Full wwPDB EM Validation Report

Sep 22, 2022 – 06:10 pm BST

PDB ID	:	7Z0T
EMDB ID	:	EMD-14430
Title	:	Structure of the Escherichia coli formate hydrogenlyase complex (aerobic preparation, composite structure)
Authors	:	Steinhilper, R.; Murphy, B.J.
Deposited on	:	2022-02-23
Resolution	:	3.40 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:

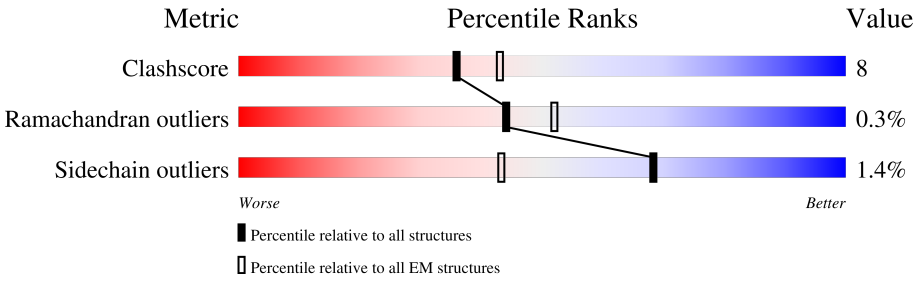
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.40 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	C	608	6% 84% 14%
2	E	581	8% 69% 20% 8%
3	B	203	73% 10% 16%
4	G	255	33% 80% 18%
5	F	180	61% 14% 24%
6	D	307	12% 74% 19% 7%
7	A	715	76% 23%

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
10	SF4	A	800	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20634 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 Formate hydrogenlyase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	603	Total	C	N	O	S	0	0
			4469	2955	738	741	35		

- Molecule 2 is a protein called Formate hydrogenlyase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	532	Total	C	N	O	S	0	0
			4244	2689	746	782	27		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	82B	HIS	-	insertion	UNP P16431
E	82C	HIS	-	insertion	UNP P16431
E	82D	HIS	-	insertion	UNP P16431
E	82E	HIS	-	insertion	UNP P16431
E	82F	HIS	-	insertion	UNP P16431
E	82G	HIS	-	insertion	UNP P16431
E	82H	HIS	-	insertion	UNP P16431
E	82I	HIS	-	insertion	UNP P16431
E	82J	HIS	-	insertion	UNP P16431
E	82K	HIS	-	insertion	UNP P16431
E	82L	GLY	-	insertion	UNP P16431
E	82M	SER	-	insertion	UNP P16431

- Molecule 3 is a protein called Formate hydrogenlyase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	170	Total	C	N	O	S	0	0
			1254	775	227	232	20		

- Molecule 4 is a protein called Formate hydrogenlyase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	249	Total	C	N	O	S	0	0
			1703	1069	311	311	12		

- Molecule 5 is a protein called Formate hydrogenlyase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	136	Total	C	N	O	S	1	0
			1075	664	196	201	14		

- Molecule 6 is a protein called Formate hydrogenlyase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	287	Total	C	N	O	S	0	0
			2152	1430	345	366	11		

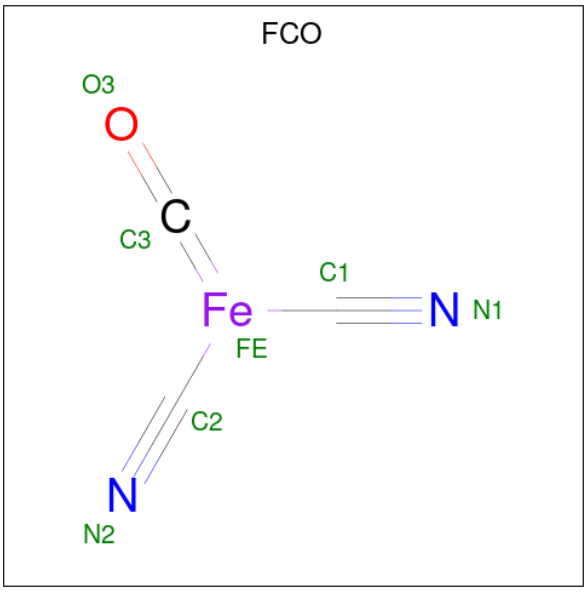
- Molecule 7 is a protein called Formate dehydrogenase H.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A	714	Total	C	N	O	S	Se	0	0
			5569	3505	972	1058	33	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

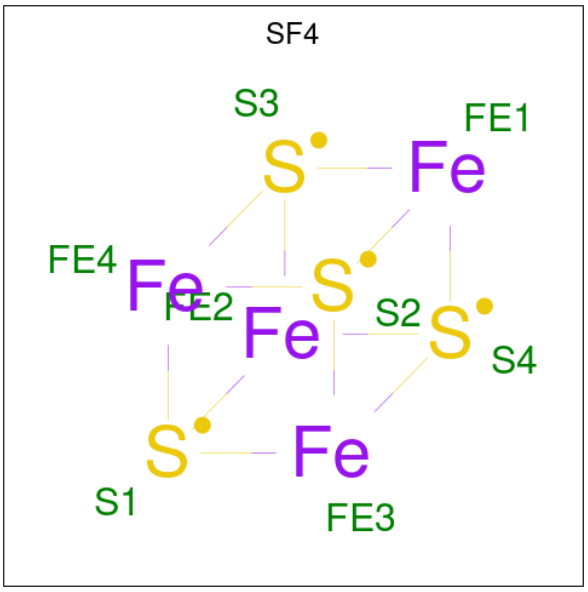
Mol	Chain	Residues	Atoms		AltConf
8	E	1	Total	Ni	0
			1	1	

- Molecule 9 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: C_3FeN_2O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	E	1	Total	C	Fe	N	O	0
			7	3	1	2	1	

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	B	1	Total	Fe	S	0
			32	16	16	
10	B	1	Total	Fe	S	0
			32	16	16	

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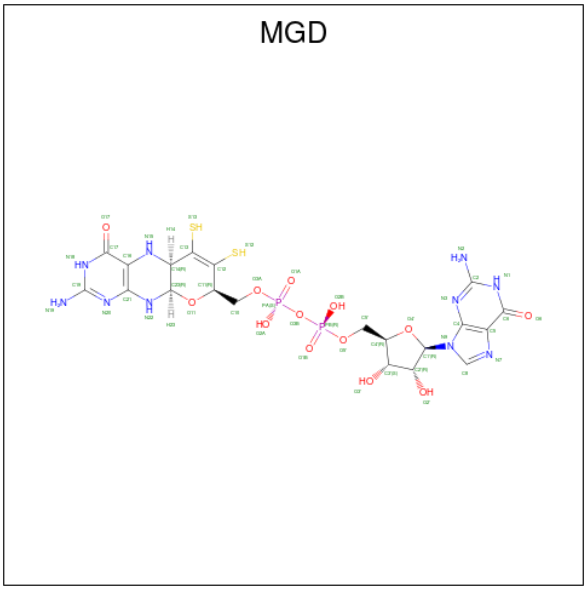
Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total Fe S 32 16 16	0
10	B	1	Total Fe S 32 16 16	0
10	G	1	Total Fe S 8 4 4	0
10	F	1	Total Fe S 16 8 8	0
10	F	1	Total Fe S 16 8 8	0
10	A	1	Total Fe S 8 4 4	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	F	1	Total Fe 1 1	0

- Molecule 12 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO -8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
12	A	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	
12	A	1	Total	C	N	O	P	S	0
			94	40	20	26	4	4	

