H:10:GLU:O	3:H:14:GLU:HG2	2.11	0.50
4:I:232:ASP:OD1	4:I:232:ASP:N	2.42	0.49
2:B:210:GLU:O	2:B:246:ARG:NH1	2.39	0.49
5:E:137:ASP:OD2	5:E:145:TYR:OH	2.30	0.49
4:D:312:PHE:CZ	4:D:316:LYS:HE2	2.48	0.49
2:G:212:ASP:OD2	2:G:215:SER:OG	2.28	0.49
5:J:4:ALA:O	5:J:36:GLU:HG2	2.13	0.49
5:E:157:TYR:O	5:E:161:LYS:HG3	2.13	0.49
4:I:312:PHE:CZ	4:I:316:LYS:HE2	2.48	0.49
1:F:283:PRO:HB3	1:F:616:LEU:HD23	1.95	0.49
2:G:165:ARG:O	2:G:167:ARG:NH2	2.46	0.49
4:I:20:LYS:NZ	5:J:125:ASP:O	2.33	0.49
2:B:165:ARG:O	2:B:167:ARG:NH2	2.46	0.49
2:B:360:ILE:HB	2:B:432:VAL:HG11	1.95	0.49
4:I:431:PHE:O	4:I:435:GLU:HG3	2.12	0.49
4:I:4:VAL:HG13	4:I:27:GLU:HG3	1.94	0.49
2:B:510:PRO:HA	2:B:513:THR:HG22	1.95	0.49
4:D:124:ASP:OD1	4:D:124:ASP:N	2.44	0.49
5:E:4:ALA:O	5:E:36:GLU:HG2	2.13	0.49
1:A:383:ILE:HB	1:A:412:LEU:HD12	1.95	0.48
2:G:405:THR:HG23	2:G:407:GLU:OE2	2.13	0.48
2:G:510:PRO:HA	2:G:513:THR:HG22	1.95	0.48
1:A:533:LYS:HA	1:A:535:PHE:CE2	2.48	0.48
1:F:533:LYS:HA	1:F:535:PHE:CE2	2.48	0.48
5:J:157:TYR:O	5:J:161:LYS:HG3	2.13	0.48
2:B:405:THR:HG23	2:B:407:GLU:OE2	2.13	0.48
1:A:240:THR:HG21	1:A:641:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ILE:HB	1:F:412:LEU:HD12	1.95	0.48
1:A:162:VAL:HG12	1:A:164:ALA:H	1.79	0.48
2:B:408:HIS:HE1	2:B:517:TYR:CZ	2.32	0.48
1:A:120:MET:O	5:E:178:TYR:OH	2.20	0.48
2:G:360:ILE:HB	2:G:432:VAL:HG11	1.95	0.48
2:G:362:ASN:HB2	2:G:382:GLY:HA2	1.94	0.48
2:G:408:HIS:HE1	2:G:517:TYR:CZ	2.32	0.48
2:B:362:ASN:HB2	2:B:382:GLY:HA2	1.94	0.48
2:B:288:THR:HA	2:B:291:MET:HE2	1.96	0.48
1:A:555:ARG:HA	1:A:559:VAL:HB	1.95	0.48
1:F:578:THR:O	1:F:580:MET:N	2.47	0.48
1:F:162:VAL:HG12	1:F:164:ALA:H	1.79	0.47
5:J:137:ASP:OD2	5:J:145:TYR:OH	2.30	0.47
1:A:283:PRO:HB3	1:A:616:LEU:HD23	1.95	0.47
2:B:196:ASP:OD1	2:B:237:ARG:NH1	2.48	0.47
1:F:61:LEU:HB3	1:F:66:THR:HG21	1.96	0.47
2:G:304:ARG:HA	2:G:304:ARG:HD3	1.73	0.47
1:F:231:LEU:HD13	1:F:266:MET:HB3	1.95	0.47
2:G:196:ASP:OD1	2:G:237:ARG:NH1	2.48	0.47
3:H:46:LEU:HG	3:H:50:ARG:HH22	1.80	0.47
2:B:199:ASP:HB3	2:B:202:ALA:HB3	1.96	0.47
4:I:80:ASP:OD1	4:I:173:GLY:N	2.46	0.47
5:J:136:ILE:O	5:J:140:VAL:HG22	2.15	0.47
1:A:61:LEU:HB3	1:A:66:THR:HG21	1.96	0.47
2:B:347:LYS:HA	2:B:347:LYS:HD3	1.74	0.47
3:C:46:LEU:HG	3:C:50:ARG:HH22	1.80	0.47
4:D:20:LYS:NZ	5:E:125:ASP:O	2.33	0.47
4:D:331:HIS:CE1	4:D:440:ALA:HA	2.49	0.47
5:E:136:ILE:O	5:E:140:VAL:HG22	2.15	0.47
1:F:555:ARG:HA	1:F:559:VAL:HB	1.95	0.47
2:G:181:ALA:O	2:G:189:LYS:NZ	2.43	0.47
4:I:331:HIS:CE1	4:I:440:ALA:HA	2.49	0.47
1:A:231:LEU:HD13	1:A:266:MET:HB3	1.95	0.47
1:A:630:THR:OG1	1:A:631:ILE:N	2.48	0.47
1:F:630:THR:OG1	1:F:631:ILE:N	2.48	0.47
2:G:187:ASP:OD1	2:G:187:ASP:N	2.47	0.47
1:A:69:GLN:O	1:A:72:MET:HG2	2.15	0.47
2:B:357:THR:OG1	2:B:358:GLY:N	2.48	0.47
2:G:357:THR:OG1	2:G:358:GLY:N	2.48	0.47
1:F:240:THR:HG21	1:F:641:ILE:HG21	1.95	0.47
5:J:62:ASN:HB2	5:J:65:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:VAL:HG22	5:E:53:VAL:HB	1.97	0.46
3:C:43:GLU:O	3:C:47:THR:HG23	2.16	0.46
2:G:347:LYS:HA	2:G:347:LYS:HD3	1.74	0.46
2:G:439:MET:HG3	2:G:518:PHE:CD2	2.50	0.46
4:D:97:LEU:HD23	4:D:160:LEU:HD11	1.98	0.46
5:E:24:LEU:HB2	5:E:28:LEU:HD13	1.97	0.46
1:F:69:GLN:O	1:F:72:MET:HG2	2.15	0.46
5:E:62:ASN:HB2	5:E:65:GLU:OE1	2.15	0.46
2:G:195:ALA:HB2	2:G:323:VAL:HG21	1.98	0.46
2:B:319:ASN:ND2	2:B:319:ASN:O	2.49	0.46
2:G:199:ASP:HB3	2:G:202:ALA:HB3	1.96	0.46
2:G:237:ARG:NH2	2:G:280:GLY:O	2.49	0.46
5:J:24:LEU:HB2	5:J:28:LEU:HD13	1.97	0.46
1:A:411:LYS:NZ	1:A:500:MET:SD	2.85	0.46
2:B:181:ALA:O	2:B:189:LYS:NZ	2.43	0.46
2:B:187:ASP:OD1	2:B:187:ASP:N	2.47	0.46
2:B:195:ALA:HB2	2:B:323:VAL:HG21	1.98	0.46
3:C:12:VAL:O	3:C:16:VAL:HG23	2.16	0.46
3:H:43:GLU:O	3:H:47:THR:HG23	2.16	0.46
5:J:8:THR:O	5:J:40:SER:HA	2.16	0.46
3:H:12:VAL:O	3:H:16:VAL:HG23	2.16	0.46
4:I:124:ASP:OD1	4:I:124:ASP:N	2.44	0.46
1:A:429:ASP:OD1	1:A:429:ASP:N	2.44	0.46
2:G:494:MET:O	2:G:498:THR:OG1	2.17	0.46
4:I:97:LEU:HD23	4:I:160:LEU:HD11	1.98	0.46
1:A:319:ILE:HD12	1:A:573:LEU:HD21	1.98	0.46
1:A:412:LEU:HB3	1:A:426:VAL:HA	1.97	0.46
2:B:439:MET:HG3	2:B:518:PHE:CD2	2.50	0.45
4:D:87:ILE:HA	4:D:361:VAL:HG21	1.99	0.45
1:F:412:LEU:HB3	1:F:426:VAL:HA	1.97	0.45
5:J:6:VAL:HG22	5:J:53:VAL:HB	1.97	0.45
1:A:210:ARG:NH2	4:D:390:SER:O	2.49	0.45
1:F:387:PHE:HA	1:F:416:SER:HB2	1.98	0.45
2:G:319:ASN:ND2	2:G:319:ASN:O	2.49	0.45
2:G:328:ASN:HD22	2:G:328:ASN:HA	1.55	0.45
1:A:578:THR:O	1:A:580:MET:N	2.47	0.45
4:D:296:ARG:HD3	4:D:375:GLU:CG	2.46	0.45
1:A:387:PHE:HA	1:A:416:SER:HB2	1.98	0.45
2:G:204:MET:HG2	2:G:353:ILE:HG13	1.99	0.45
2:B:257:MET:SD	2:B:257:MET:N	2.90	0.45
5:E:8:THR:O	5:E:40:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:311:GLU:OE1	4:I:332:TYR:OH	2.18	0.45
2:B:237:ARG:NH2	2:B:280:GLY:O	2.49	0.45
4:D:248:ARG:HD3	1:F:569:ARG:NH1	2.32	0.45
1:F:319:ILE:HD12	1:F:573:LEU:HD21	1.98	0.45
1:F:527:ASN:ND2	1:F:689:ILE:H	2.15	0.45
4:D:6:LYS:HG2	4:D:8:GLU:OE2	2.17	0.45
1:F:154:CYS:HA	1:F:157:THR:HG22	1.99	0.45
4:I:156:ILE:HG12	4:I:187:ILE:HD13	1.99	0.45
2:B:426:GLY:C	2:B:428:GLY:H	2.20	0.44
2:G:288:THR:HA	2:G:291:MET:HE2	1.99	0.44
4:I:296:ARG:HD3	4:I:375:GLU:CG	2.46	0.44
1:A:379:ASP:N	1:A:379:ASP:OD1	2.50	0.44
2:B:458:CYS:SG	7:B:702:SF4:S2	3.04	0.44
4:D:128:LYS:HE2	4:D:128:LYS:HB2	1.78	0.44
4:I:128:LYS:HE2	4:I:128:LYS:HB2	1.78	0.44
4:D:80:ASP:OD1	4:D:173:GLY:N	2.46	0.44
4:D:260:TYR:OH	4:D:397:ASN:ND2	2.43	0.44
1:F:652:HIS:CE1	1:F:666:LEU:HD23	2.53	0.44
2:G:385:ILE:HD11	2:G:391:PHE:HB2	2.00	0.44
1:A:578:THR:O	1:A:578:THR:OG1	2.32	0.44
1:A:652:HIS:CE1	1:A:666:LEU:HD23	2.53	0.44
4:D:156:ILE:HG12	4:D:187:ILE:HD13	1.99	0.44
4:D:413:VAL:HG13	4:D:434:LEU:HD22	1.99	0.44
5:E:70:LYS:O	5:E:74:GLU:HG3	2.17	0.44
1:F:235:GLY:HA3	1:F:636:ARG:NH1	2.33	0.44
1:F:426:VAL:HG22	1:F:428:LEU:H	1.82	0.44
4:I:87:ILE:HA	4:I:361:VAL:HG21	1.99	0.44
4:I:260:TYR:OH	4:I:397:ASN:ND2	2.43	0.44
1:A:527:ASN:ND2	1:A:689:ILE:H	2.15	0.44
1:A:569:ARG:NH1	4:I:248:ARG:HD3	2.32	0.44
2:G:257:MET:SD	2:G:257:MET:N	2.90	0.44
1:A:327:GLU:OE1	1:A:327:GLU:N	2.47	0.44
4:D:390:SER:HB2	4:D:392:VAL:HG23	2.00	0.44
4:D:373:VAL:HG22	4:D:382:ILE:HG12	2.00	0.44
4:D:414:GLU:O	4:D:418:LYS:HG2	2.18	0.44
2:G:329:VAL:N	2:G:330:PRO:HD2	2.33	0.44
4:I:6:LYS:HG2	4:I:8:GLU:OE2	2.17	0.44
4:I:405:ASN:O	4:I:409:MET:HG3	2.18	0.44
5:J:70:LYS:O	5:J:74:GLU:HG3	2.17	0.44
2:B:385:ILE:HD11	2:B:391:PHE:HB2	2.00	0.44
4:D:405:ASN:O	4:D:409:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:CYS:O	1:F:106:SER:HB3	2.18	0.44
1:A:103:CYS:O	1:A:106:SER:HB3	2.18	0.44
1:A:426:VAL:HG22	1:A:428:LEU:H	1.82	0.44
1:F:313:GLN:O	1:F:315:LYS:HG3	2.18	0.44
2:G:145:LYS:O	2:G:150:MET:HG2	2.18	0.44
1:A:235:GLY:HA3	1:A:636:ARG:NH1	2.33	0.43
4:I:165:ILE:HB	5:J:150:PRO:HG3	2.00	0.43
4:I:223:ASP:N	4:I:223:ASP:OD1	2.51	0.43
1:A:154:CYS:HA	1:A:157:THR:HG22	1.99	0.43
5:E:10:TRP:HD1	5:E:10:TRP:O	2.01	0.43
1:F:379:ASP:N	1:F:379:ASP:OD1	2.50	0.43
4:I:110:SER:HB2	4:I:442:ASP:CG	2.39	0.43
1:A:164:ALA:HB1	1:A:191:THR:O	2.18	0.43
2:B:329:VAL:N	2:B:330:PRO:HD2	2.33	0.43
1:F:164:ALA:HB1	1:F:191:THR:O	2.18	0.43
1:F:391:GLN:HE21	1:F:402:ARG:HH12	1.66	0.43
2:B:132:GLU:OE2	2:B:132:GLU:N	2.49	0.43
2:B:204:MET:HG2	2:B:353:ILE:HG13	1.99	0.43
4:I:151:LYS:NZ	4:I:155:GLU:OE1	2.34	0.43
4:I:390:SER:HB2	4:I:392:VAL:HG23	2.00	0.43
4:D:110:SER:HB2	4:D:442:ASP:CG	2.39	0.43
4:I:414:GLU:O	4:I:418:LYS:HG2	2.18	0.43
1:A:198:CYS:HB2	1:A:207:ILE:HD13	2.01	0.43
1:F:210:ARG:NH2	4:I:390:SER:O	2.49	0.43
2:G:426:GLY:C	2:G:428:GLY:H	2.20	0.43
4:I:413:VAL:HG13	4:I:434:LEU:HD22	1.99	0.43
4:D:14:ARG:HH22	4:D:118:ASP:CG	2.21	0.43
1:F:309:LYS:HE3	1:F:309:LYS:HB3	1.90	0.43
4:D:223:ASP:N	4:D:223:ASP:OD1	2.51	0.43
2:G:151:THR:HG23	2:G:154:GLU:H	1.84	0.43
4:I:14:ARG:HH22	4:I:118:ASP:CG	2.21	0.43
4:I:373:VAL:HG22	4:I:382:ILE:HG12	2.00	0.43
1:A:243:ARG:HG2	1:A:244:THR:HG23	2.00	0.43
1:A:313:GLN:O	1:A:315:LYS:HG3	2.18	0.43
1:A:391:GLN:HE21	1:A:402:ARG:HH12	1.66	0.43
2:B:151:THR:HG23	2:B:154:GLU:H	1.84	0.43
8:B:701:NAD:H2D	8:B:701:NAD:H6N	1.78	0.43
4:D:165:ILE:HB	5:E:150:PRO:HG3	2.00	0.43
5:J:10:TRP:HD1	5:J:10:TRP:O	2.01	0.43
1:A:264:CYS:SG	7:A:704:SF4:S2	3.17	0.43
4:D:373:VAL:HG22	4:D:382:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:424:ILE:HD12	2:G:424:ILE:HA	1.94	0.43
4:I:373:VAL:HG22	4:I:382:ILE:HG23	2.00	0.43
1:F:198:CYS:HB2	1:F:207:ILE:HD13	2.01	0.42
1:F:243:ARG:HG2	1:F:244:THR:HG23	2.00	0.42
8:G:701:NAD:H6N	8:G:701:NAD:H2D	1.78	0.42
4:I:13:THR:OG1	5:J:44:ASP:OD1	2.31	0.42
2:B:145:LYS:O	2:B:150:MET:HG2	2.18	0.42
3:C:30:LEU:HD22	3:C:40:LEU:HD13	2.01	0.42
1:F:327:GLU:OE1	1:F:327:GLU:N	2.47	0.42
1:F:527:ASN:HA	1:F:530:VAL:HG22	2.01	0.42
2:G:132:GLU:OE2	2:G:132:GLU:N	2.49	0.42
3:H:30:LEU:HD22	3:H:40:LEU:HD13	2.01	0.42
4:I:144:LYS:HB3	4:I:144:LYS:HE3	1.77	0.42
4:I:422:THR:OG1	4:I:423:GLY:N	2.52	0.42
1:A:309:LYS:HE3	1:A:309:LYS:HB3	1.90	0.42
1:A:606:ARG:HD2	1:A:606:ARG:HA	1.88	0.42
1:F:645:LYS:H	1:F:645:LYS:HG2	1.58	0.42
2:G:264:ILE:HD12	2:G:269:PHE:HE2	1.84	0.42
1:A:55:GLU:HB2	1:A:73:VAL:HG21	2.01	0.42
4:D:6:LYS:CG	4:D:8:GLU:OE2	2.68	0.42
1:F:172:ARG:HB3	3:H:65:PHE:CD1	2.55	0.42
1:F:392:LYS:HB2	1:F:392:LYS:HE3	1.90	0.42
2:G:481:THR:HG23	2:G:484:ASP:H	1.85	0.42
1:A:172:ARG:HB3	3:C:65:PHE:CD1	2.55	0.42
2:B:199:ASP:CG	2:B:399:PRO:HD3	2.40	0.42
2:B:481:THR:HG23	2:B:484:ASP:H	1.85	0.42
4:D:422:THR:OG1	4:D:423:GLY:N	2.52	0.42
1:F:660:LYS:HG2	1:F:661:LYS:H	1.85	0.42
2:G:291:MET:HE1	2:G:302:ARG:HH11	1.83	0.42
2:G:520:ASP:OD1	2:G:520:ASP:N	2.53	0.42
1:A:660:LYS:HG2	1:A:661:LYS:H	1.85	0.42
4:D:296:ARG:HD3	4:D:375:GLU:HG2	2.02	0.42
1:F:152:GLN:HE22	2:G:457:LYS:HG3	1.85	0.42
2:G:346:GLU:O	2:G:347:LYS:HD3	2.20	0.42
2:G:361:THR:OG1	2:G:382:GLY:O	2.23	0.42
5:J:66:VAL:HG13	5:J:139:GLU:HG3	2.01	0.42
2:B:264:ILE:HD12	2:B:269:PHE:HE2	1.84	0.42
5:J:106:GLU:O	5:J:106:GLU:HG2	2.20	0.42
1:A:257:GLU:HB2	1:A:259:ASP:OD1	2.20	0.42
2:B:424:ILE:HD12	2:B:424:ILE:HA	1.94	0.42
2:B:520:ASP:OD1	2:B:520:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:LEU:HD23	5:E:163:LEU:HA	1.89	0.42
1:F:264:CYS:SG	7:F:704:SF4:S2	3.17	0.42
2:G:199:ASP:CG	2:G:399:PRO:HD3	2.40	0.42
1:A:182:LEU:HD23	3:C:60:TYR:HB2	2.02	0.42
3:C:11:LYS:O	3:C:15:ILE:HG13	2.20	0.42
4:D:13:THR:OG1	5:E:44:ASP:OD1	2.31	0.42
4:D:190:GLN:O	4:D:194:MET:HG2	2.20	0.42
4:D:248:ARG:HD2	4:D:248:ARG:HA	1.79	0.42
4:D:331:HIS:HE1	4:D:440:ALA:HA	1.85	0.42
4:D:400:VAL:HG12	4:D:401:ALA:N	2.31	0.42
5:E:66:VAL:HG13	5:E:139:GLU:HG3	2.01	0.42
2:G:461:CYS:HB3	7:G:702:SF4:S2	2.60	0.42
1:A:384:ILE:HD13	1:A:509:PHE:CZ	2.55	0.41
1:F:606:ARG:HD2	1:F:606:ARG:HA	1.94	0.41
4:I:6:LYS:CG	4:I:8:GLU:OE2	2.68	0.41
5:J:73:ARG:NH1	5:J:141:LYS:O	2.53	0.41
1:A:344:HIS:HB3	1:A:564:TRP:CD2	2.55	0.41
1:A:452:ILE:HG21	1:A:502:ILE:HG21	2.02	0.41
4:D:389:GLU:CD	4:D:389:GLU:H	2.23	0.41
1:A:533:LYS:HE2	1:A:533:LYS:HB2	1.80	0.41
4:D:10:ASN:ND2	4:D:10:ASN:C	2.73	0.41
4:D:147:ILE:CG2	5:E:25:ASP:HB3	2.50	0.41
1:F:182:LEU:HD23	3:H:60:TYR:HB2	2.02	0.41
1:F:257:GLU:HB2	1:F:259:ASP:OD1	2.20	0.41
1:A:315:LYS:HD3	1:A:571:ASP:OD1	2.21	0.41
4:D:225:ALA:HB3	4:D:289:TYR:HB3	2.02	0.41
5:E:104:LEU:HD23	5:E:104:LEU:HA	1.87	0.41
4:I:10:ASN:ND2	4:I:10:ASN:C	2.73	0.41
4:I:225:ALA:HB3	4:I:289:TYR:HB3	2.02	0.41
1:A:22:LEU:HD22	1:A:64:CYS:HB3	2.02	0.41
1:A:152:GLN:HE22	2:B:457:LYS:HG3	1.85	0.41
1:A:527:ASN:HA	1:A:530:VAL:HG22	2.01	0.41
2:B:346:GLU:O	2:B:347:LYS:HD3	2.20	0.41
4:D:144:LYS:HB3	4:D:144:LYS:HE3	1.77	0.41
4:D:180:THR:OG1	4:D:183:GLU:HG2	2.20	0.41
2:G:244:ILE:HG12	2:G:275:LEU:HD21	2.03	0.41
2:G:264:ILE:HD12	2:G:269:PHE:CE2	2.55	0.41
5:J:163:LEU:HD23	5:J:163:LEU:HA	1.89	0.41
1:F:384:ILE:HD13	1:F:509:PHE:CE2	2.55	0.41
4:I:10:ASN:CB	4:I:20:LYS:CG	2.88	0.41
4:I:388:ASN:HD21	4:I:392:VAL:HB	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:TRP:CE3	2:B:326:TRP:HA	2.56	0.41
1:F:533:LYS:HB2	1:F:533:LYS:HE2	1.80	0.41
1:F:591:ILE:O	1:F:594:THR:OG1	2.36	0.41
4:I:115:SER:O	4:I:119:ILE:HG13	2.21	0.41
4:I:119:ILE:HD13	4:I:205:ILE:HD13	2.03	0.41
4:I:190:GLN:O	4:I:194:MET:HG2	2.20	0.41
4:I:296:ARG:HD3	4:I:375:GLU:HG2	2.02	0.41
1:A:296:TRP:CZ3	1:A:616:LEU:HD22	2.55	0.41
1:F:55:GLU:HB2	1:F:73:VAL:HG21	2.01	0.41
1:F:144:ASP:O	1:F:206:THR:HG23	2.21	0.41
2:G:326:TRP:CE3	2:G:326:TRP:HA	2.56	0.41
1:A:133:GLU:H	1:A:133:GLU:HG2	1.69	0.41
1:A:384:ILE:HD13	1:A:509:PHE:CE2	2.55	0.41
4:D:10:ASN:CB	4:D:20:LYS:CG	2.88	0.41
4:D:119:ILE:HD13	4:D:205:ILE:HD13	2.03	0.41
1:F:296:TRP:CZ3	1:F:616:LEU:HD22	2.55	0.41
1:F:344:HIS:HB3	1:F:564:TRP:CD2	2.55	0.41
1:F:599:VAL:HB	1:F:615:LEU:HD12	2.03	0.41
4:I:147:ILE:CG2	5:J:25:ASP:HB3	2.50	0.41
4:I:331:HIS:HE1	4:I:440:ALA:HA	1.85	0.41
4:I:389:GLU:CD	4:I:389:GLU:H	2.23	0.41
2:B:461:CYS:HB3	7:B:702:SF4:S2	2.60	0.41
4:D:388:ASN:HD21	4:D:392:VAL:HB	1.85	0.41
1:F:106:SER:HA	7:F:705:SF4:S2	2.61	0.41
1:F:271:LEU:HD22	1:F:621:TRP:CZ2	2.56	0.41
1:F:384:ILE:HD13	1:F:509:PHE:CZ	2.55	0.41
1:F:521:LEU:HD12	1:F:521:LEU:HA	1.93	0.41
1:A:420:SER:O	1:A:422:PHE:N	2.54	0.40
1:A:683:ARG:HD2	1:A:684:ALA:HB3	2.04	0.40
1:F:20:THR:OG1	1:F:23:ASP:OD2	2.38	0.40
1:F:151:CYS:SG	7:F:702:SF4:S2	3.19	0.40
2:G:245:LYS:O	2:G:249:ILE:HG22	2.21	0.40
2:G:403:CYS:N	2:G:513:THR:HG21	2.36	0.40
4:I:135:LEU:O	4:I:139:TYR:N	2.51	0.40
1:A:144:ASP:O	1:A:206:THR:HG23	2.21	0.40
1:A:151:CYS:SG	7:A:702:SF4:S2	3.19	0.40
1:A:344:HIS:HB3	1:A:564:TRP:CE2	2.56	0.40
2:B:214:HIS:CE1	2:B:250:ALA:HB1	2.57	0.40
2:B:244:ILE:HG12	2:B:275:LEU:HD21	2.03	0.40
1:F:420:SER:O	1:F:422:PHE:N	2.54	0.40
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:CYS:N	2:B:513:THR:HG21	2.36	0.40
4:D:417:ALA:O	4:D:421:ILE:HB	2.22	0.40
5:E:106:GLU:O	5:E:106:GLU:HG2	2.20	0.40
1:F:344:HIS:HB3	1:F:564:TRP:CE2	2.56	0.40
1:F:496:GLU:HB2	1:F:499:LEU:HD22	2.03	0.40
2:G:357:THR:O	2:G:431:VAL:HA	2.21	0.40
3:H:11:LYS:O	3:H:15:ILE:HG13	2.20	0.40
4:I:180:THR:OG1	4:I:183:GLU:HG2	2.20	0.40
1:A:106:SER:HA	7:A:705:SF4:S2	2.61	0.40
3:C:8:VAL:O	3:C:12:VAL:HG23	2.22	0.40
3:C:46:LEU:HG	3:C:50:ARG:NH2	2.36	0.40
4:D:140:PRO:HG2	4:D:141:GLU:OE1	2.22	0.40
1:A:537:GLU:OE2	1:A:537:GLU:N	2.55	0.40
2:B:212:ASP:OD2	2:B:215:SER:OG	2.28	0.40
4:D:115:SER:O	4:D:119:ILE:HG13	2.21	0.40
1:F:452:ILE:HG21	1:F:502:ILE:HG21	2.02	0.40
3:H:8:VAL:O	3:H:12:VAL:HG23	2.22	0.40
3:H:46:LEU:HG	3:H:50:ARG:NH2	2.36	0.40