- Molecule 13 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

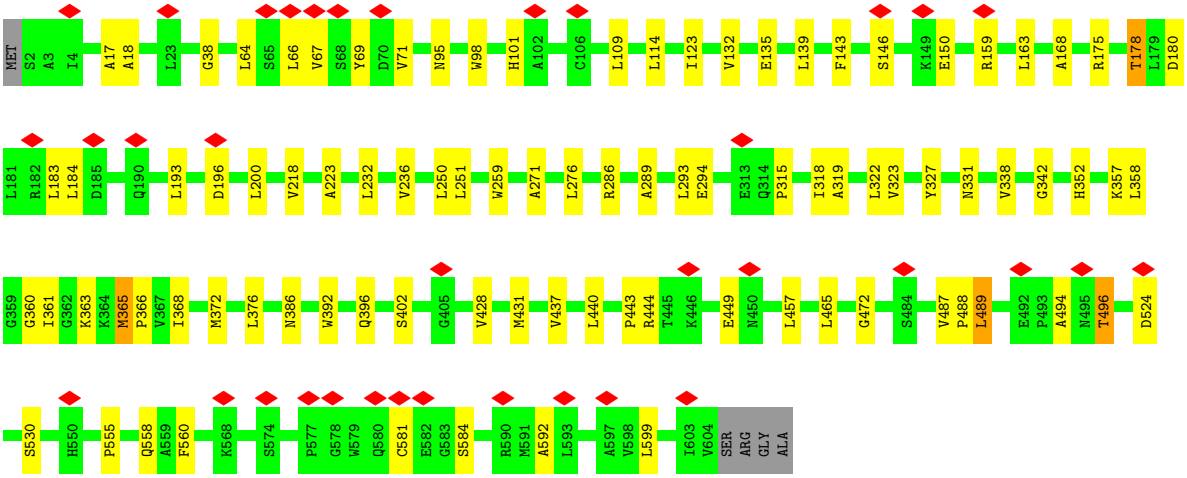
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mo	0
			1	1	

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.

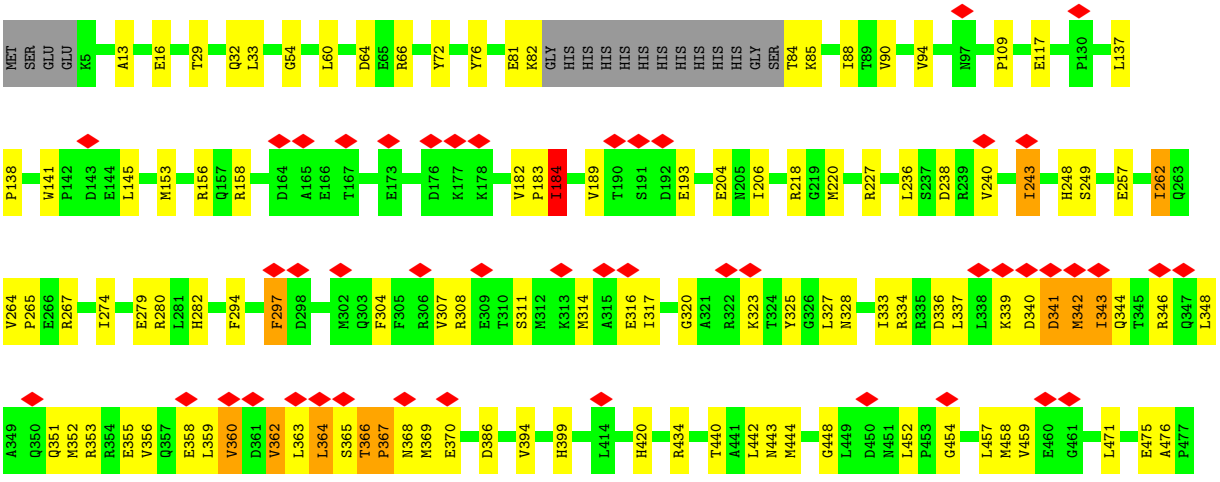
• Molecule 1: Formate hydrogenlyase subunit 3

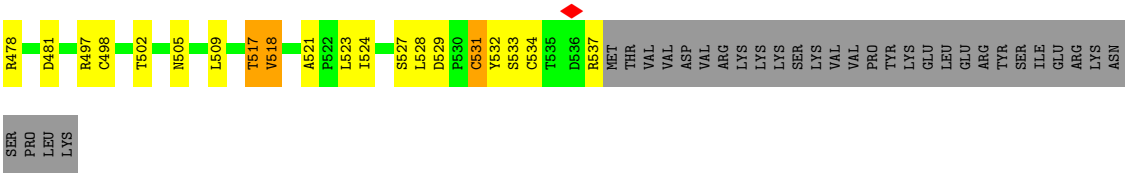
Chain C:



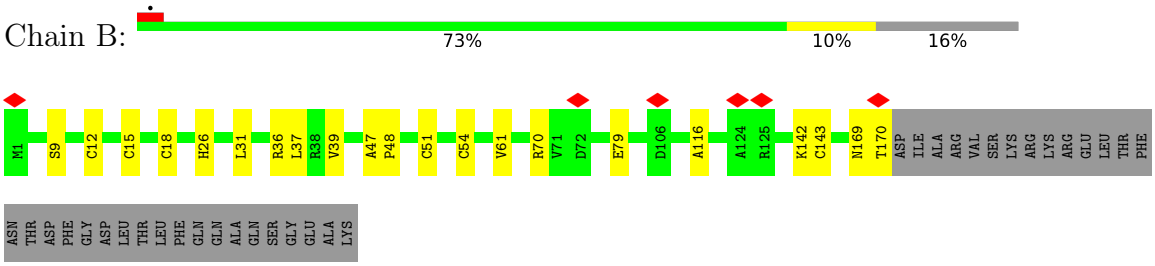
• Molecule 2: Formate hydrogenlyase subunit 5

Chain E:

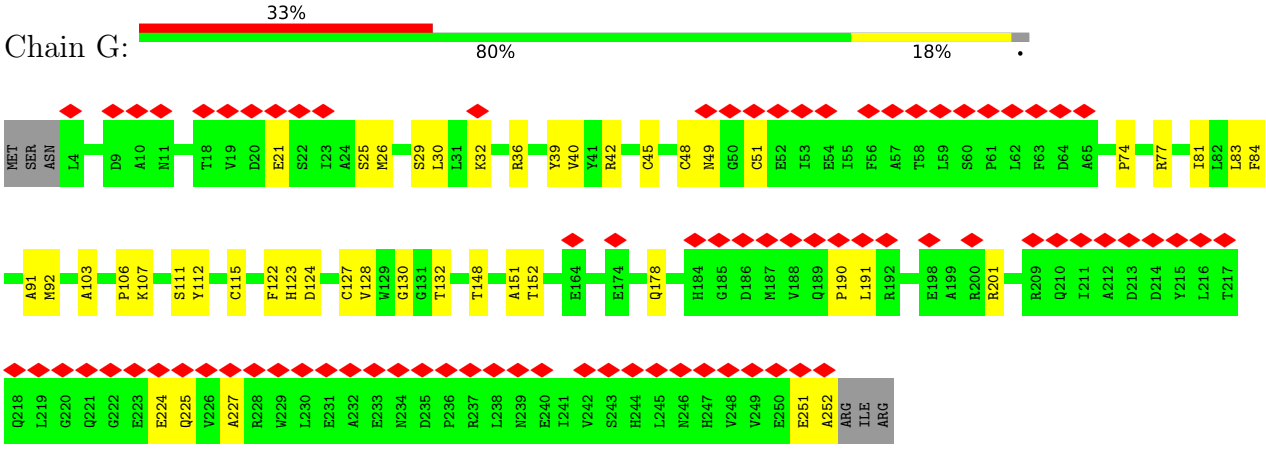




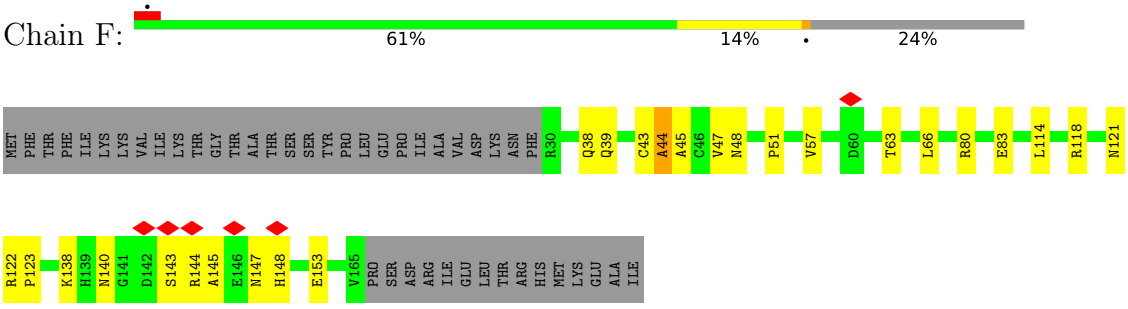
• Molecule 3: Formate hydrogenlyase subunit 2



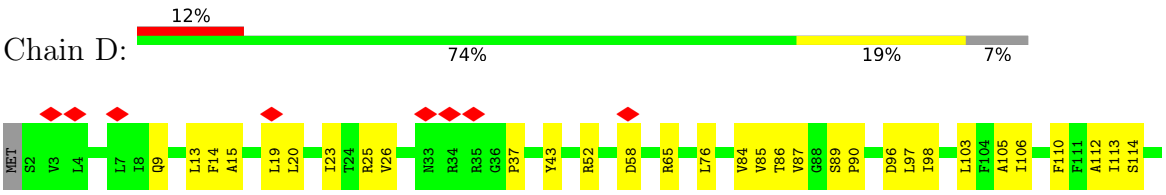
• Molecule 4: Formate hydrogenlyase subunit 7

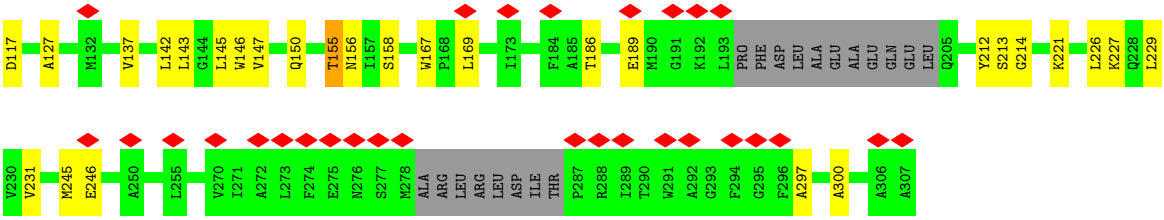


• Molecule 5: Formate hydrogenlyase subunit 6

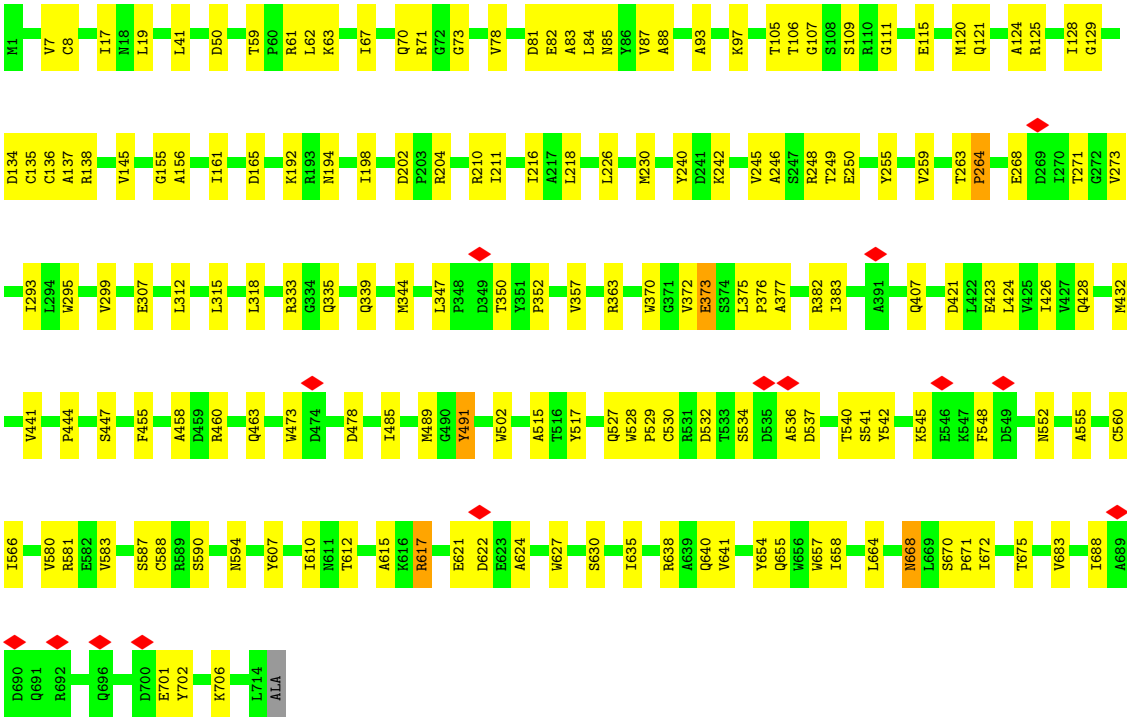


• Molecule 6: Formate hydrogenlyase subunit 4





• Molecule 7: Formate dehydrogenase H



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90459	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	72	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	69.052	Depositor
Minimum map value	-27.956	Depositor
Average map value	0.002	Depositor
Map value standard deviation	1.105	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	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: FCO, SF4, NI, FE, SEC, 6MO, MGD

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	C	0.32	1/4573 (0.0%)	0.62	3/6238 (0.0%)
2	E	0.39	1/4345 (0.0%)	0.78	9/5898 (0.2%)
3	B	0.27	0/1281	0.59	1/1748 (0.1%)
4	G	0.44	0/1736	0.72	1/2369 (0.0%)
5	F	0.47	0/1095	0.77	0/1479
6	D	0.31	0/2201	0.62	2/3003 (0.1%)
7	A	0.41	1/5684 (0.0%)	0.77	11/7712 (0.1%)
All	All	0.38	3/20915 (0.0%)	0.71	27/28447 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
5	F	0	4
7	A	0	1
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	264	PRO	N-CD	-9.45	1.34	1.47
2	E	362	VAL	C-O	5.82	1.34	1.23
1	C	366	PRO	N-CD	-5.18	1.40	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	517	THR	N-CA-C	15.26	152.19	111.00
2	E	518	VAL	N-CA-CB	12.54	139.08	111.50
7	A	81	ASP	CB-CA-C	-12.11	86.17	110.40
6	D	156	ASN	CB-CA-C	-8.63	93.15	110.40
2	E	517	THR	CB-CA-C	-8.01	89.97	111.60
3	B	116	ALA	N-CA-CB	-7.90	99.04	110.10
4	G	225	GLN	CB-CA-C	7.13	124.66	110.40
2	E	297	PHE	CB-CA-C	6.63	123.67	110.40
7	A	491	TYR	N-CA-CB	-6.49	98.91	110.60
2	E	370	GLU	CB-CA-C	-6.30	97.81	110.40
7	A	617	ARG	CB-CA-C	6.27	122.94	110.40
7	A	85	ASN	N-CA-CB	6.09	121.56	110.60
7	A	264	PRO	CA-N-CD	5.87	119.92	111.70
7	A	668	ASN	N-CA-C	-5.63	95.81	111.00
1	C	488	PRO	N-CA-C	5.61	126.69	112.10
1	C	357	LYS	CB-CA-C	-5.54	99.32	110.40
6	D	155	THR	CB-CA-C	-5.46	96.87	111.60
7	A	318	LEU	CA-CB-CG	5.39	127.71	115.30
2	E	518	VAL	N-CA-C	-5.28	96.76	111.00
7	A	137	ALA	N-CA-CB	5.27	117.48	110.10
7	A	373	GLU	N-CA-CB	-5.24	101.16	110.60
7	A	135	CYS	CB-CA-C	5.24	120.88	110.40
2	E	355	GLU	CB-CA-C	-5.14	100.12	110.40
7	A	136	CYS	CB-CA-C	-5.08	100.24	110.40
2	E	341	ASP	N-CA-CB	5.03	119.65	110.60
1	C	163	LEU	N-CA-CB	5.01	120.43	110.40
2	E	325	TYR	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	268	GLU	Mainchain
2	E	360	VAL	Mainchain
5	F	121	ASN	Mainchain
5	F	122[A]	ARG	Mainchain
5	F	122[B]	ARG	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4469	0	4723	63	0
2	E	4244	0	4145	81	0
3	B	1254	0	1235	14	0
4	G	1703	0	1551	29	0
5	F	1075	0	1032	18	0
6	D	2152	0	2239	47	0
7	A	5569	0	5448	120	0
8	E	1	0	0	0	0
9	E	7	0	0	1	0
10	A	8	0	0	2	0
10	B	32	0	0	0	0
10	F	16	0	0	0	0
10	G	8	0	0	0	0
11	F	1	0	0	0	0
12	A	94	0	44	3	0
13	A	1	0	0	0	0
All	All	20634	0	20417	349	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 8.