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 PDB entries followed by that with respect to all EM entries.

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	662/692 (96%)	589 (89%)	73 (11%)	0	100	100
1	F	662/692 (96%)	590 (89%)	72 (11%)	0	100	100
2	B	423/597 (71%)	389 (92%)	34 (8%)	0	100	100
2	G	423/597 (71%)	389 (92%)	34 (8%)	0	100	100
3	C	70/156 (45%)	67 (96%)	3 (4%)	0	100	100
3	H	70/156 (45%)	67 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	445/475 (94%)	423 (95%)	22 (5%)	0	100	100
4	I	445/475 (94%)	423 (95%)	22 (5%)	0	100	100
5	E	177/179 (99%)	163 (92%)	14 (8%)	0	100	100
5	J	177/179 (99%)	163 (92%)	14 (8%)	0	100	100
All	All	3554/4198 (85%)	3263 (92%)	291 (8%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	565/583 (97%)	514 (91%)	51 (9%)	9	35
1	F	565/583 (97%)	514 (91%)	51 (9%)	9	35
2	B	341/488 (70%)	313 (92%)	28 (8%)	11	39
2	G	341/488 (70%)	313 (92%)	28 (8%)	11	39
3	C	60/133 (45%)	54 (90%)	6 (10%)	7	29
3	H	60/133 (45%)	54 (90%)	6 (10%)	7	29
4	D	378/402 (94%)	359 (95%)	19 (5%)	24	60
4	I	378/402 (94%)	359 (95%)	19 (5%)	24	60
5	E	154/154 (100%)	149 (97%)	5 (3%)	39	74
5	J	154/154 (100%)	149 (97%)	5 (3%)	39	74
All	All	2996/3520 (85%)	2778 (93%)	218 (7%)	18	44

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	39	LYS
1	A	51	VAL
1	A	52	VAL

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Mol	Chain	Res	Type
1	A	59	LYS
1	A	73	VAL
1	A	82	LYS
1	A	101	MET
1	A	106	SER
1	A	127	TYR
1	A	148	CYS
1	A	150	LEU
1	A	154	CYS
1	A	158	CYS
1	A	171	ARG
1	A	172	ARG
1	A	187	ARG
1	A	189	SER
1	A	222	ASP
1	A	227	SER
1	A	246	SER
1	A	269	TRP
1	A	276	GLU
1	A	282	VAL
1	A	341	LYS
1	A	364	ARG
1	A	365	GLU
1	A	371	PHE
1	A	379	ASP
1	A	393	GLU
1	A	416	SER
1	A	417	TYR
1	A	442	LEU
1	A	496	GLU
1	A	499	LEU
1	A	500	MET
1	A	505	ARG
1	A	517	LYS
1	A	528	LEU
1	A	595	ARG
1	A	611	LEU
1	A	624	ARG
1	A	628	PHE
1	A	634	GLU
1	A	640	THR
1	A	649	LYS

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Mol	Chain	Res	Type
1	A	661	LYS
1	A	670	GLU
1	A	674	CYS
1	A	680	SER
1	A	686	GLU
2	B	125	TYR
2	B	131	ILE
2	B	147	LEU
2	B	151	THR
2	B	161	LYS
2	B	193	CYS
2	B	207	SER
2	B	247	LEU
2	B	255	GLU
2	B	257	MET
2	B	262	ASP
2	B	268	ASN
2	B	272	HIS
2	B	286	GLU
2	B	293	SER
2	B	313	LEU
2	B	328	ASN
2	B	329	VAL
2	B	339	TRP
2	B	407	GLU
2	B	410	ASP
2	B	414	ASP
2	B	416	GLU
2	B	417	SER
2	B	458	CYS
2	B	499	SER
2	B	520	ASP
2	B	530	ARG
3	C	7	ASP
3	C	11	LYS
3	C	27	ILE
3	C	50	ARG
3	C	54	MET
3	C	74	ARG
4	D	10	ASN
4	D	24	MET
4	D	67	CYS

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Mol	Chain	Res	Type
4	D	75	SER
4	D	115	SER
4	D	144	LYS
4	D	155	GLU
4	D	175	VAL
4	D	200	GLU
4	D	203	LYS
4	D	222	LEU
4	D	239	ASP
4	D	248	ARG
4	D	252	LEU
4	D	301	ASP
4	D	303	VAL
4	D	354	ILE
4	D	425	ASN
4	D	450	HIS
5	E	1	MET
5	E	10	TRP
5	E	20	SER
5	E	25	ASP
5	E	160	PHE
1	F	7	THR
1	F	39	LYS
1	F	51	VAL
1	F	52	VAL
1	F	59	LYS
1	F	73	VAL
1	F	82	LYS
1	F	101	MET
1	F	106	SER
1	F	127	TYR
1	F	148	CYS
1	F	150	LEU
1	F	154	CYS
1	F	158	CYS
1	F	171	ARG
1	F	172	ARG
1	F	187	ARG
1	F	189	SER
1	F	222	ASP
1	F	227	SER
1	F	246	SER

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Mol	Chain	Res	Type
1	F	269	TRP
1	F	276	GLU
1	F	282	VAL
1	F	341	LYS
1	F	364	ARG
1	F	365	GLU
1	F	371	PHE
1	F	379	ASP
1	F	393	GLU
1	F	416	SER
1	F	417	TYR
1	F	442	LEU
1	F	496	GLU
1	F	499	LEU
1	F	500	MET
1	F	505	ARG
1	F	517	LYS
1	F	528	LEU
1	F	595	ARG
1	F	611	LEU
1	F	624	ARG
1	F	628	PHE
1	F	634	GLU
1	F	640	THR
1	F	649	LYS
1	F	661	LYS
1	F	670	GLU
1	F	674	CYS
1	F	680	SER
1	F	686	GLU
2	G	125	TYR
2	G	131	ILE
2	G	147	LEU
2	G	151	THR
2	G	161	LYS
2	G	193	CYS
2	G	207	SER
2	G	247	LEU
2	G	255	GLU
2	G	257	MET
2	G	262	ASP
2	G	268	ASN

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Mol	Chain	Res	Type
2	G	272	HIS
2	G	286	GLU
2	G	293	SER
2	G	313	LEU
2	G	328	ASN
2	G	329	VAL
2	G	339	TRP
2	G	407	GLU
2	G	410	ASP
2	G	414	ASP
2	G	416	GLU
2	G	417	SER
2	G	458	CYS
2	G	499	SER
2	G	520	ASP
2	G	530	ARG
3	H	7	ASP
3	H	11	LYS
3	H	27	ILE
3	H	50	ARG
3	H	54	MET
3	H	74	ARG
4	I	10	ASN
4	I	24	MET
4	I	67	CYS
4	I	75	SER
4	I	115	SER
4	I	144	LYS
4	I	155	GLU
4	I	175	VAL
4	I	200	GLU
4	I	203	LYS
4	I	222	LEU
4	I	239	ASP
4	I	248	ARG
4	I	252	LEU
4	I	301	ASP
4	I	303	VAL
4	I	354	ILE
4	I	425	ASN
4	I	450	HIS
5	J	1	MET