All (349) 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:E:204:GLU:HG3	2:E:517:THR:O	1.55	1.07
2:E:145:LEU:HD11	2:E:153:MET:HB3	1.55	0.88
7:A:529:PRO:HD2	7:A:540:THR:HB	1.57	0.87
7:A:622:ASP:OD1	7:A:622:ASP:O	1.95	0.84
7:A:156:ALA:HA	7:A:333:ARG:HH21	1.46	0.80
2:E:297:PHE:HZ	2:E:362:VAL:HB	1.44	0.80
7:A:84:LEU:HD22	7:A:485:ILE:HG13	1.63	0.79
7:A:84:LEU:HD22	7:A:485:ILE:CG1	2.13	0.79
7:A:542:TYR:HE1	7:A:545:LYS:HD3	1.48	0.78
2:E:340:ASP:OD1	2:E:341:ASP:N	2.17	0.76
6:D:155:THR:O	6:D:155:THR:OG1	1.98	0.76
6:D:97:LEU:HD21	6:D:142:LEU:CD1	2.17	0.75
7:A:424:LEU:HD21	7:A:426:ILE:HG13	1.69	0.75
7:A:307:GLU:HG2	7:A:560:CYS:SG	2.29	0.73
7:A:8:CYS:HB3	10:A:800:SF4:S1	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE2	1:C:139:LEU:CD1	2.38	0.71
2:E:238:ASP:OD1	2:E:249:SER:OG	2.09	0.70
1:C:180:ASP:O	1:C:184:LEU:HD23	1.92	0.70
7:A:372:VAL:HG22	7:A:373:GLU:HG2	1.76	0.68
7:A:121:GLN:NE2	7:A:344:MET:O	2.28	0.67
7:A:155:GLY:O	7:A:333:ARG:NH2	2.27	0.67
6:D:97:LEU:HD21	6:D:142:LEU:HD12	1.76	0.67
2:E:248:HIS:CE1	2:E:534:CYS:SG	2.87	0.67
1:C:178:THR:HG22	1:C:184:LEU:HD22	1.77	0.66
7:A:670:SER:OG	7:A:671:PRO:HD2	1.96	0.66
7:A:124:ALA:O	7:A:128:ILE:HB	1.96	0.65
3:B:61:VAL:HG11	5:F:140:ASN:ND2	2.12	0.64
7:A:87:VAL:HG13	7:A:426:ILE:HD13	1.79	0.64
7:A:542:TYR:CE1	7:A:545:LYS:HD3	2.31	0.64
2:E:340:ASP:HA	2:E:343:ILE:CG1	2.28	0.64
7:A:610:ILE:HG21	7:A:615:ALA:HB2	1.79	0.64
7:A:263:THR:OG1	7:A:264:PRO:HD2	1.98	0.64
2:E:363:LEU:O	2:E:366:THR:HG23	1.98	0.63
7:A:211:ILE:HD12	7:A:211:ILE:O	1.98	0.63
7:A:460:ARG:HB2	7:A:528:TRP:NE1	2.13	0.63
2:E:420:HIS:NE2	2:E:440:THR:OG1	2.32	0.63
7:A:424:LEU:HD21	7:A:426:ILE:CD1	2.28	0.62
7:A:109:SER:HB3	7:A:335:GLN:OE1	1.99	0.62
2:E:257:GLU:HA	2:E:262:ILE:HD12	1.81	0.62
7:A:8:CYS:CB	10:A:800:SF4:S1	2.88	0.62
7:A:161:ILE:HD11	7:A:458:ALA:HB3	1.80	0.62
7:A:106:THR:HG22	7:A:107:GLY:N	2.14	0.61
7:A:424:LEU:CD2	7:A:426:ILE:HG13	2.30	0.61
2:E:363:LEU:HD12	2:E:364:LEU:N	2.16	0.61
2:E:340:ASP:HA	2:E:343:ILE:HG13	1.81	0.61
5:F:138:LYS:HG2	5:F:145:ALA:HB3	1.82	0.61
6:D:96:ASP:OD1	6:D:97:LEU:N	2.27	0.61
6:D:97:LEU:CD2	6:D:142:LEU:CD1	2.77	0.61
5:F:43:CYS:O	5:F:45:ALA:N	2.33	0.60
7:A:424:LEU:HD21	7:A:426:ILE:CG1	2.31	0.60
1:C:232:LEU:O	1:C:236:VAL:HB	2.02	0.60
7:A:240:TYR:OH	7:A:242:LYS:HE3	2.01	0.60
5:F:43:CYS:O	5:F:43:CYS:SG	2.60	0.60
6:D:86:THR:HA	6:D:245:MET:H	1.67	0.60
2:E:363:LEU:HD12	2:E:363:LEU:C	2.23	0.59
2:E:521:ALA:HA	2:E:524:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:327:LEU:O	2:E:333:ILE:HG23	2.03	0.59
1:C:581:CYS:HB2	1:C:584:SER:HB3	1.84	0.59
7:A:216:ILE:HG21	7:A:226:LEU:HD11	1.85	0.58
7:A:421:ASP:OD1	7:A:421:ASP:O	2.21	0.58
7:A:407:GLN:NE2	7:A:654:TYR:O	2.36	0.58
4:G:77:ARG:HB3	6:D:213:SER:HB2	1.86	0.58
7:A:121:GLN:OE1	7:A:125:ARG:NH1	2.37	0.58
2:E:227:ARG:NH2	5:F:51:PRO:O	2.36	0.58
7:A:527:GLN:OE1	7:A:541:SER:HA	2.02	0.58
1:C:524:ASP:OD2	4:G:29:SER:OG	2.18	0.58
4:G:251:GLU:O	4:G:252:ALA:C	2.41	0.58
5:F:118:ARG:HD2	5:F:153:GLU:HB2	1.85	0.58
7:A:240:TYR:CE2	7:A:242:LYS:HG2	2.39	0.58
7:A:529:PRO:HD2	7:A:540:THR:CB	2.31	0.58
3:B:61:VAL:CG1	5:F:140:ASN:ND2	2.67	0.57
2:E:336:ASP:OD1	2:E:457:LEU:HD13	2.04	0.57
1:C:178:THR:HG22	1:C:184:LEU:CD2	2.34	0.57
1:C:193:LEU:HB3	1:C:259:TRP:HH2	1.68	0.57
2:E:458:MET:HB3	4:G:201:ARG:HG3	1.86	0.57
1:C:271:ALA:HA	1:C:294:GLU:HA	1.87	0.57
7:A:129:GLY:C	7:A:376:PRO:HG3	2.26	0.57
1:C:132:VAL:HG13	1:C:599:LEU:HD21	1.86	0.56
1:C:66:LEU:HD12	1:C:67:VAL:HG23	1.87	0.56
7:A:78:VAL:HG11	7:A:82:GLU:HG3	1.86	0.56
1:C:218:VAL:HG12	1:C:289:ALA:HB1	1.87	0.56
7:A:93:ALA:O	7:A:97:LYS:HG2	2.05	0.56
6:D:15:ALA:O	6:D:43:TYR:OH	2.23	0.56
1:C:496:THR:HG21	6:D:155:THR:OG1	2.06	0.56
7:A:87:VAL:CG2	7:A:441:VAL:HG11	2.35	0.56
6:D:103:LEU:HD23	6:D:106:ILE:HD12	1.89	0.55
4:G:30:LEU:HD22	4:G:106:PRO:HG2	1.88	0.55
6:D:97:LEU:HD11	6:D:145:LEU:CB	2.37	0.55
4:G:103:ALA:HB3	4:G:107:LYS:HD3	1.88	0.55
1:C:319:ALA:O	1:C:323:VAL:HG12	2.06	0.55
7:A:88:ALA:HB1	7:A:489:MET:HB3	1.89	0.55
2:E:76:TYR:HB2	2:E:90:VAL:HB	1.89	0.55
2:E:336:ASP:HB2	2:E:457:LEU:HD22	1.88	0.54
3:B:39:VAL:HG22	3:B:48:PRO:HG3	1.89	0.54
5:F:144:ARG:CG	5:F:147:ASN:HB2	2.38	0.54
6:D:13:LEU:HD22	6:D:229:LEU:HD21	1.89	0.54
2:E:274:ILE:HD11	2:E:448:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:THR:HG23	1:C:180:ASP:H	1.73	0.54
4:G:122:PHE:O	4:G:128:VAL:HG21	2.07	0.54
2:E:117:GLU:OE1	2:E:497:ARG:NH2	2.40	0.54
2:E:366:THR:N	2:E:367:PRO:HD3	2.21	0.54
1:C:392:TRP:HZ2	1:C:496:THR:HG23	1.72	0.54
1:C:175:ARG:NH2	1:C:196:ASP:OD2	2.39	0.54
1:C:322:LEU:HB3	1:C:487:VAL:HG21	1.88	0.54
7:A:372:VAL:HG22	7:A:373:GLU:N	2.23	0.54
2:E:297:PHE:CZ	2:E:362:VAL:HB	2.34	0.53
7:A:249:THR:HG22	7:A:555:ALA:HB3	1.89	0.53
6:D:97:LEU:HD11	6:D:145:LEU:HB2	1.89	0.53
1:C:555:PRO:HA	1:C:558:GLN:HB3	1.91	0.53
5:F:44:ALA:O	5:F:48:ASN:ND2	2.41	0.53
2:E:189:VAL:HG11	4:G:74:PRO:HA	1.90	0.53
1:C:402:SER:OG	6:D:150:GLN:OE1	2.27	0.53
4:G:21:GLU:O	4:G:25:SER:HB3	2.09	0.53
6:D:84:VAL:HG23	6:D:85:VAL:HG13	1.91	0.53
1:C:135:GLU:OE2	1:C:139:LEU:HD11	2.09	0.53
3:B:36:ARG:NH2	3:B:79:GLU:OE2	2.42	0.53
4:G:191:LEU:HD21	4:G:252:ALA:HB2	1.90	0.53
7:A:581:ARG:NH1	12:A:802:MGD:O2B	2.42	0.53
6:D:147:VAL:HG11	6:D:300:ALA:HB1	1.89	0.53
7:A:61:ARG:HH12	7:A:447:SER:HB2	1.72	0.53
7:A:621:GLU:HG2	7:A:624:ALA:HB2	1.91	0.53
7:A:106:THR:HG22	7:A:107:GLY:O	2.09	0.53
2:E:72:TYR:HB2	2:E:94:VAL:HB	1.91	0.52
7:A:587:SER:HA	7:A:655:GLN:HG3	1.90	0.52
2:E:316:GLU:O	2:E:320:GLY:HA2	2.09	0.52
2:E:262:ILE:HG22	2:E:264:VAL:HG13	1.90	0.52
3:B:12:CYS:O	7:A:210:ARG:NH2	2.43	0.52
7:A:590:SER:O	7:A:594:ASN:ND2	2.41	0.52
7:A:588:CYS:O	7:A:657:TRP:NE1	2.43	0.52
7:A:630:SER:HB2	7:A:683:VAL:HG12	1.90	0.52
1:C:146:SER:OG	1:C:150:GLU:OE1	2.28	0.52
2:E:282:HIS:HE1	2:E:308:ARG:HH21	1.56	0.52
2:E:267:ARG:HH21	2:E:454:GLY:HA2	1.75	0.52
2:E:220:MET:HB2	2:E:236:LEU:HD21	1.92	0.52
4:G:42:ARG:HG3	4:G:83:LEU:HD23	1.91	0.52
7:A:17:ILE:HG12	7:A:41:LEU:HD21	1.92	0.52
7:A:370:TRP:HE3	7:A:375:LEU:HD21	1.75	0.52
7:A:372:VAL:HG22	7:A:373:GLU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:534:SER:C	7:A:536:ALA:H	2.12	0.51
6:D:14:PHE:HB2	6:D:76:LEU:HD21	1.91	0.51
7:A:248:ARG:HB3	7:A:548:PHE:HE2	1.75	0.51
7:A:532:ASP:C	7:A:534:SER:H	2.13	0.51
4:G:112:TYR:HH	4:G:152:THR:HG1	1.57	0.51
5:F:144:ARG:HH12	5:F:148:HIS:CE1	2.28	0.51
6:D:97:LEU:CD1	6:D:145:LEU:HB3	2.40	0.51
7:A:658:ILE:HD12	7:A:701:GLU:HG3	1.92	0.51
6:D:89:SER:N	6:D:158:SER:OG	2.37	0.51
7:A:134:ASP:HB3	7:A:383:ILE:HG23	1.92	0.51
1:C:64:LEU:HB2	1:C:69:TYR:HB3	1.91	0.51
2:E:109:PRO:HG2	2:E:386:ASP:HB3	1.92	0.51
2:E:156:ARG:HG2	4:G:124:ASP:HB2	1.92	0.51
2:E:394:VAL:HG22	2:E:399:HIS:HB2	1.92	0.51
6:D:114:SER:OG	6:D:212:TYR:OH	2.26	0.51
7:A:82:GLU:O	7:A:83:ALA:C	2.45	0.51
7:A:7:VAL:HG21	7:A:463:GLN:HB3	1.93	0.50
1:C:178:THR:HG21	1:C:183:LEU:HB3	1.93	0.50
1:C:315:PRO:HA	1:C:318:ILE:HD12	1.92	0.50
7:A:165:ASP:O	7:A:194:ASN:ND2	2.41	0.50
2:E:476:ALA:HB1	9:E:602:FCO:N1	2.26	0.50
7:A:612:THR:HA	7:A:641:VAL:HG13	1.94	0.50
2:E:348:LEU:HA	2:E:351:GLN:HG3	1.93	0.50
2:E:434:ARG:NH1	2:E:527:SER:O	2.43	0.50
2:E:314:MET:HA	2:E:317:ILE:HG12	1.94	0.50
6:D:186:THR:HG23	6:D:231:VAL:HG12	1.94	0.50
7:A:428:GLN:NE2	7:A:478:ASP:OD1	2.44	0.50
1:C:193:LEU:HB3	1:C:259:TRP:CH2	2.46	0.49
4:G:49:ASN:OD1	4:G:49:ASN:O	2.29	0.49
1:C:315:PRO:O	1:C:489:LEU:HD11	2.11	0.49
2:E:353:ARG:NH1	2:E:443:ASN:OD1	2.45	0.49
4:G:191:LEU:HD21	4:G:252:ALA:CB	2.42	0.49
7:A:67:ILE:HD11	7:A:83:ALA:HA	1.93	0.49
2:E:204:GLU:CG	2:E:517:THR:O	2.44	0.49
6:D:189:GLU:OE1	6:D:227:LYS:NZ	2.46	0.49
1:C:437:VAL:O	1:C:444:ARG:NH2	2.46	0.49
2:E:294:PHE:HB2	2:E:523:LEU:HD13	1.94	0.49
1:C:396:GLN:HE21	1:C:494:ALA:H	1.60	0.49
1:C:496:THR:HG21	6:D:155:THR:HG1	1.78	0.49
3:B:15:CYS:HA	7:A:583:VAL:HG11	1.93	0.49
4:G:148:THR:HG23	4:G:151:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:25:ARG:HH21	6:D:37:PRO:HG3	1.75	0.49
4:G:40:VAL:HG22	4:G:81:ILE:HB	1.95	0.49
6:D:9:GLN:HG2	6:D:90:PRO:HG2	1.94	0.49
1:C:440:LEU:HB3	6:D:117:ASP:HA	1.95	0.49
4:G:45:CYS:HA	4:G:92:MET:HG2	1.95	0.49
1:C:396:GLN:OE1	6:D:155:THR:HG21	2.13	0.48
7:A:295:TRP:HB2	7:A:299:VAL:HG21	1.94	0.48
3:B:169:ASN:O	3:B:170:THR:C	2.51	0.48
4:G:111:SER:OG	4:G:132:THR:OG1	2.29	0.48
7:A:192:LYS:HG3	7:A:198:ILE:CD1	2.44	0.48
2:E:356:VAL:O	2:E:360:VAL:HG23	2.14	0.48
6:D:142:LEU:O	6:D:146:TRP:HB2	2.13	0.48
7:A:156:ALA:HA	7:A:333:ARG:NH2	2.21	0.48
7:A:202:ASP:OD1	12:A:802:MGD:H1'	2.14	0.48
1:C:135:GLU:OE2	1:C:159:ARG:NH2	2.46	0.48
2:E:280:ARG:HH22	2:E:475:GLU:HG3	1.78	0.48
2:E:117:GLU:OE2	2:E:537:ARG:NH2	2.47	0.48
7:A:145:VAL:HG23	7:A:155:GLY:HA3	1.95	0.48
2:E:478:ARG:NE	2:E:529:ASP:O	2.47	0.48
1:C:114:LEU:HD22	1:C:232:LEU:HD13	1.95	0.47
5:F:144:ARG:O	5:F:144:ARG:HG2	2.14	0.47
4:G:128:VAL:HG23	4:G:130:GLY:H	1.78	0.47
6:D:14:PHE:HD1	6:D:226:LEU:HD22	1.79	0.47
7:A:115:GLU:OE2	7:A:517:TYR:OH	2.30	0.47
6:D:19:LEU:HD22	6:D:43:TYR:HE1	1.80	0.47
6:D:23:ILE:HA	6:D:26:VAL:HG12	1.96	0.47
1:C:368:ILE:O	1:C:372:MET:HG2	2.14	0.47
3:B:18:CYS:HB2	3:B:37:LEU:HD11	1.96	0.47
7:A:70:GLN:O	7:A:73:GLY:N	2.46	0.47
7:A:635:ILE:HG12	7:A:664:LEU:HD21	1.97	0.47
2:E:265:PRO:HD3	2:E:459:VAL:HG23	1.97	0.47
7:A:121:GLN:HE22	7:A:352:PRO:HD3	1.80	0.47
1:C:530:SER:HB2	6:D:65:ARG:HH22	1.79	0.47
4:G:39:TYR:OH	6:D:221:LYS:NZ	2.48	0.47
1:C:392:TRP:CZ2	1:C:496:THR:HG23	2.51	0.46
7:A:370:TRP:CE3	7:A:375:LEU:HD21	2.50	0.46
7:A:105:THR:CG2	7:A:120:MET:SD	3.04	0.46
5:F:144:ARG:HG2	5:F:147:ASN:HB2	1.97	0.46
7:A:106:THR:CG2	7:A:107:GLY:N	2.78	0.46
2:E:54:GLY:HA3	2:E:82:LYS:HE2	1.98	0.46
1:C:196:ASP:OD1	1:C:196:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:66:LEU:HB2	5:F:114:LEU:HD21	1.98	0.46
4:G:178:GLN:HB3	5:F:38:GLN:HG2	1.97	0.46
7:A:71:ARG:NH2	7:A:423:GLU:HA	2.30	0.46
7:A:87:VAL:CG1	7:A:426:ILE:HD13	2.45	0.46
3:B:61:VAL:HG11	5:F:140:ASN:HD21	1.79	0.46
3:B:51:CYS:HB3	3:B:143:CYS:HB3	1.98	0.46
7:A:230:MET:HG3	7:A:315:LEU:HD11	1.98	0.46
7:A:363:ARG:CZ	7:A:377:ALA:HB2	2.46	0.46
4:G:224:GLU:O	4:G:227:ALA:HB3	2.16	0.46
6:D:97:LEU:HD21	6:D:142:LEU:HD13	1.95	0.46
7:A:502:TRP:NE1	7:A:515:ALA:O	2.37	0.46
1:C:18:ALA:HB1	1:C:109:LEU:HD12	1.98	0.46
4:G:84:PHE:HB3	4:G:132:THR:HG21	1.98	0.46
2:E:531:CYS:HB3	2:E:534:CYS:HB2	1.98	0.45
7:A:670:SER:HB2	7:A:675:THR:HG22	1.97	0.45
1:C:361:ILE:HG22	1:C:365:MET:HG3	1.98	0.45
3:B:9:SER:HB3	3:B:47:ALA:HB2	1.98	0.45
6:D:112:ALA:HA	6:D:127:ALA:HB1	1.98	0.45
1:C:342:GLY:HA3	1:C:372:MET:SD	2.57	0.45
2:E:32:GLN:NE2	2:E:471:LEU:O	2.46	0.45