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Mol	Chain	Res	Type
5	J	10	TRP
5	J	20	SER
5	J	25	ASP
5	J	160	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	118	HIS
1	A	145	HIS
1	A	146	ASN
1	A	152	GLN
1	A	313	GLN
1	A	391	GLN
1	A	414	ASN
1	A	527	ASN
1	A	610	ASN
1	A	652	HIS
2	B	253	GLN
2	B	274	HIS
2	B	328	ASN
2	B	362	ASN
4	D	10	ASN
4	D	166	HIS
4	D	210	GLN
4	D	425	ASN
4	D	450	HIS
1	F	97	ASN
1	F	118	HIS
1	F	145	HIS
1	F	146	ASN
1	F	152	GLN
1	F	313	GLN
1	F	391	GLN
1	F	414	ASN
1	F	527	ASN
1	F	652	HIS
2	G	253	GLN
2	G	274	HIS
2	G	328	ASN
2	G	362	ASN

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Mol	Chain	Res	Type
4	I	10	ASN
4	I	166	HIS
4	I	210	GLN
4	I	425	ASN
4	I	450	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
7	SF4	E	201	5	0,12,12	-	-	-		
6	FES	G	704	2	0,4,4	-	-	-		
7	SF4	F	703	1	0,12,12	-	-	-		
7	SF4	F	702	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
7	SF4	F	704	1	0,12,12	-	-	-		
7	SF4	F	705	1	0,12,12	-	-	-		
6	FES	A	701	1	0,4,4	-	-	-		
9	FMN	B	703	-	33,33,33	0.63	0	48,50,50	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	FCO	I	502	4	0,6,6	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	G	702	-	0,12,12	-	-	-		
6	FES	B	704	2	0,4,4	-	-	-		
7	SF4	A	702	1	0,12,12	-	-	-		
8	NAD	B	701	-	42,48,48	1.35	3 (7%)	50,73,73	1.13	5 (10%)
9	FMN	G	703	-	33,33,33	0.63	0	48,50,50	0.67	0
11	FCO	D	502	4	0,6,6	-	-	-		
6	FES	F	701	1	0,4,4	-	-	-		
7	SF4	B	702	-	0,12,12	-	-	-		
7	SF4	J	201	5	0,12,12	-	-	-		
8	NAD	G	701	-	42,48,48	1.35	3 (7%)	50,73,73	1.13	5 (10%)

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
7	SF4	E	201	5	-	-	0/6/5/5
6	FES	G	704	2	-	-	0/1/1/1
7	SF4	F	703	1	-	-	0/6/5/5
7	SF4	F	702	1	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
7	SF4	F	704	1	-	-	0/6/5/5
7	SF4	F	705	1	-	-	0/6/5/5
6	FES	A	701	1	-	-	0/1/1/1
9	FMN	B	703	-	-	7/18/18/18	0/3/3/3
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	G	702	-	-	-	0/6/5/5
6	FES	B	704	2	-	-	0/1/1/1
7	SF4	A	702	1	-	-	0/6/5/5
8	NAD	B	701	-	-	10/26/62/62	0/5/5/5
9	FMN	G	703	-	-	7/18/18/18	0/3/3/3
6	FES	F	701	1	-	-	0/1/1/1
7	SF4	B	702	-	-	-	0/6/5/5
7	SF4	J	201	5	-	-	0/6/5/5
8	NAD	G	701	-	-	10/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	701	NAD	C4N-C3N	5.63	1.48	1.39
8	G	701	NAD	C4N-C3N	5.63	1.48	1.39
8	B	701	NAD	C5N-C4N	3.91	1.47	1.38
8	G	701	NAD	C5N-C4N	3.91	1.47	1.38
8	B	701	NAD	C6N-C5N	-3.13	1.31	1.38
8	G	701	NAD	C6N-C5N	-3.13	1.31	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	701	NAD	C5N-C4N-C3N	-4.71	114.77	120.34
8	G	701	NAD	C5N-C4N-C3N	-4.71	114.77	120.34
8	B	701	NAD	C3D-C2D-C1D	2.67	105.00	100.98
8	G	701	NAD	C3D-C2D-C1D	2.67	105.00	100.98
8	B	701	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
8	G	701	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
8	B	701	NAD	O4D-C1D-C2D	-2.44	103.37	106.93
8	G	701	NAD	O4D-C1D-C2D	-2.44	103.37	106.93
8	B	701	NAD	C5A-C6A-N6A	2.23	123.73	120.35
8	G	701	NAD	C5A-C6A-N6A	2.23	123.73	120.35

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	701	NAD	C5B-O5B-PA-O3
8	B	701	NAD	O4D-C1D-N1N-C2N
8	B	701	NAD	O4D-C1D-N1N-C6N
8	B	701	NAD	C2D-C1D-N1N-C2N
8	B	701	NAD	C2D-C1D-N1N-C6N
8	G	701	NAD	C5B-O5B-PA-O3
8	G	701	NAD	O4D-C1D-N1N-C2N
8	G	701	NAD	O4D-C1D-N1N-C6N
8	G	701	NAD	C2D-C1D-N1N-C2N
8	G	701	NAD	C2D-C1D-N1N-C6N
9	B	703	FMN	N10-C1'-C2'-O2'
9	B	703	FMN	N10-C1'-C2'-C3'
9	B	703	FMN	C1'-C2'-C3'-O3'
9	B	703	FMN	C1'-C2'-C3'-C4'
9	G	703	FMN	N10-C1'-C2'-O2'
9	G	703	FMN	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
9	G	703	FMN	C1'-C2'-C3'-O3'
9	G	703	FMN	C1'-C2'-C3'-C4'
9	B	703	FMN	O2'-C2'-C3'-O3'
9	G	703	FMN	O2'-C2'-C3'-O3'
8	B	701	NAD	O4D-C4D-C5D-O5D
8	B	701	NAD	C3D-C4D-C5D-O5D
8	G	701	NAD	O4D-C4D-C5D-O5D
8	G	701	NAD	C3D-C4D-C5D-O5D
9	B	703	FMN	O2'-C2'-C3'-C4'
9	G	703	FMN	O2'-C2'-C3'-C4'
8	B	701	NAD	C4D-C5D-O5D-PN
8	G	701	NAD	C4D-C5D-O5D-PN
9	B	703	FMN	C4'-C5'-O5'-P
9	G	703	FMN	C4'-C5'-O5'-P
8	B	701	NAD	C5B-O5B-PA-O2A
8	G	701	NAD	C5B-O5B-PA-O2A
8	B	701	NAD	O4B-C4B-C5B-O5B
8	G	701	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

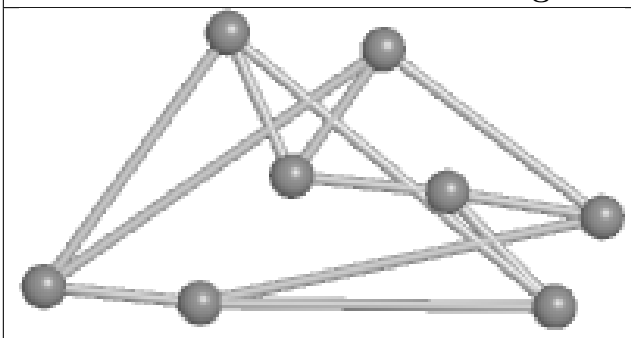
16 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	703	SF4	2	0
7	F	702	SF4	6	0
7	A	704	SF4	8	0
7	F	704	SF4	8	0
7	F	705	SF4	1	0
6	A	701	FES	2	0
11	I	502	FCO	4	0
7	A	705	SF4	1	0
7	A	703	SF4	2	0
7	G	702	SF4	13	0
7	A	702	SF4	6	0
8	B	701	NAD	1	0
11	D	502	FCO	4	0
6	F	701	FES	2	0
7	B	702	SF4	13	0
8	G	701	NAD	1	0

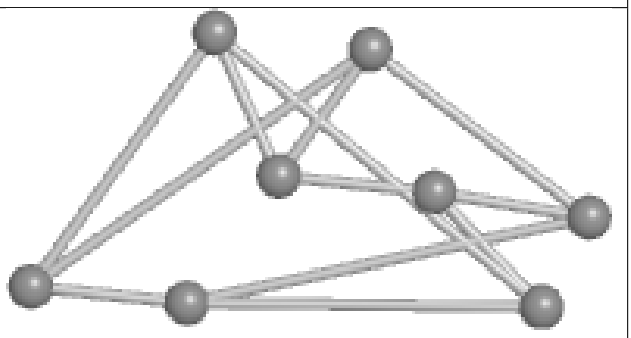
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

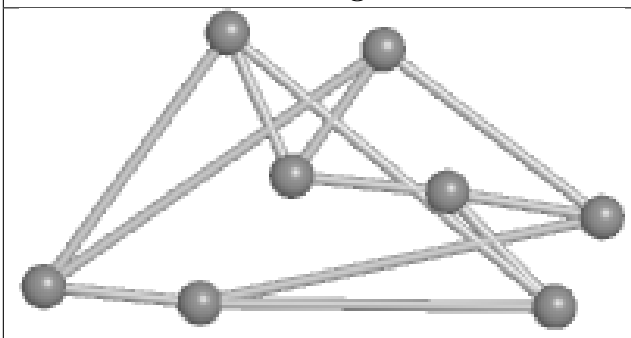
Ligand SF4 E 201



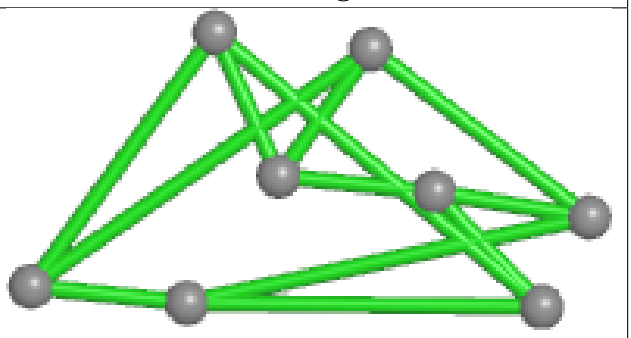
Bond lengths



Bond angles

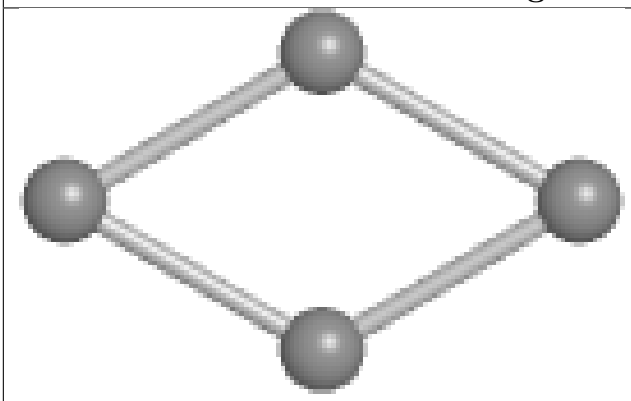


Torsions



Rings

Ligand FES G 704



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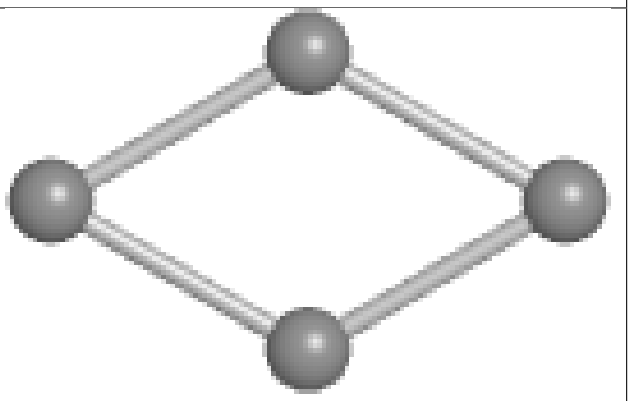
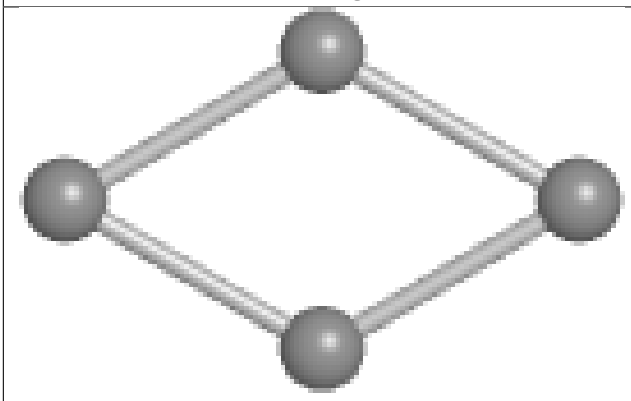


Bond angles



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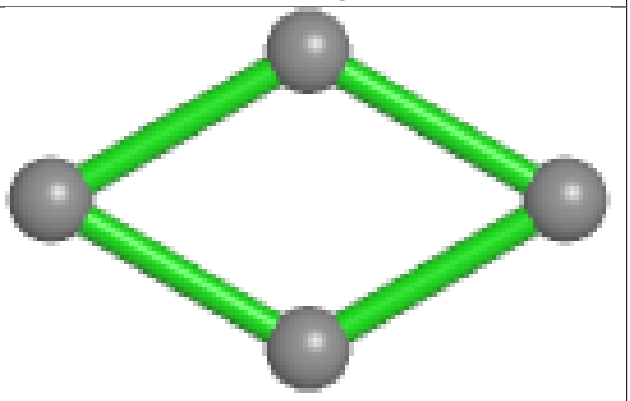
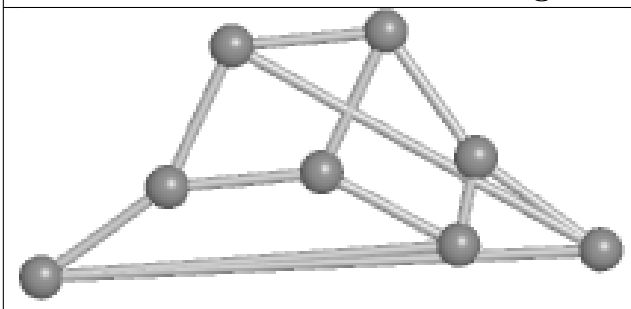


Rings

Ligand SF4 F 703



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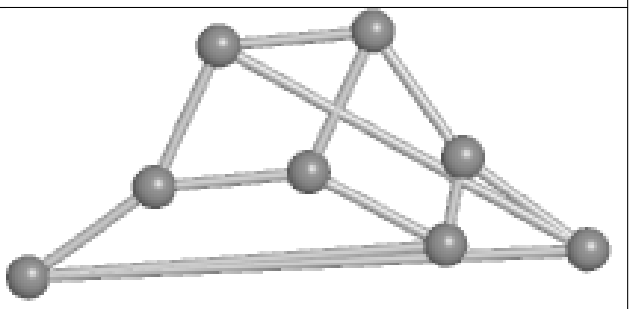

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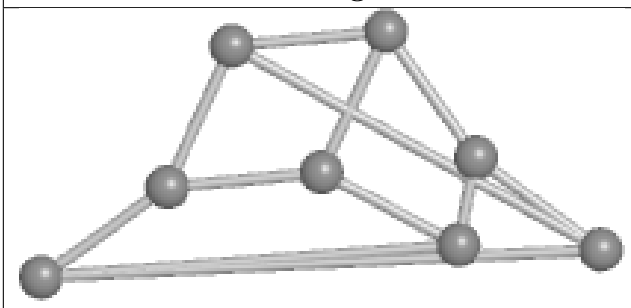

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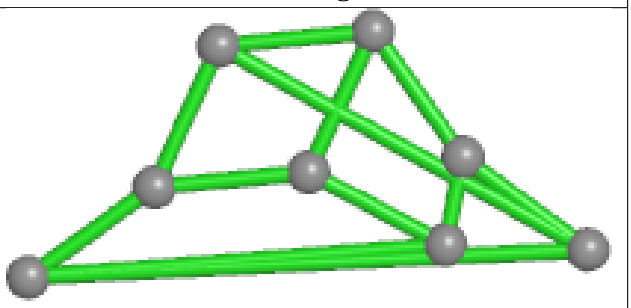
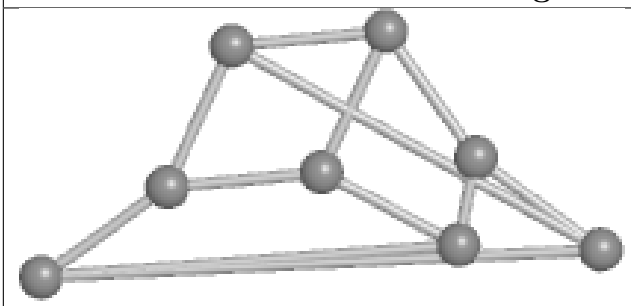


Rings

Ligand SF4 F 702



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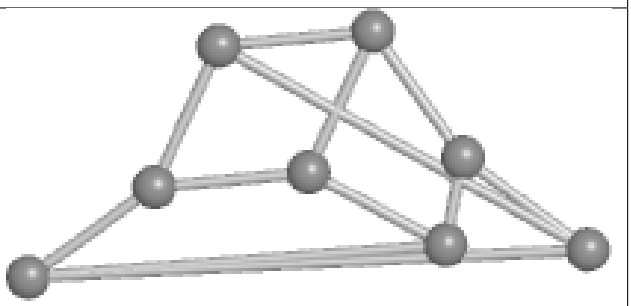

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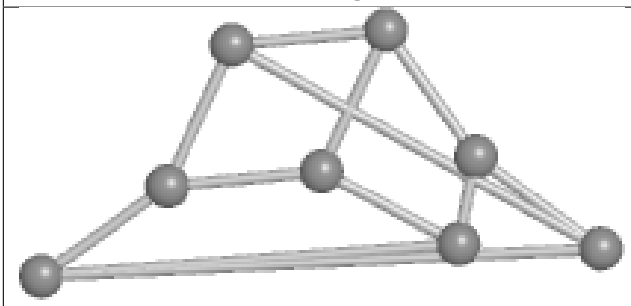