2:E:304:PHE:HA	2:E:307:VAL:HG12	1.98	0.45
7:A:242:LYS:O	7:A:246:ALA:N	2.48	0.45
7:A:534:SER:C	7:A:536:ALA:N	2.69	0.45
1:C:250:LEU:HD11	1:C:322:LEU:HD21	1.99	0.45
7:A:250:GLU:OE1	7:A:552:ASN:ND2	2.49	0.45
7:A:610:ILE:CG2	7:A:615:ALA:HB2	2.46	0.45
6:D:167:TRP:HD1	6:D:169:LEU:HD22	1.82	0.45
7:A:566:ILE:HD12	7:A:668:ASN:HB3	1.99	0.45
7:A:333:ARG:HG3	7:A:339:GLN:HB2	1.99	0.45
7:A:293:ILE:HG21	7:A:312:LEU:HD22	1.99	0.44
7:A:581:ARG:NH2	12:A:801:MGD:H15	2.15	0.44
2:E:183:PRO:C	2:E:184:ILE:HG12	2.37	0.44
2:E:183:PRO:O	2:E:184:ILE:HG12	2.18	0.44
1:C:327:TYR:OH	1:C:472:GLY:O	2.34	0.44
7:A:424:LEU:HD21	7:A:426:ILE:HD11	1.97	0.44
1:C:352:HIS:HB2	1:C:358:LEU:HD13	2.00	0.44
2:E:193:GLU:HG2	2:E:532:TYR:HB2	2.00	0.44
7:A:70:GLN:O	7:A:71:ARG:C	2.56	0.44
7:A:111:GLY:HA2	7:A:455:PHE:HZ	1.82	0.44
7:A:192:LYS:HD2	7:A:211:ILE:HB	2.00	0.44
7:A:607:TYR:HE1	7:A:638:ARG:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:47:VAL:HG11	5:F:57:VAL:HG22	2.00	0.44
2:E:249:SER:HB3	2:E:328:ASN:OD1	2.18	0.44
2:E:158:ARG:NH2	4:G:123:HIS:O	2.49	0.44
1:C:457:LEU:HD23	1:C:457:LEU:HA	1.84	0.43
2:E:84:THR:OG1	2:E:85:LYS:N	2.38	0.43
7:A:240:TYR:CZ	7:A:242:LYS:HE3	2.53	0.43
7:A:532:ASP:C	7:A:534:SER:N	2.70	0.43
7:A:218:LEU:HD13	7:A:226:LEU:HD13	1.99	0.43
2:E:64:ASP:OD1	2:E:66:ARG:NH1	2.50	0.43
5:F:144:ARG:HG3	5:F:147:ASN:HB2	2.01	0.43
7:A:357:VAL:O	7:A:363:ARG:HD2	2.18	0.43
1:C:428:VAL:HG21	6:D:105:ALA:HB1	2.00	0.43
3:B:142:LYS:HB3	3:B:142:LYS:HE3	1.84	0.43
2:E:29:THR:H	2:E:32:GLN:HB2	1.84	0.43
2:E:243:ILE:O	2:E:279:GLU:OE2	2.37	0.43
4:G:29:SER:HA	4:G:32:LYS:HE3	2.00	0.43
1:C:363:LYS:NZ	6:D:58:ASP:O	2.51	0.43
1:C:443:PRO:HG2	1:C:449:GLU:HG3	2.01	0.43
7:A:50:ASP:N	7:A:50:ASP:OD1	2.47	0.43
1:C:67:VAL:HB	1:C:69:TYR:HB2	2.00	0.43
2:E:240:VAL:O	2:E:533:SER:OG	2.28	0.43
6:D:110:PHE:HA	6:D:113:ILE:HG12	2.00	0.43
6:D:143:LEU:HD23	6:D:297:ALA:HB1	2.00	0.43
2:E:343:ILE:O	2:E:346:ARG:HB2	2.19	0.43
7:A:271:THR:OG1	7:A:273:VAL:HG12	2.19	0.43
2:E:340:ASP:O	2:E:341:ASP:C	2.57	0.42
1:C:168:ALA:HB2	1:C:200:LEU:HD23	2.00	0.42
1:C:218:VAL:HG21	1:C:293:LEU:HD21	2.01	0.42
7:A:59:THR:OG1	7:A:432:MET:O	2.29	0.42
7:A:87:VAL:HG13	7:A:426:ILE:CD1	2.46	0.42
7:A:617:ARG:HE	7:A:617:ARG:HB2	1.32	0.42
2:E:81:GLU:HA	2:E:85:LYS:HG2	2.00	0.42
2:E:352:MET:HG2	2:E:442:LEU:HD11	2.00	0.42
2:E:33:LEU:HD22	2:E:88:ILE:HG12	2.01	0.42
2:E:206:ILE:HD11	2:E:521:ALA:HB2	2.02	0.42
6:D:98:ILE:H	6:D:98:ILE:HG12	1.53	0.42
6:D:87:VAL:HG22	6:D:246:GLU:HA	2.02	0.42
7:A:607:TYR:HB3	7:A:640:GLN:HB2	2.01	0.42
7:A:702:TYR:CZ	7:A:706:LYS:HE3	2.54	0.42
5:F:80:ARG:NH1	5:F:83:GLU:OE1	2.43	0.42
1:C:17:ALA:HB2	1:C:38:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:LEU:HD22	1:C:487:VAL:HG13	2.02	0.41
2:E:137:LEU:HD13	2:E:141:TRP:CD1	2.54	0.41
2:E:339:LYS:O	2:E:342:MET:HG3	2.19	0.41
2:E:481:ASP:OD1	2:E:481:ASP:N	2.49	0.41
2:E:502:THR:HA	2:E:505:ASN:HB2	2.01	0.41
3:B:26:HIS:HD2	3:B:31:LEU:HD12	1.85	0.41
3:B:54:CYS:O	3:B:70:ARG:NH2	2.53	0.41
1:C:178:THR:HG21	1:C:183:LEU:CB	2.50	0.41
2:E:138:PRO:HB3	4:G:91:ALA:HB2	2.03	0.41
7:A:138:ARG:HE	7:A:382:ARG:HG2	1.85	0.41
2:E:13:ALA:HA	2:E:16:GLU:HG2	2.01	0.41
2:E:340:ASP:O	2:E:344:GLN:HB3	2.20	0.41
2:E:444:MET:O	2:E:448:GLY:N	2.51	0.41
7:A:245:VAL:HG12	7:A:245:VAL:O	2.19	0.41
1:C:223:ALA:HA	1:C:286:ARG:HG3	2.02	0.41
1:C:376:LEU:HD22	1:C:431:MET:SD	2.60	0.41
7:A:204:ARG:NH1	7:A:580:VAL:HG11	2.36	0.41
2:E:337:LEU:HD11	2:E:452:LEU:HD11	2.03	0.41
7:A:627:TRP:HD1	7:A:688:ILE:HG12	1.86	0.41
1:C:338:VAL:HG22	1:C:465:LEU:HB3	2.03	0.41
2:E:497:ARG:NH1	2:E:498:CYS:O	2.52	0.41
4:G:36:ARG:HD2	4:G:36:ARG:HA	1.73	0.41
7:A:63:LYS:HG3	7:A:473:TRP:CD1	2.56	0.41
1:C:71:VAL:HG23	1:C:123:ILE:HB	2.03	0.41
2:E:367:PRO:HD2	2:E:368:ASN:H	1.86	0.41
6:D:137:VAL:HG21	6:D:189:GLU:HG2	2.02	0.41
7:A:105:THR:HG21	7:A:120:MET:SD	2.61	0.41
7:A:532:ASP:HB2	7:A:537:ASP:OD2	2.21	0.41
6:D:20:LEU:HA	6:D:23:ILE:HG22	2.03	0.41
1:C:276:LEU:HD21	1:C:560:PHE:HB3	2.03	0.40
1:C:331:ASN:ND2	1:C:386:ASN:O	2.53	0.40
2:E:182:VAL:HA	2:E:183:PRO:HD3	1.93	0.40
7:A:621:GLU:CG	7:A:624:ALA:HB2	2.50	0.40
2:E:311:SER:HB3	2:E:352:MET:HE1	2.02	0.40
2:E:509:LEU:HD21	2:E:528:LEU:HD21	2.03	0.40
4:G:124:ASP:OD1	4:G:124:ASP:N	2.50	0.40
6:D:52:ARG:HB2	6:D:214:GLY:HA2	2.04	0.40
6:D:97:LEU:HD12	6:D:145:LEU:HB3	2.02	0.40
7:A:255:TYR:CZ	7:A:259:VAL:HG21	2.56	0.40
1:C:95:ASN:HA	1:C:98:TRP:HB3	2.02	0.40
7:A:62:LEU:HB3	7:A:444:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:PHE:HE1	1:C:592:ALA:HB1	1.87	0.40
2:E:60:LEU:HD22	2:E:76:TYR:CE2	2.56	0.40
6:D:13:LEU:HD23	6:D:13:LEU:HA	1.92	0.40
7:A:19:LEU:HD23	7:A:19:LEU:HA	1.97	0.40
1:C:360:GLY:HA3	1:C:443:PRO:HG3	2.04	0.40
7:A:347:LEU:HB2	7:A:350:THR:HG22	2.03	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	C	601/608 (99%)	572 (95%)	29 (5%)	0	100	100
2	E	528/581 (91%)	493 (93%)	29 (6%)	6 (1%)	14	44
3	B	168/203 (83%)	165 (98%)	3 (2%)	0	100	100
4	G	247/255 (97%)	237 (96%)	10 (4%)	0	100	100
5	F	135/180 (75%)	129 (96%)	4 (3%)	2 (2%)	10	36
6	D	281/307 (92%)	275 (98%)	6 (2%)	0	100	100
7	A	711/715 (99%)	673 (95%)	38 (5%)	0	100	100
All	All	2671/2849 (94%)	2544 (95%)	119 (4%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	334	ARG
2	E	367	PRO
2	E	518	VAL
5	F	44	ALA
2	E	323	LYS