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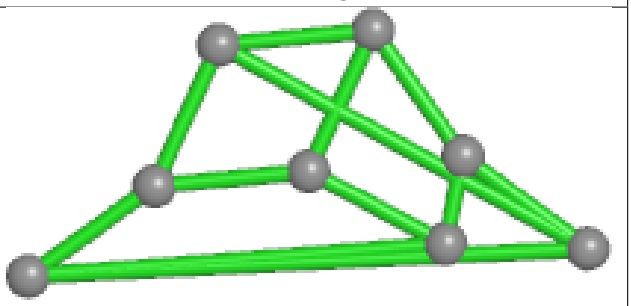
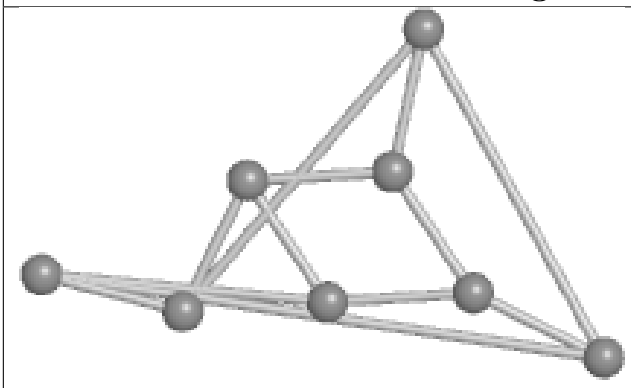


Rings

Ligand SF4 A 704



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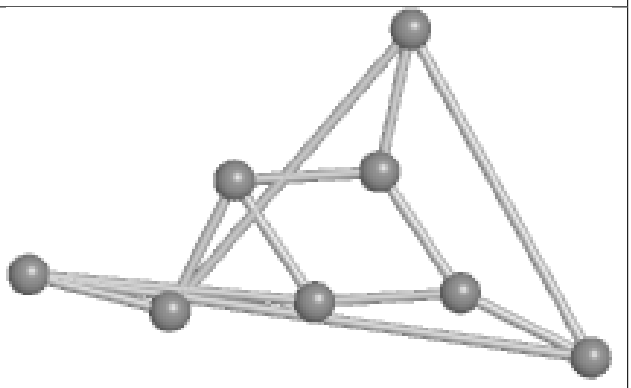

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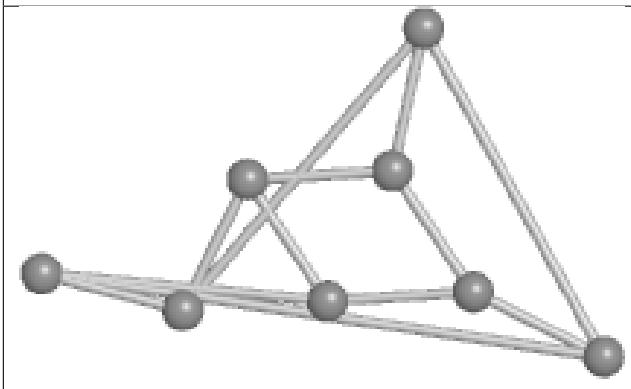

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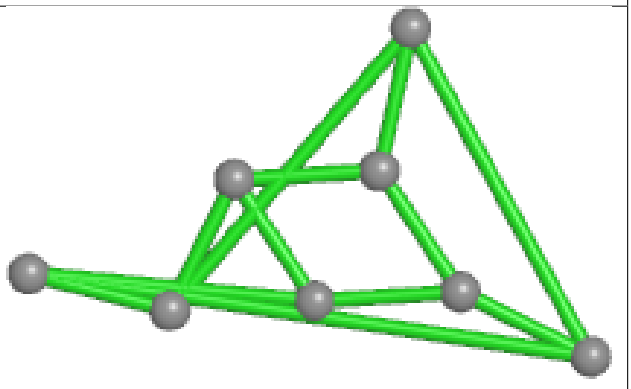
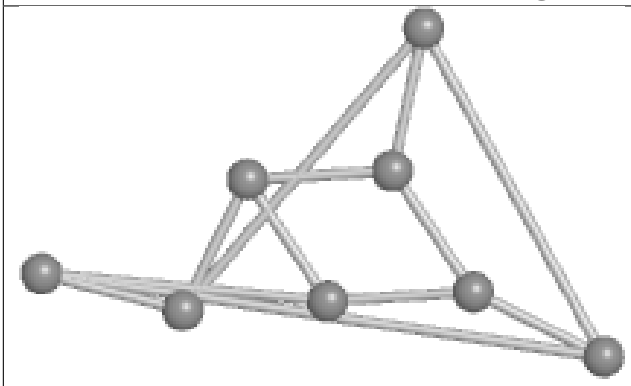


Rings

Ligand SF4 F 704



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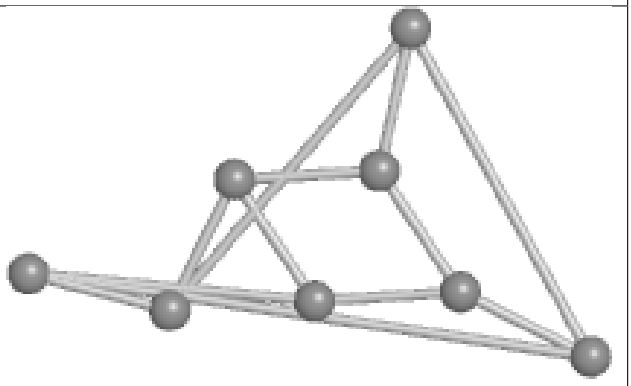

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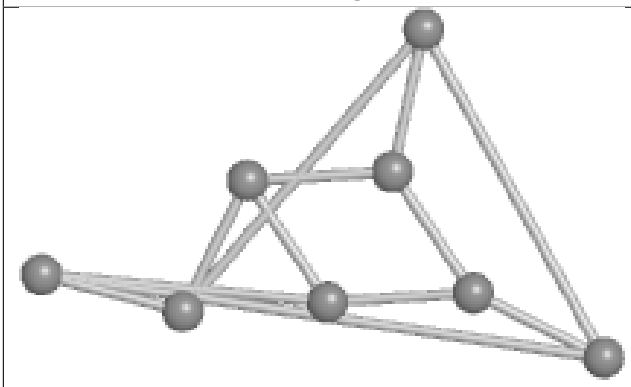

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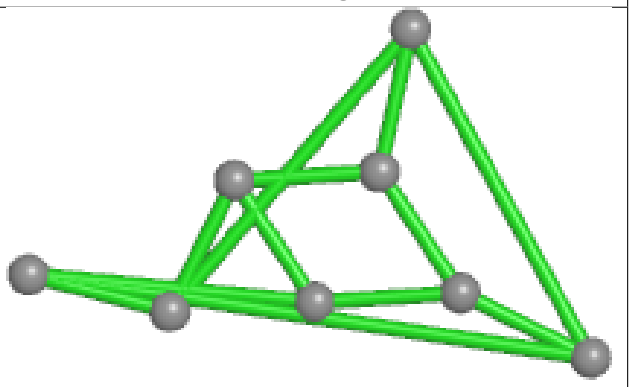

Rings

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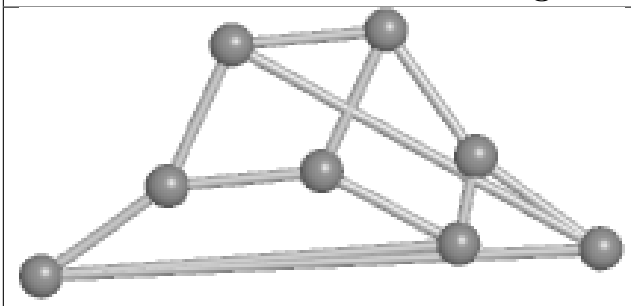

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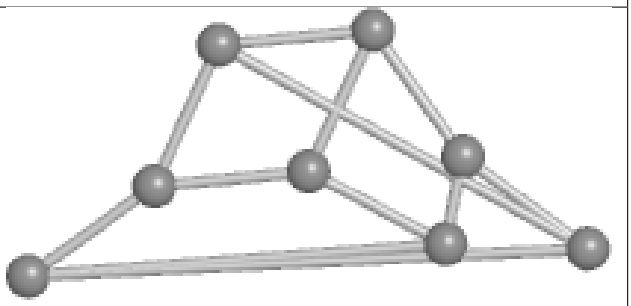

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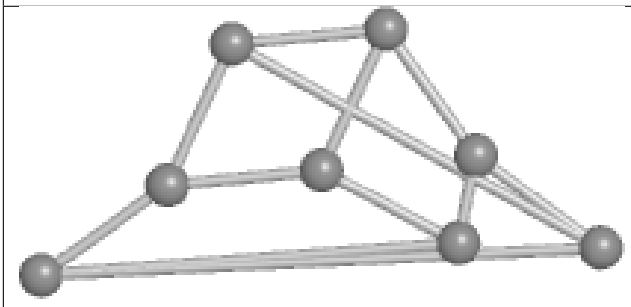

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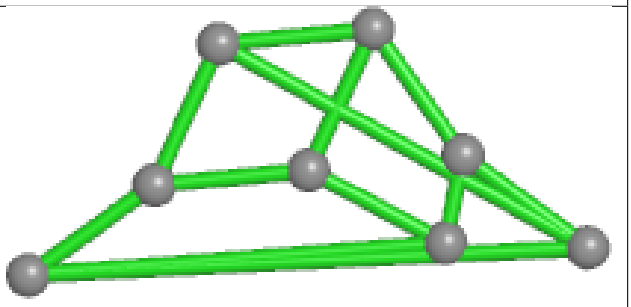
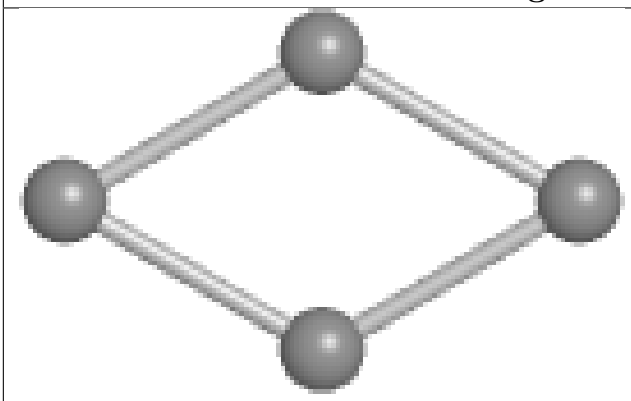


Rings

Ligand FES A 701



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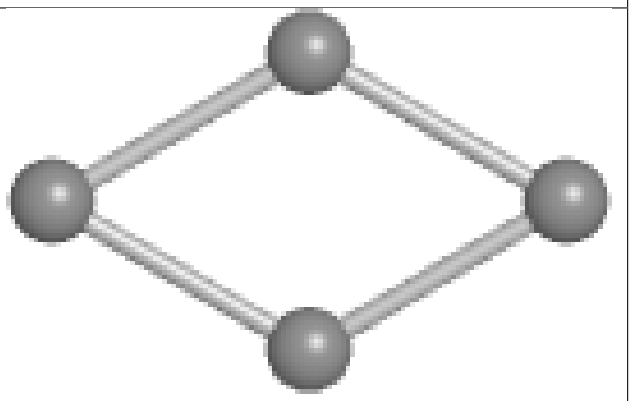

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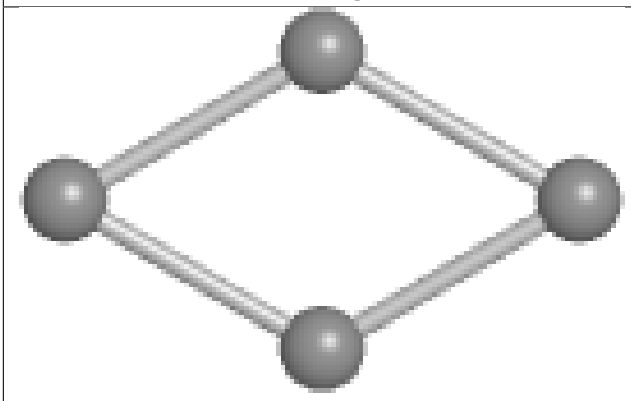

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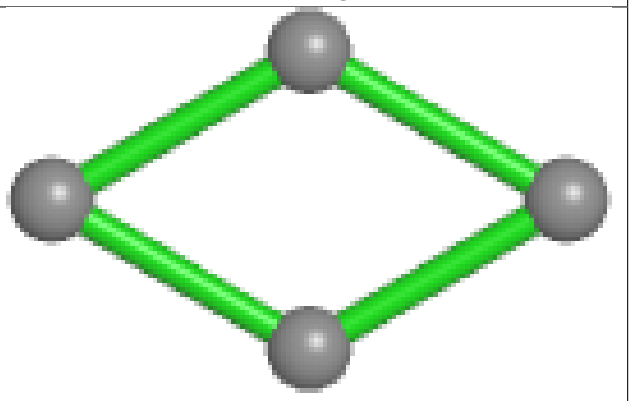
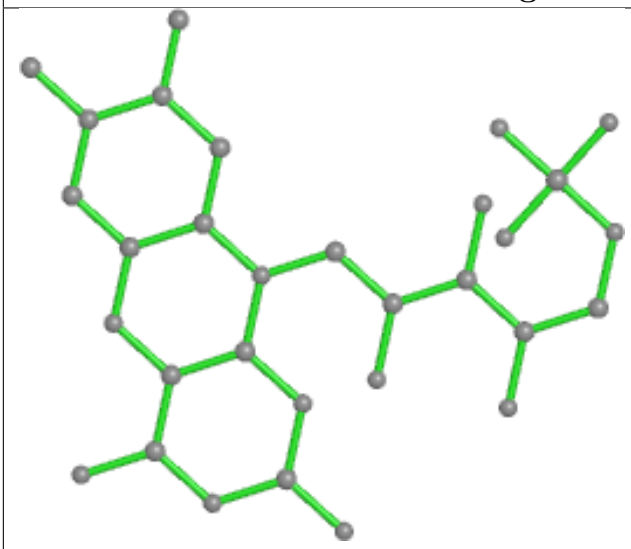


Rings

Ligand FMN B 703



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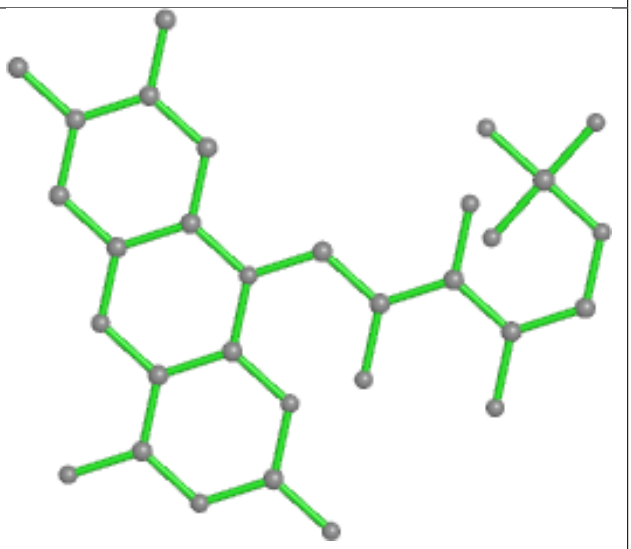

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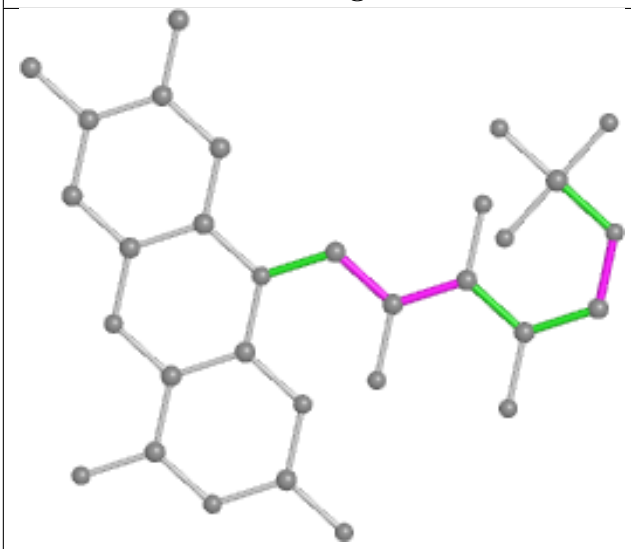

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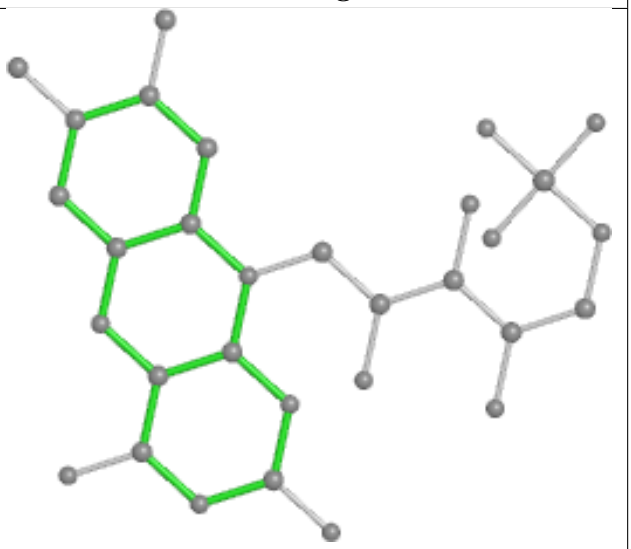
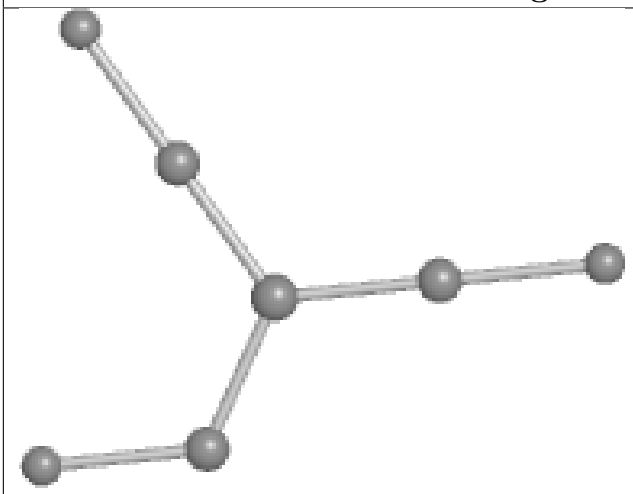


Rings

Ligand FCO I 502



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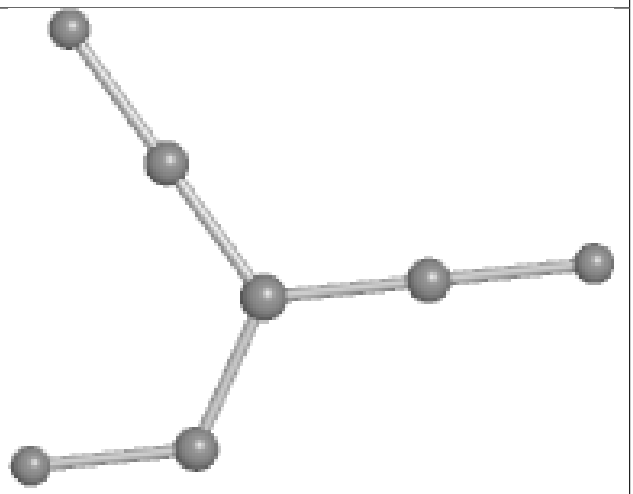

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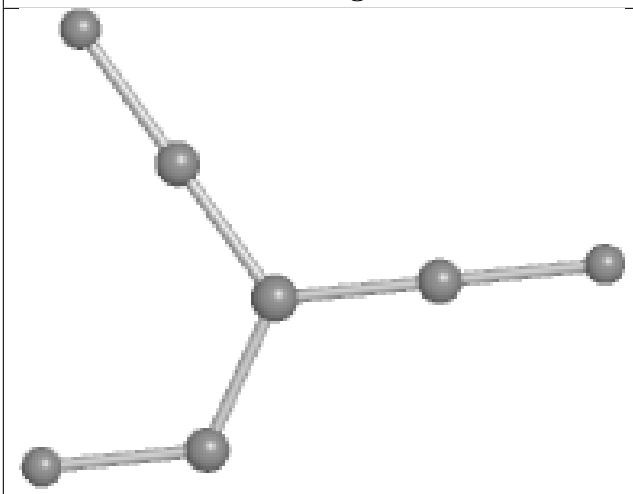

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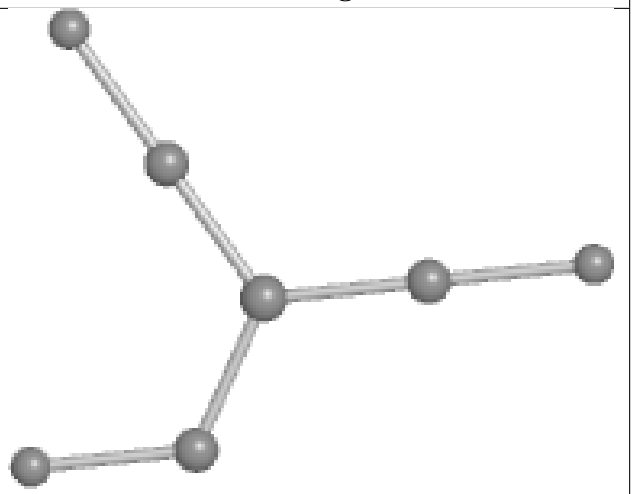
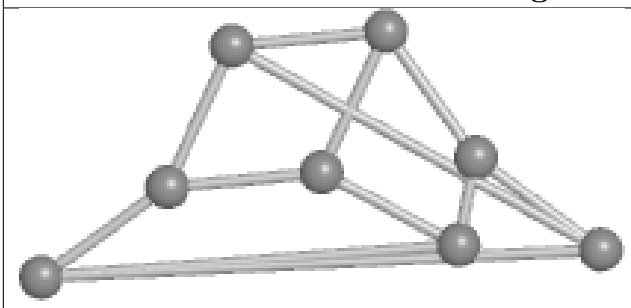


Rings

Ligand SF4 A 705



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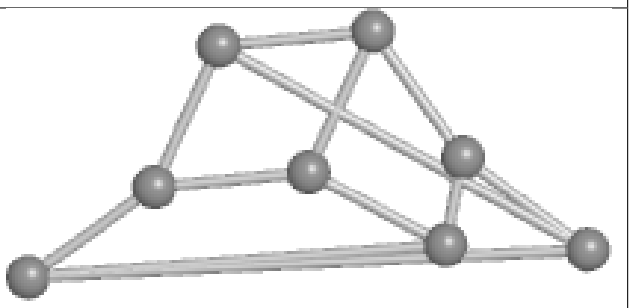

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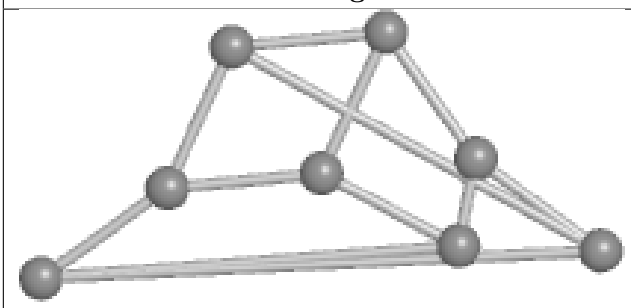

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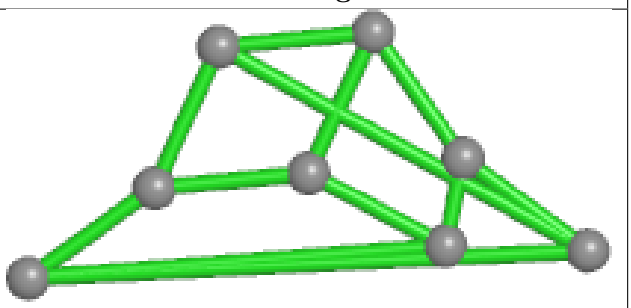
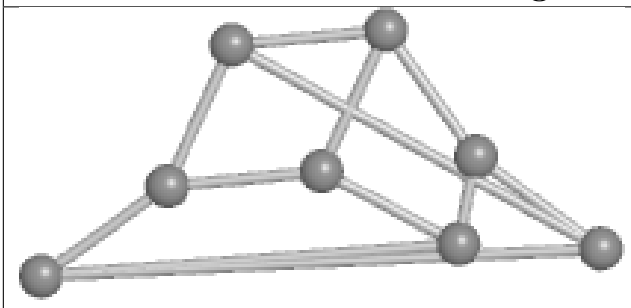


Rings

Ligand SF4 A 703



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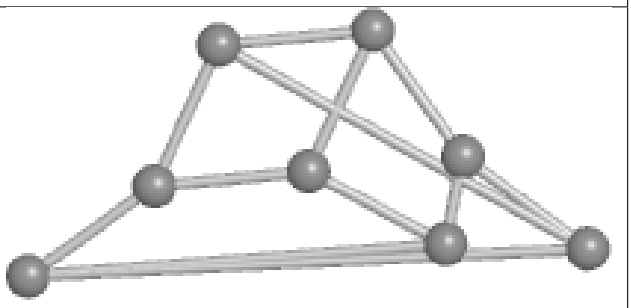
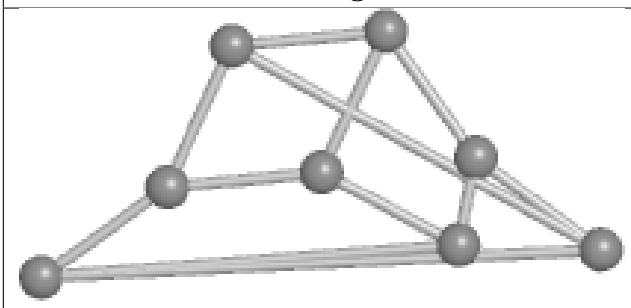


Bond angles



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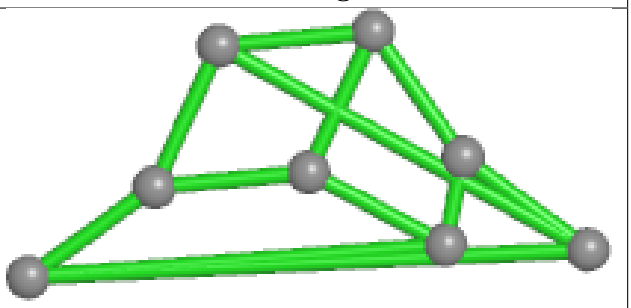
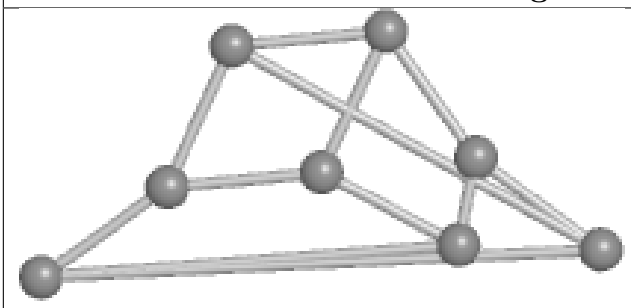
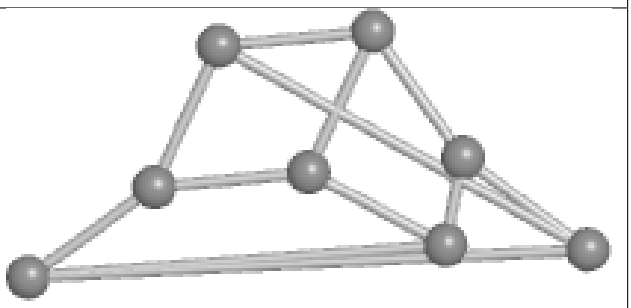