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Mol	Chain	Res	Type
2	E	262	ILE
5	F	63	THR
2	E	184	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	C	461/464 (99%)	455 (99%)	6 (1%)	69	84
2	E	454/505 (90%)	442 (97%)	12 (3%)	46	72
3	B	142/170 (84%)	142 (100%)	0	100	100
4	G	146/207 (70%)	140 (96%)	6 (4%)	30	59
5	F	117/156 (75%)	114 (97%)	3 (3%)	46	72
6	D	225/246 (92%)	225 (100%)	0	100	100
7	A	584/584 (100%)	581 (100%)	3 (0%)	88	94
All	All	2129/2332 (91%)	2099 (99%)	30 (1%)	68	83

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	101	HIS
1	C	178	THR
1	C	251	LEU
1	C	365	MET
1	C	489	LEU
1	C	496	THR
2	E	184	ILE
2	E	218	ARG
2	E	243	ILE
2	E	342	MET
2	E	343	ILE
2	E	358	GLU
2	E	359	LEU
2	E	364	LEU

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Mol	Chain	Res	Type
2	E	365	SER
2	E	366	THR
2	E	369	MET
2	E	531	CYS
4	G	26	MET
4	G	48	CYS
4	G	51	CYS
4	G	115	CYS
4	G	127	CYS
4	G	190	PRO
5	F	39	GLN
5	F	123	PRO
5	F	143	SER
7	A	491	TYR
7	A	530	CYS
7	A	672	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	254	ASN
2	E	205	ASN
2	E	248	HIS
2	E	282	HIS
2	E	368	ASN
5	F	147	ASN
5	F	148	HIS
6	D	156	ASN
7	A	104	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
10	SF4	F	201	5	0,12,12	-	-	-		
9	FCO	E	602	2	0,6,6	-	-	-		
10	SF4	B	302	3	0,12,12	-	-	-		
10	SF4	B	303	3	0,12,12	-	-	-		
10	SF4	G	301	4	0,12,12	-	-	-		
10	SF4	A	800	7	0,12,12	-	-	-		
12	MGD	A	802	13	41,52,52	0.98	4 (9%)	40,81,81	1.15	3 (7%)
10	SF4	B	304	3	0,12,12	-	-	-		
12	MGD	A	801	13	41,52,52	0.95	3 (7%)	40,81,81	0.97	3 (7%)
10	SF4	B	301	3	0,12,12	-	-	-		
10	SF4	F	202	5	0,12,12	-	-	-		