Rings

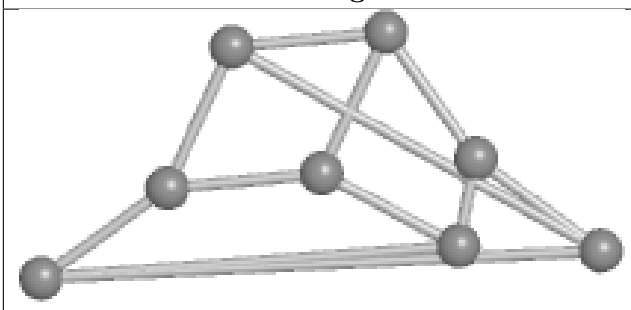
Ligand SF4 G 702



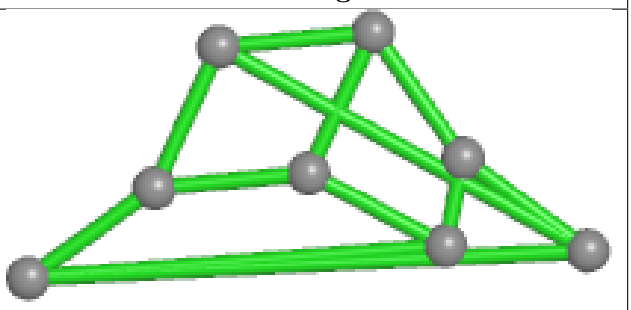
Bond lengths



Bond angles

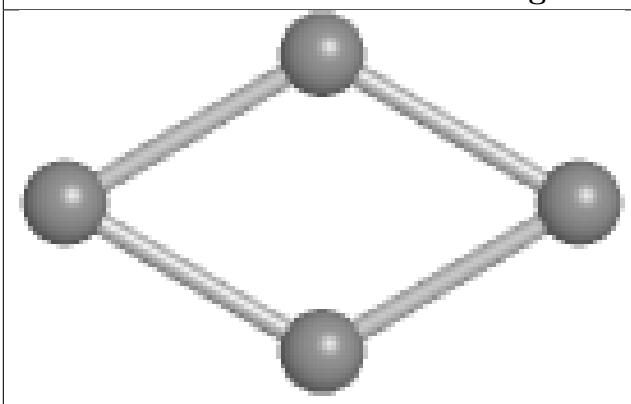


Torsions

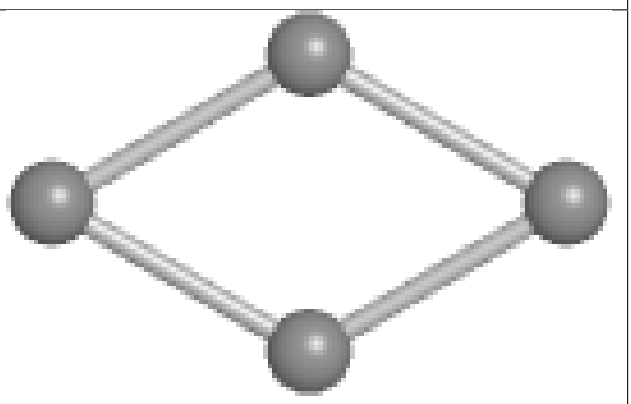


Rings

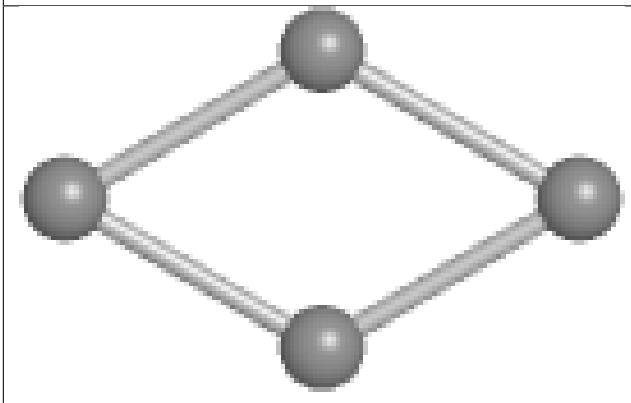
Ligand FES B 704



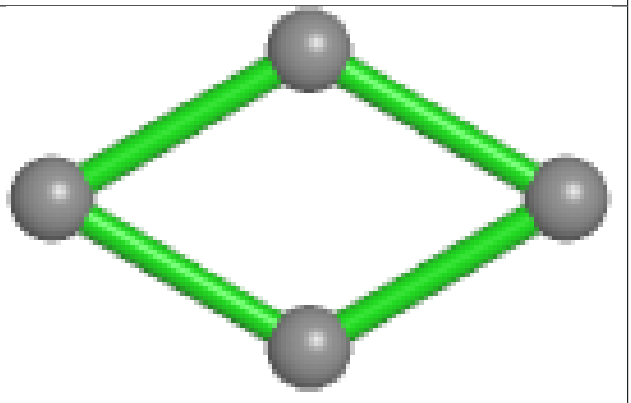
Bond lengths



Bond angles

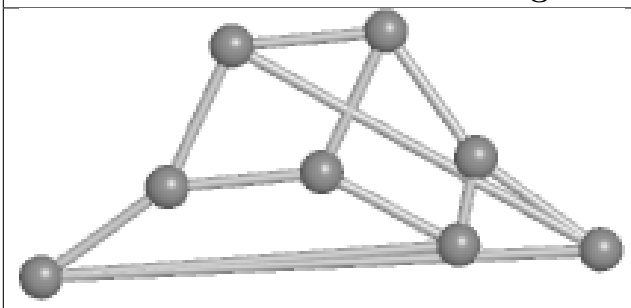


Torsions

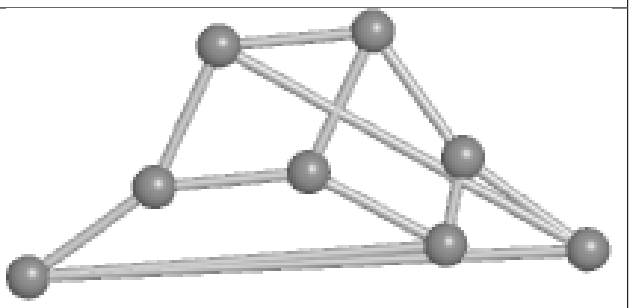


Rings

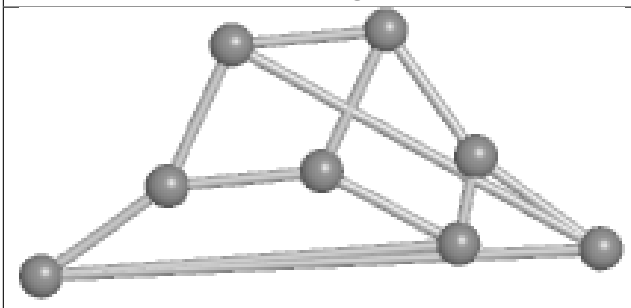
Ligand SF4 A 702



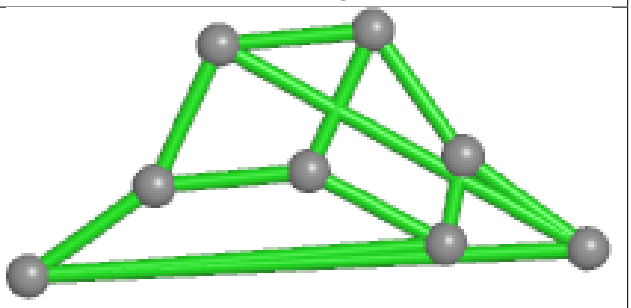
Bond lengths



Bond angles

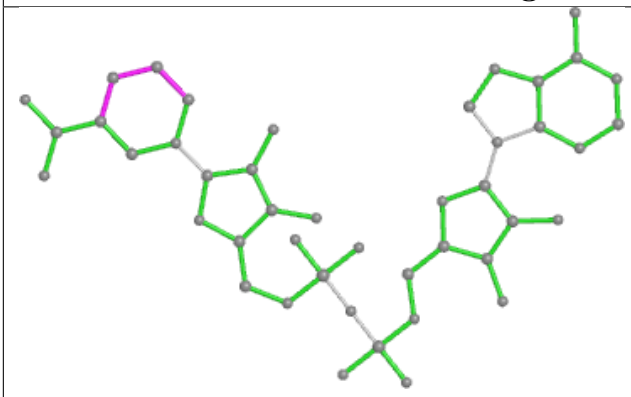


Torsions

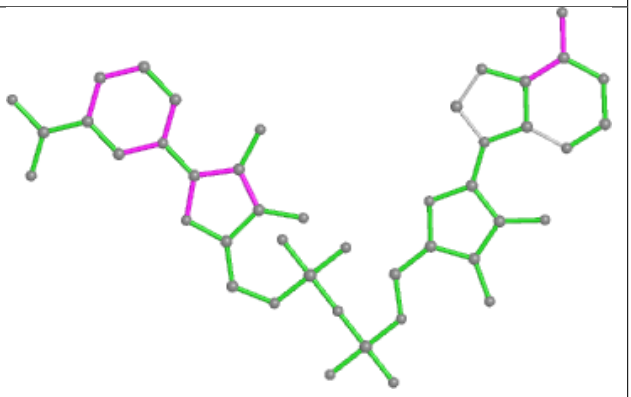


Rings

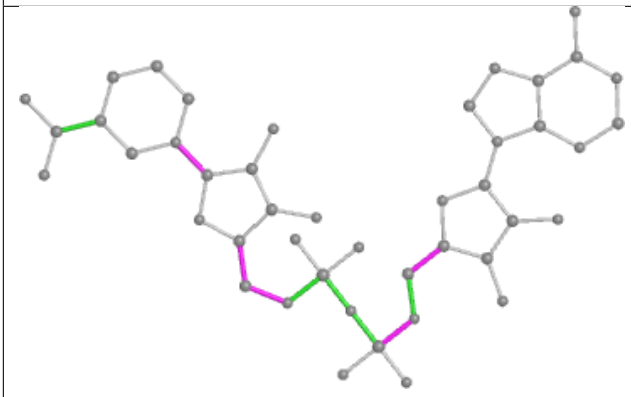
Ligand NAD B 701



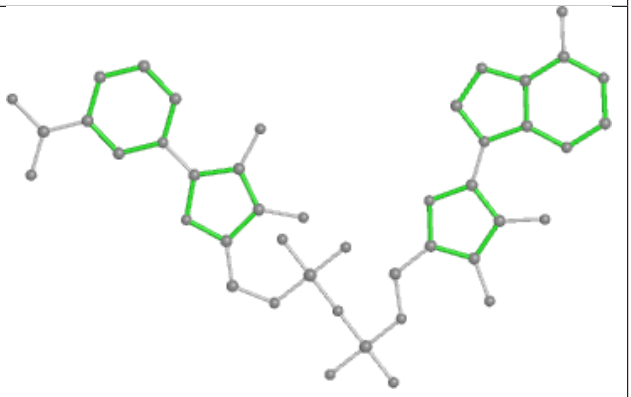
Bond lengths



Bond angles

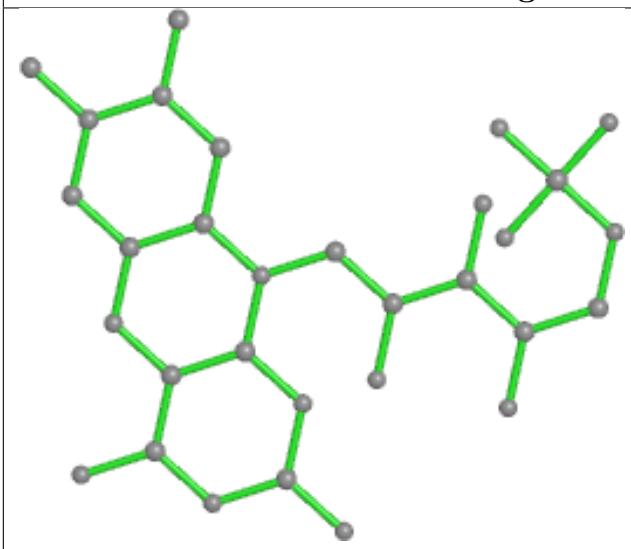


Torsions

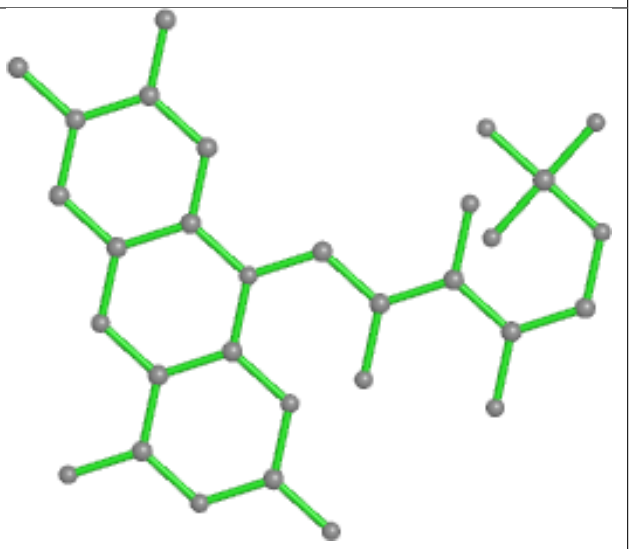


Rings

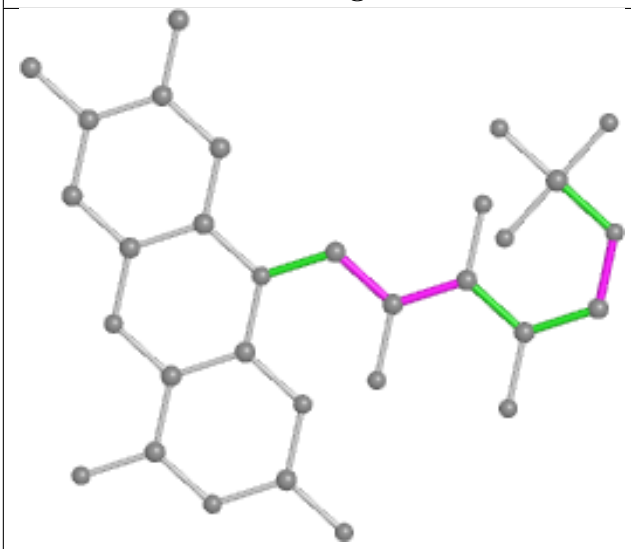
Ligand FMN G 703



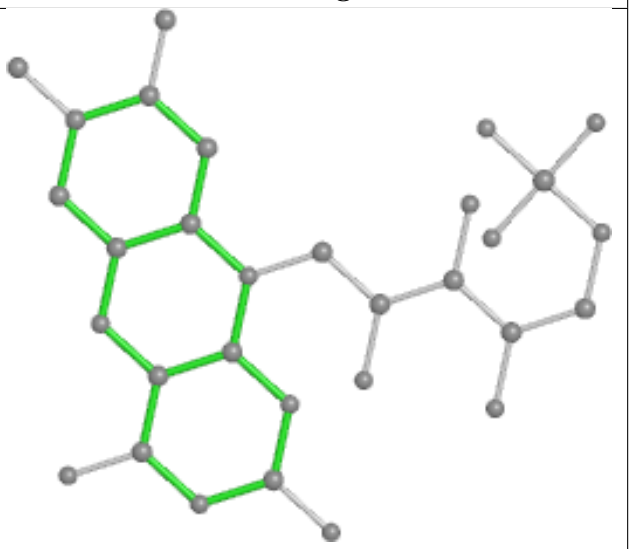
Bond lengths



Bond angles

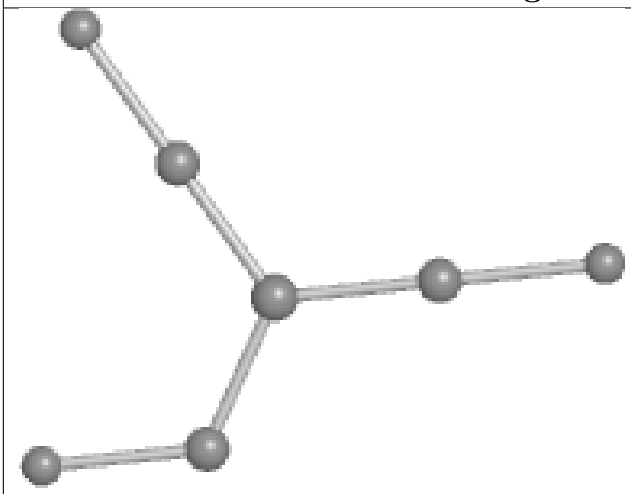


Torsions

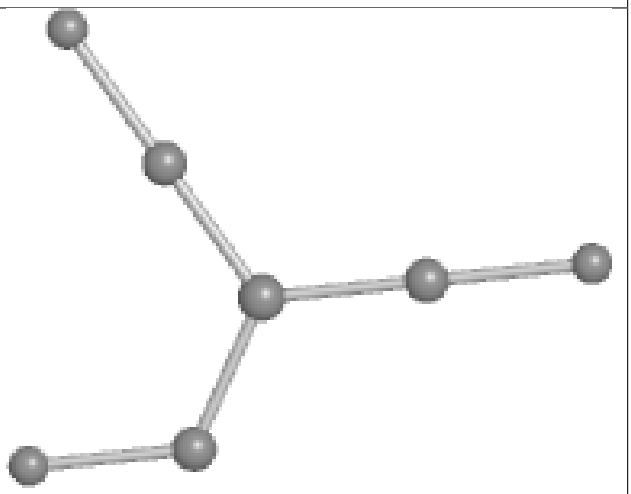


Rings

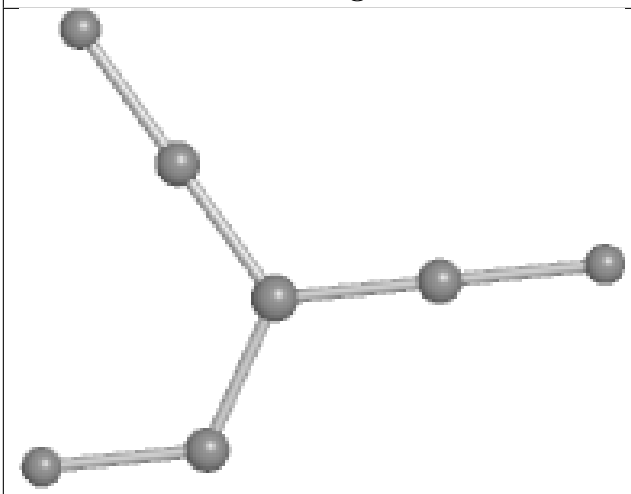
Ligand FCO D 502



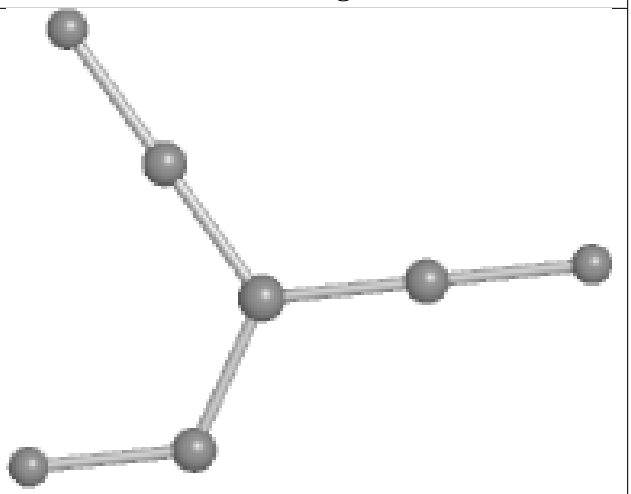
Bond lengths



Bond angles

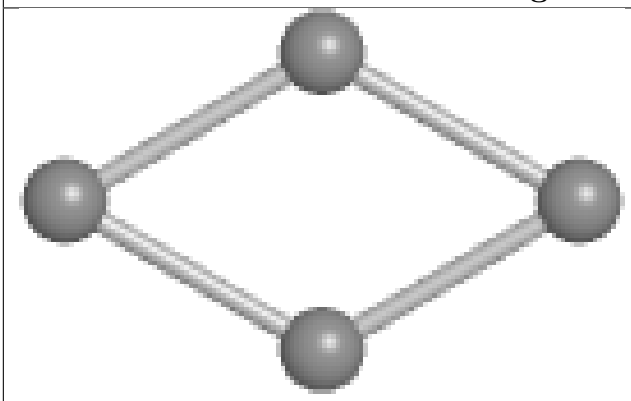


Torsions

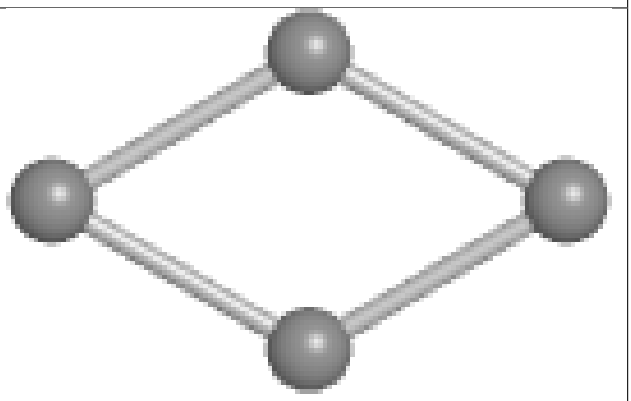


Rings

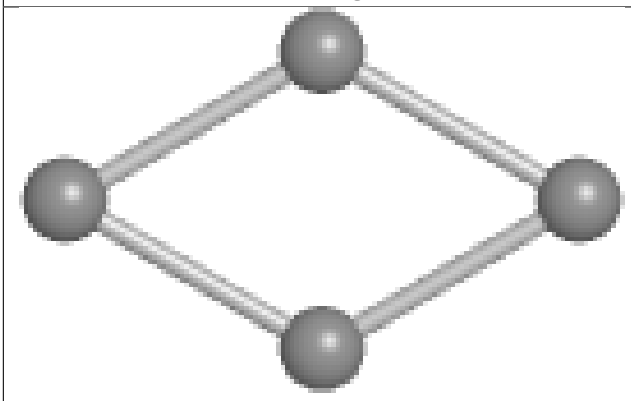
Ligand FES F 701



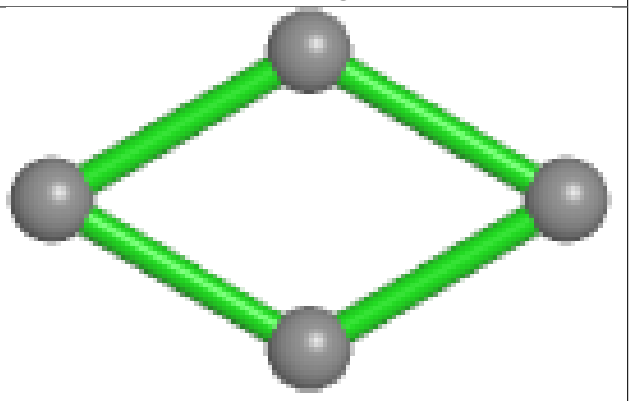
Bond lengths



Bond angles

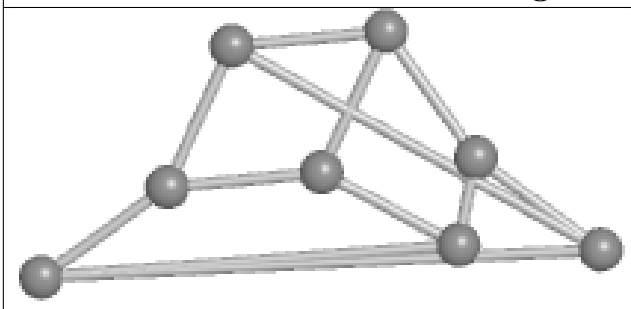


Torsions

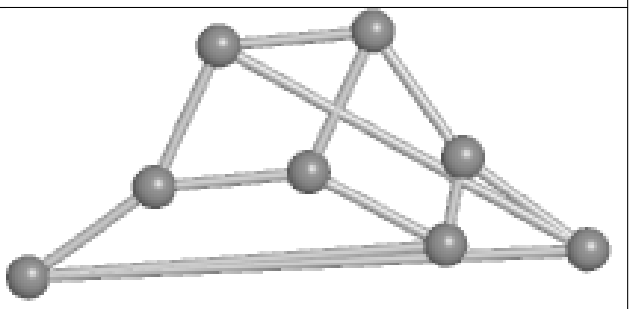


Rings

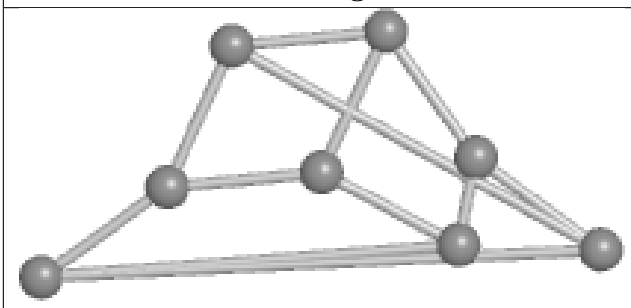
Ligand SF4 B 702



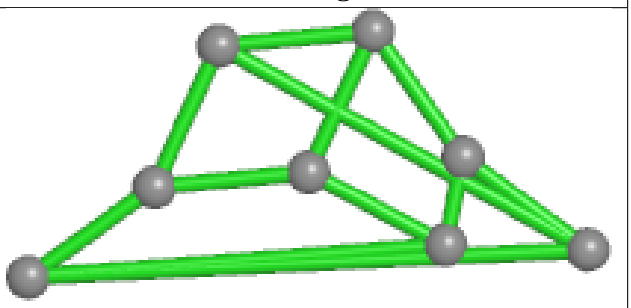
Bond lengths



Bond angles

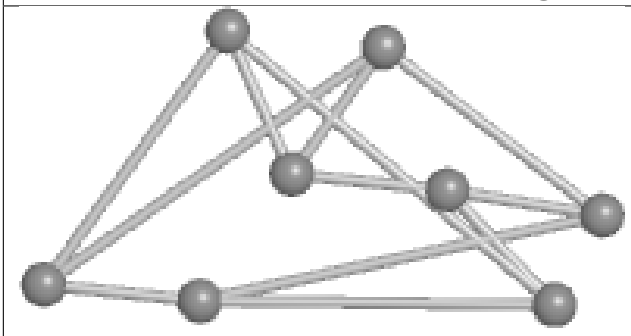


Torsions

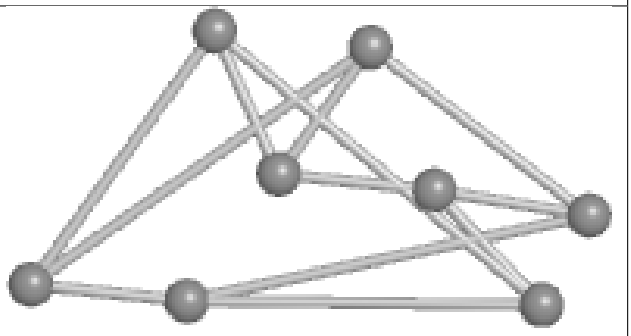


Rings

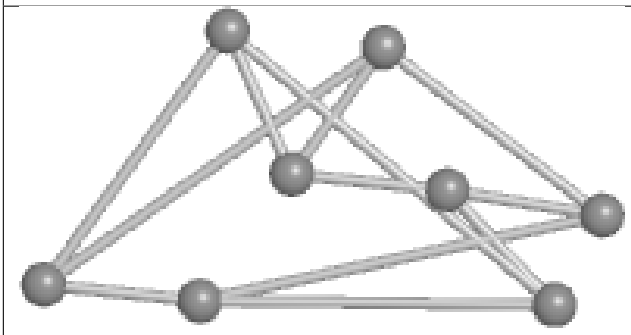
Ligand SF4 J 201



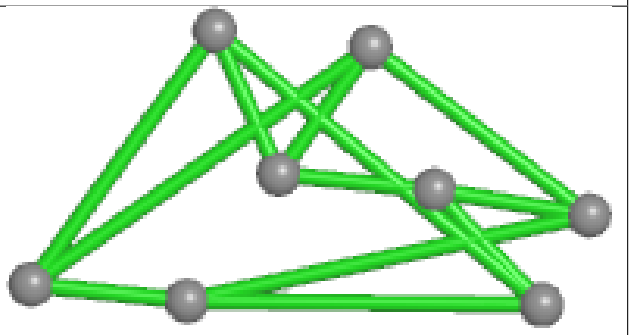
Bond lengths



Bond angles

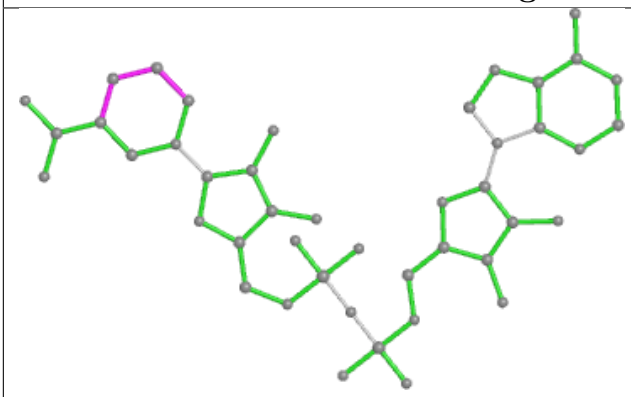


Torsions

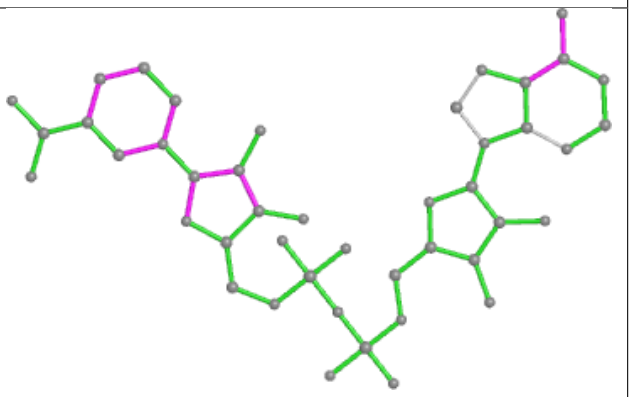


Rings

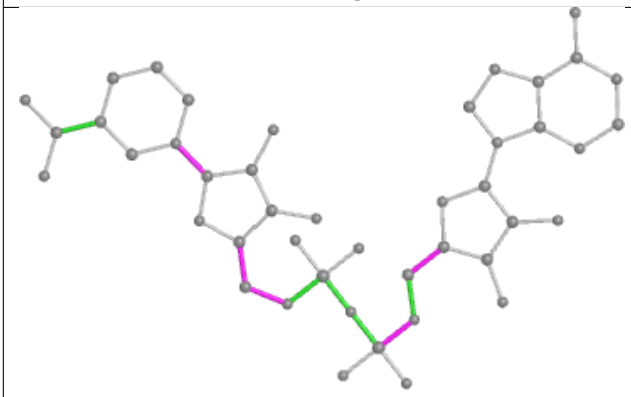
Ligand NAD G 701



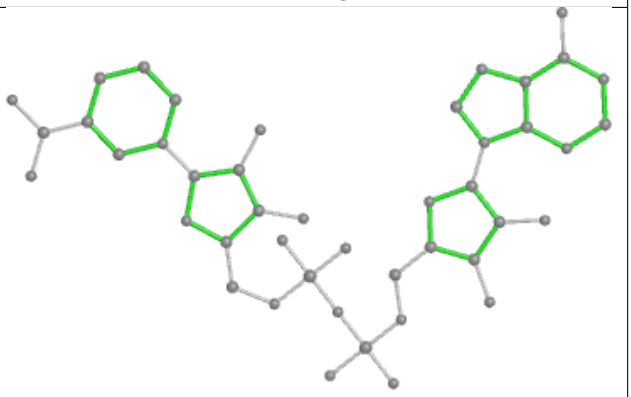
Bond lengths



Bond angles



Torsions



Rings

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.

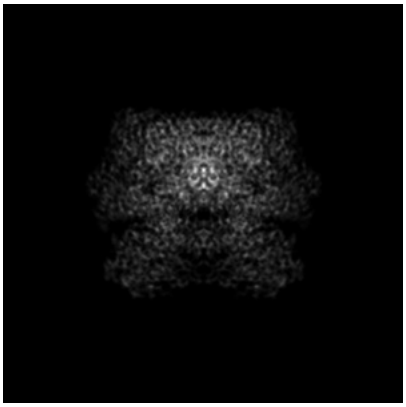
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25647. These allow visual inspection of the internal detail of the map and identification of artifacts.

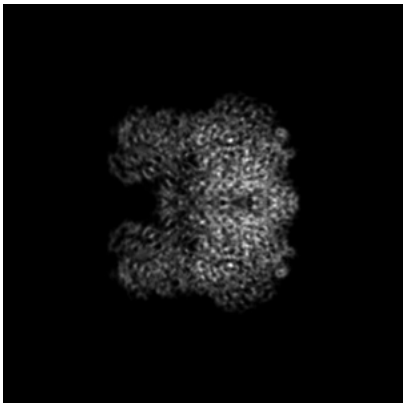
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

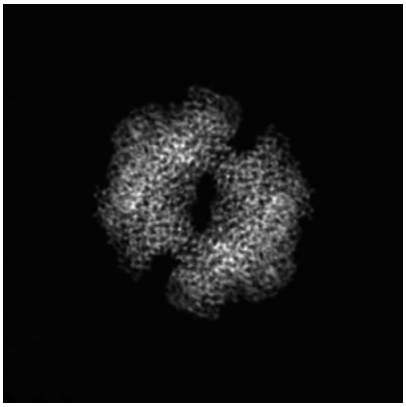
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 140

Y Index: 140

Z Index: 140

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 102

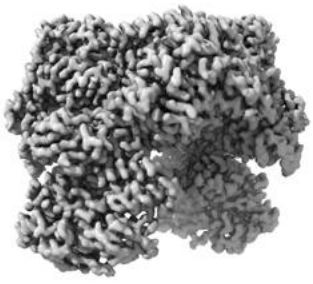
Y Index: 140

Z Index: 170

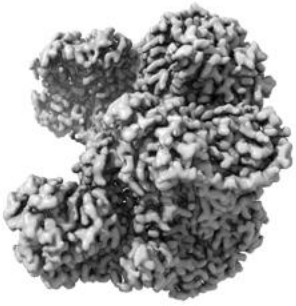
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

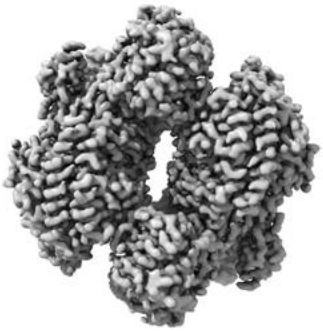
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

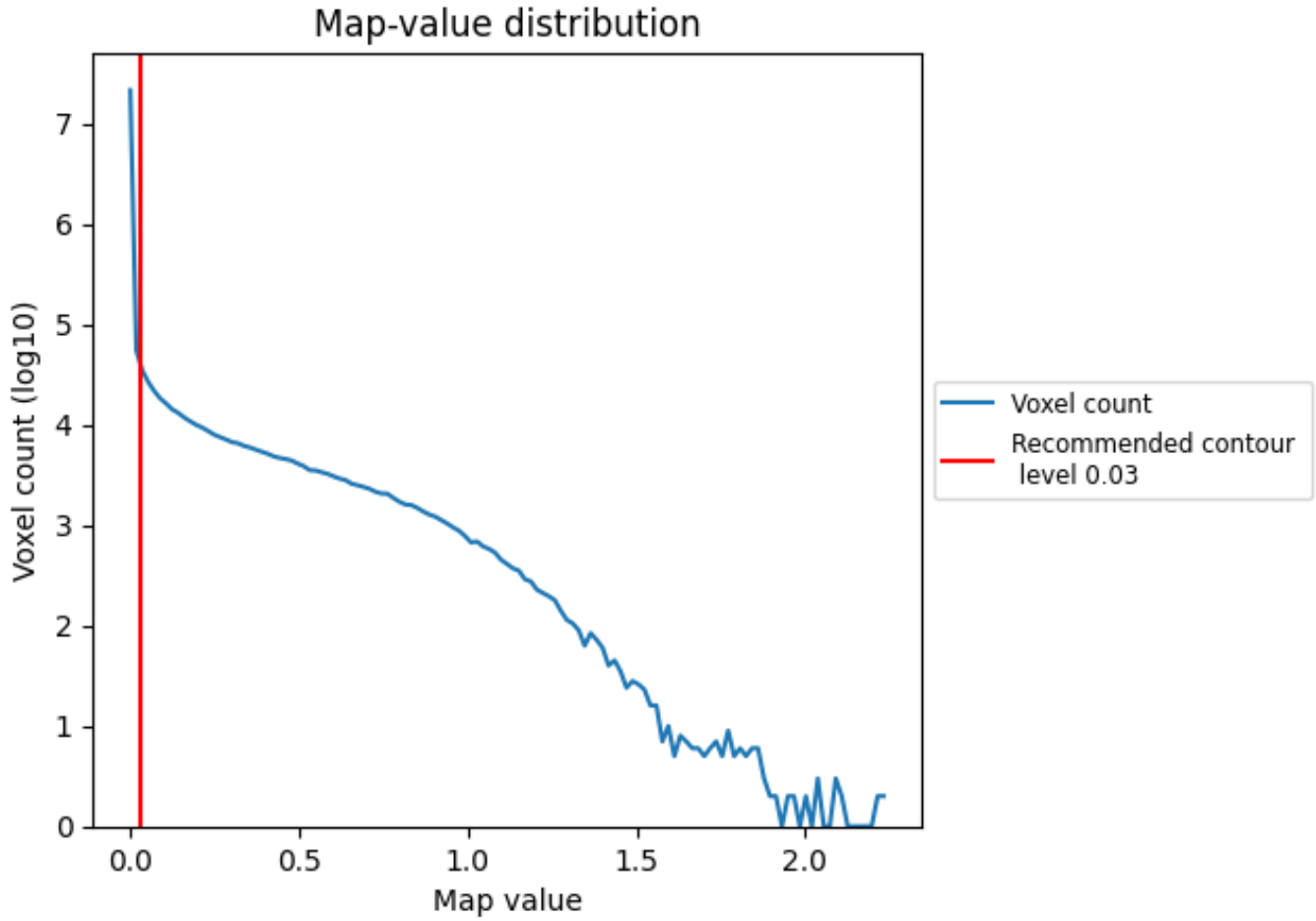
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

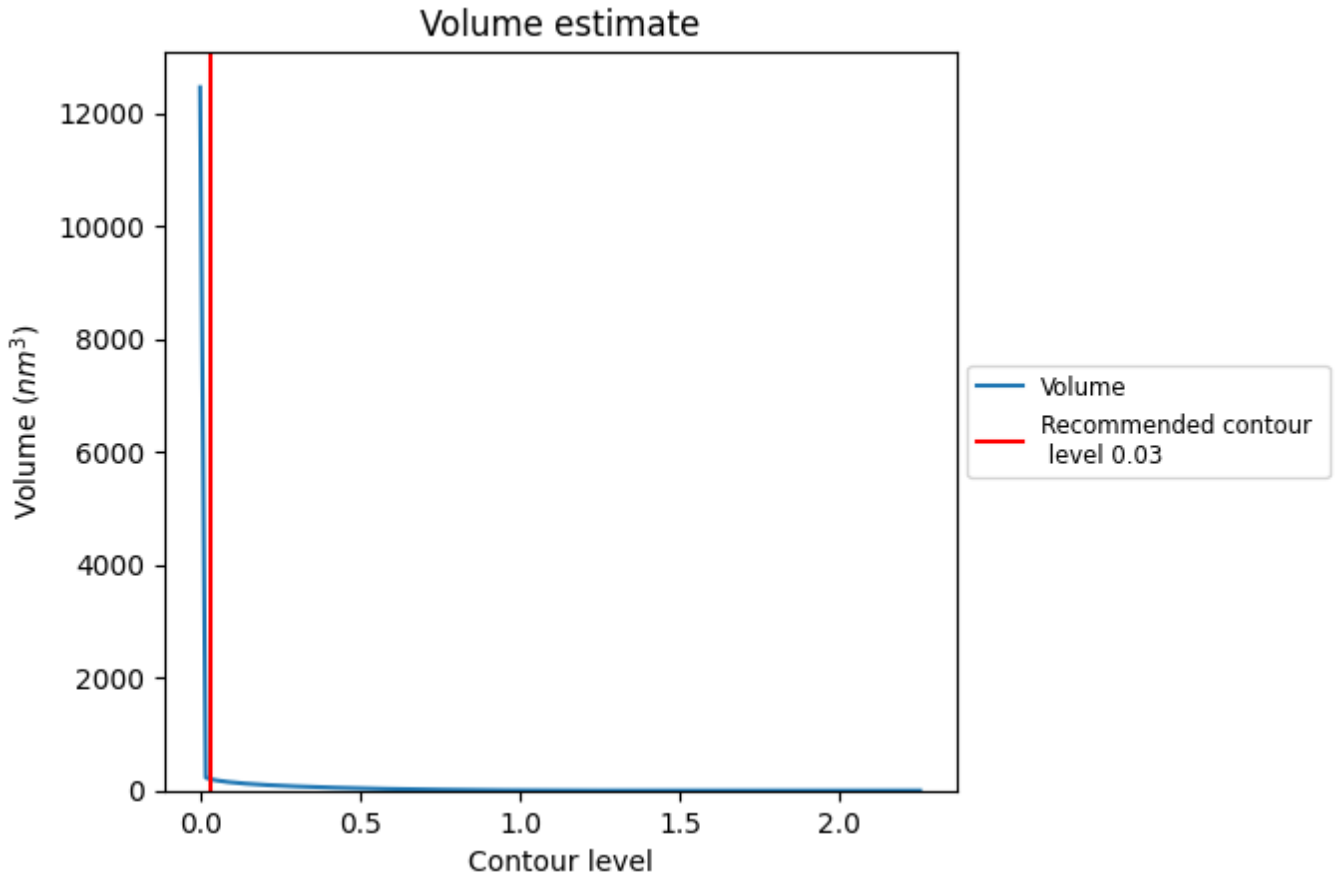
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

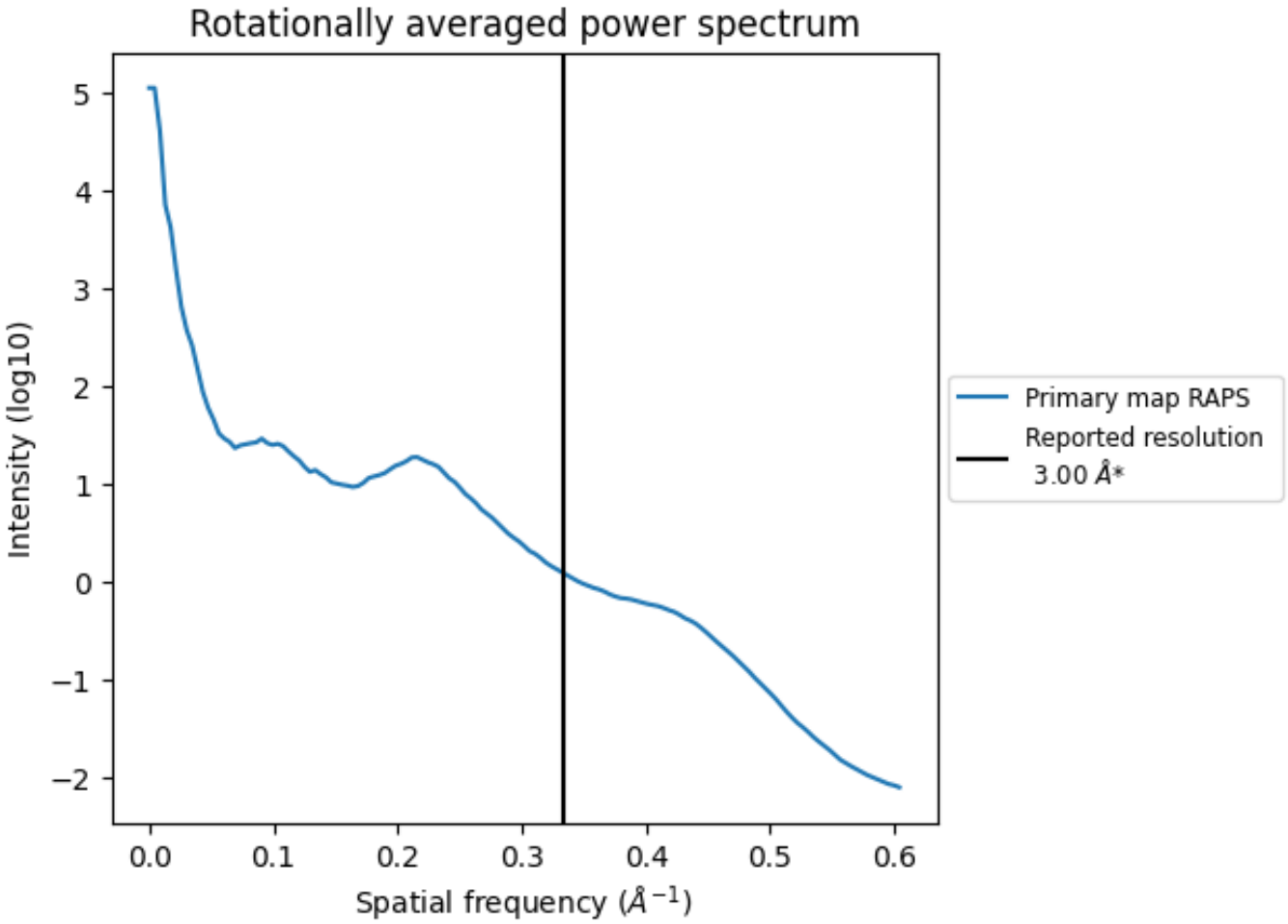
7.2 Volume estimate



The volume at the recommended contour level is 205 nm^3; this corresponds to an approximate mass of 185 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

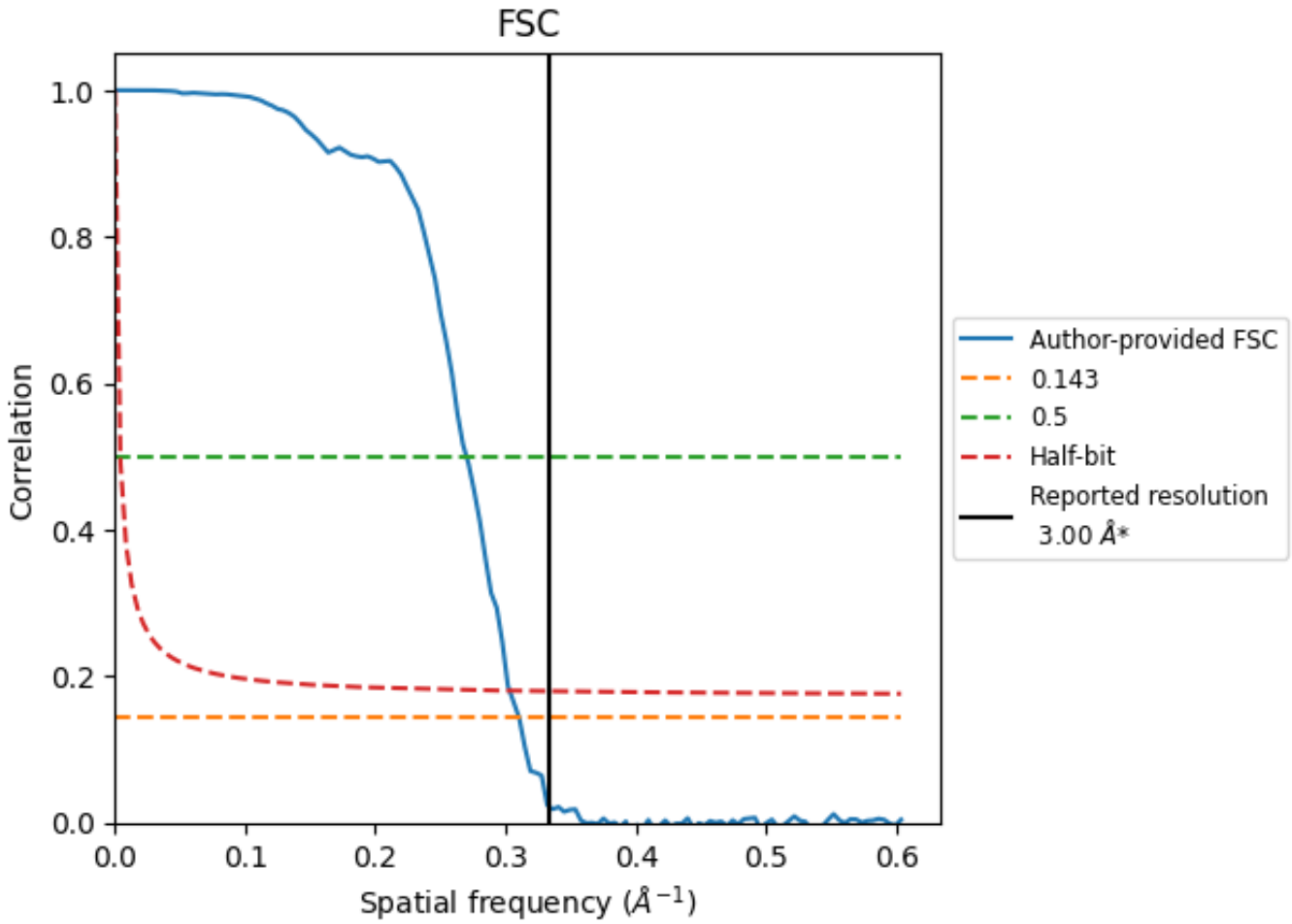


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

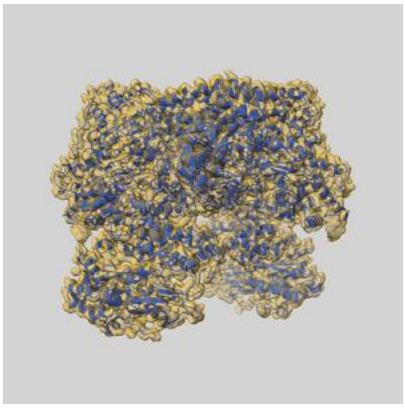
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.22	3.70	3.30
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

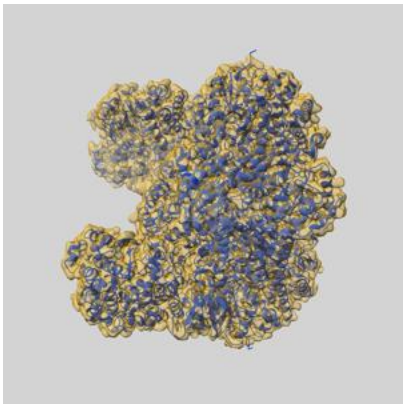
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25647 and PDB model 7T30. Per-residue inclusion information can be found in section 3 on page 9.

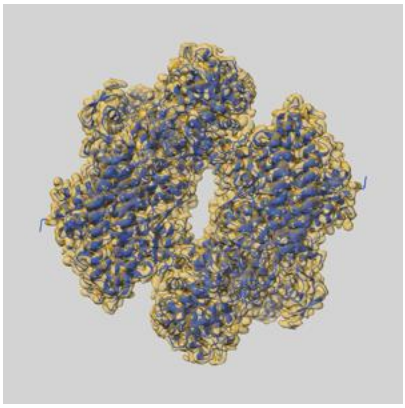
9.1 Map-model overlay



X



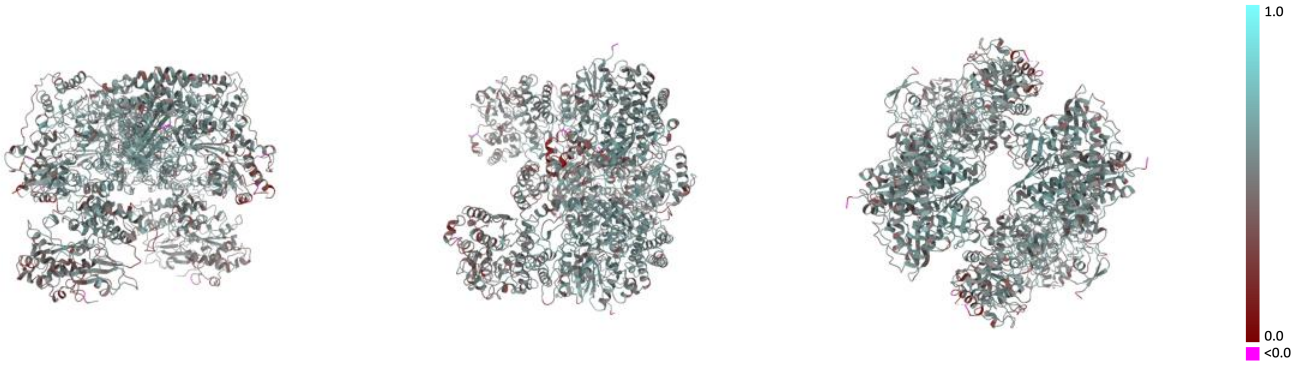
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

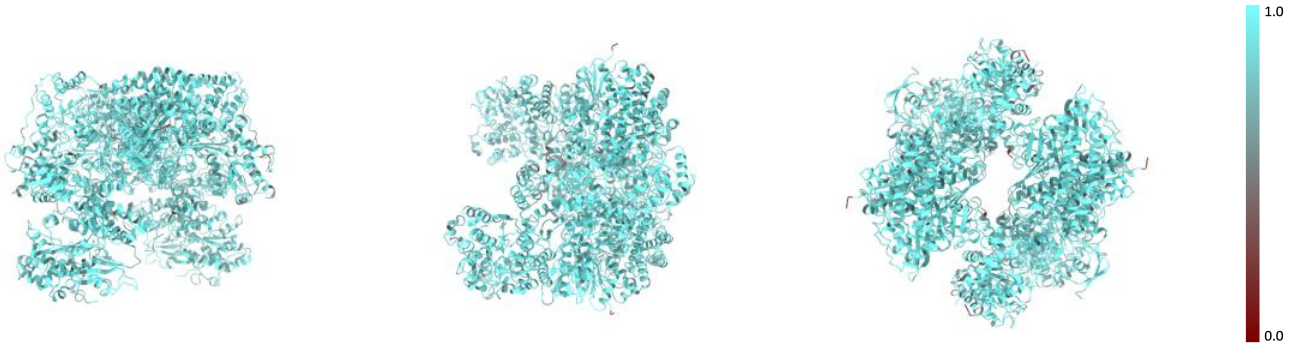
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

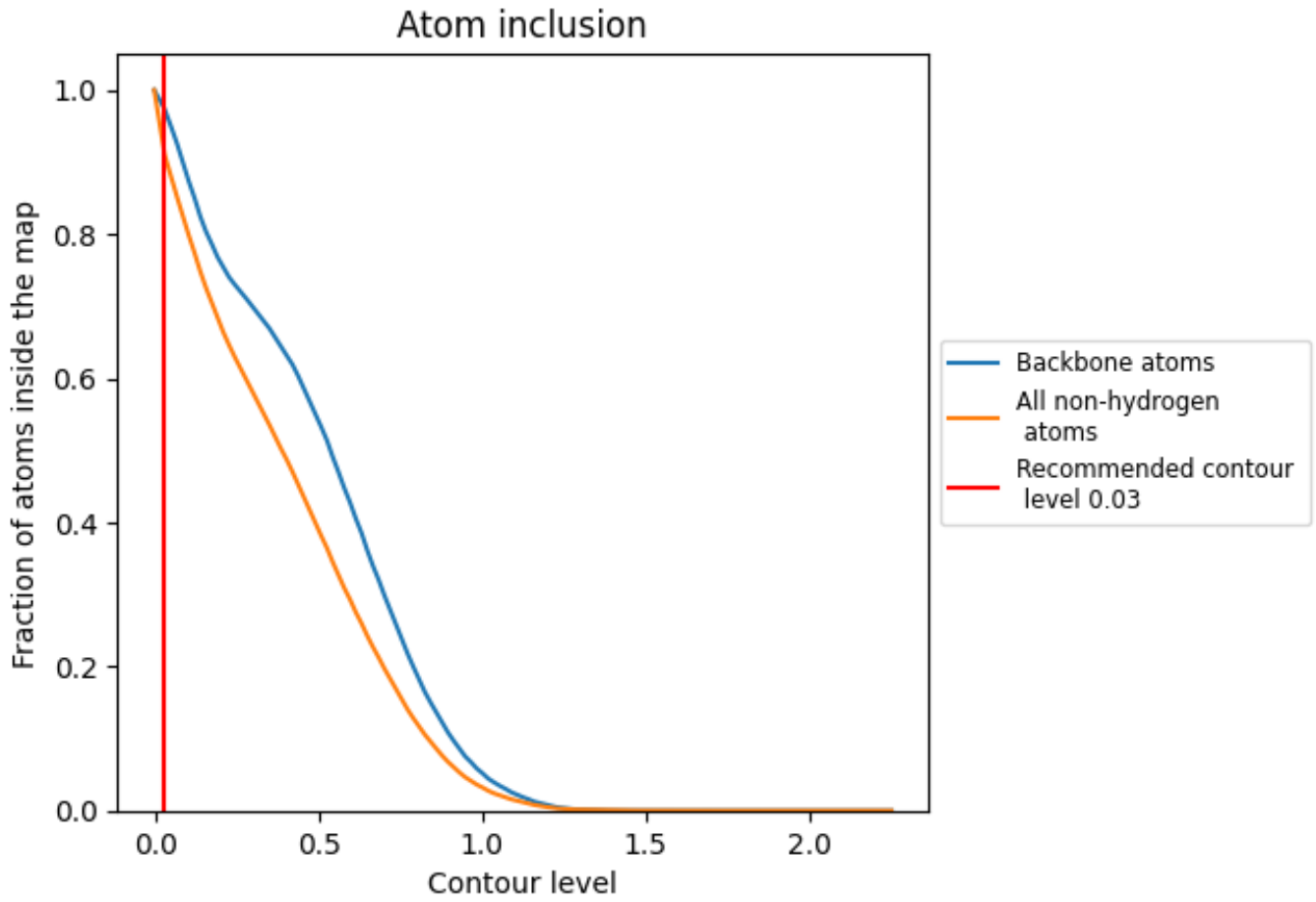
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9106	0.5100
A	0.9046	0.5060
B	0.8896	0.4720
C	0.8696	0.4770
D	0.9358	0.5550
E	0.9261	0.5310
F	0.9079	0.5020
G	0.8906	0.4710
H	0.8786	0.4850
I	0.9387	0.5510
J	0.9196	0.5260