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
10	SF4	F	201	5	-	-	0/6/5/5
10	SF4	B	302	3	-	-	0/6/5/5
10	SF4	B	303	3	-	-	0/6/5/5
10	SF4	G	301	4	-	-	0/6/5/5
10	SF4	A	800	7	-	-	0/6/5/5
12	MGD	A	802	13	-	3/18/66/66	0/6/6/6
10	SF4	B	304	3	-	-	0/6/5/5
12	MGD	A	801	13	-	5/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SF4	B	301	3	-	-	0/6/5/5
10	SF4	F	202	5	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	801	MGD	C5-C6	-3.18	1.41	1.47
12	A	802	MGD	C5-C6	-2.65	1.42	1.47
12	A	801	MGD	C5-C4	-2.39	1.37	1.43
12	A	801	MGD	C8-N7	-2.29	1.31	1.35
12	A	802	MGD	C8-N7	-2.23	1.31	1.35
12	A	802	MGD	C5-C4	-2.20	1.37	1.43
12	A	802	MGD	C23-C14	-2.07	1.52	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	802	MGD	C19-N20-C21	3.14	119.11	113.43
12	A	801	MGD	C19-N20-C21	2.91	118.69	113.43
12	A	802	MGD	O4'-C1'-C2'	-2.90	102.69	106.93
12	A	802	MGD	O6-C6-C5	2.16	128.59	124.37
12	A	801	MGD	PB-O5'-C5'	-2.11	109.29	121.68
12	A	801	MGD	C17-C16-N15	2.06	122.29	116.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	MGD	C5'-O5'-PB-O1B
12	A	801	MGD	C5'-O5'-PB-O2B
12	A	802	MGD	O3A-C10-C11-O11
12	A	801	MGD	O4'-C4'-C5'-O5'
12	A	801	MGD	C3'-C4'-C5'-O5'
12	A	802	MGD	PB-O3B-PA-O2A
12	A	801	MGD	C5'-O5'-PB-O3B
12	A	802	MGD	PB-O3B-PA-O1A

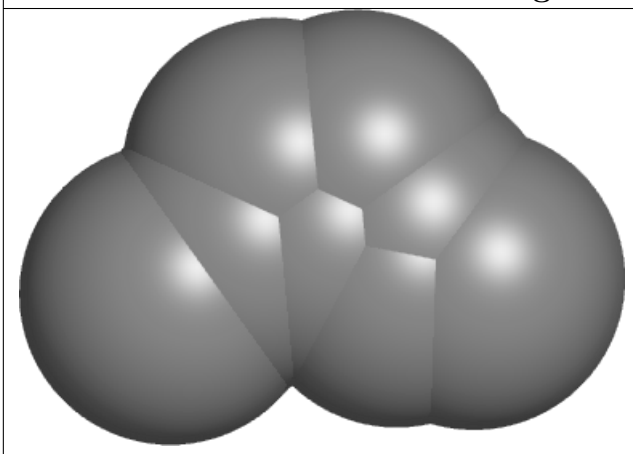
There are no ring outliers.

4 monomers are involved in 6 short contacts:

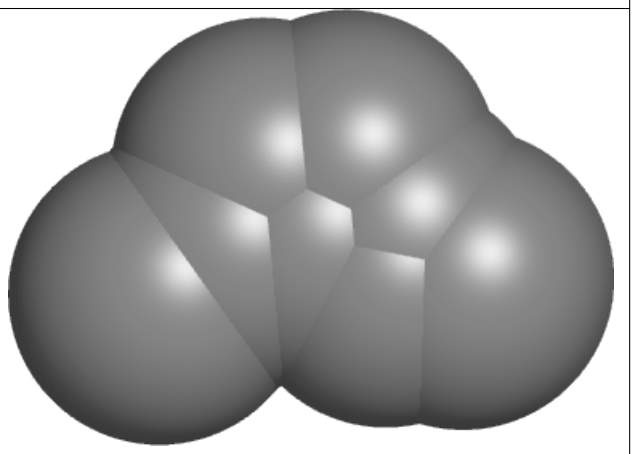
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	602	FCO	1	0
10	A	800	SF4	2	0
12	A	802	MGD	2	0
12	A	801	MGD	1	0

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.

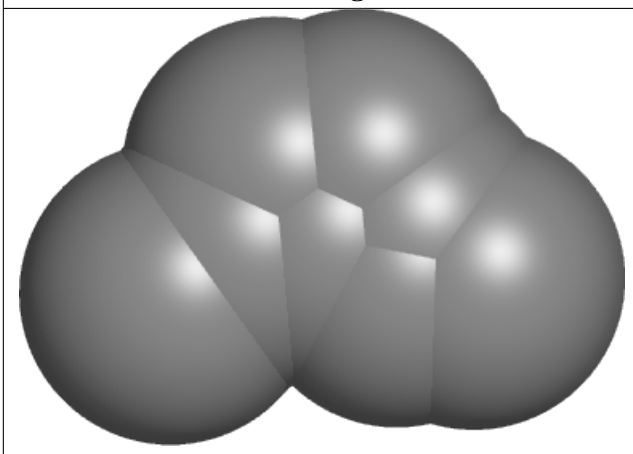
Ligand SF4 F 201



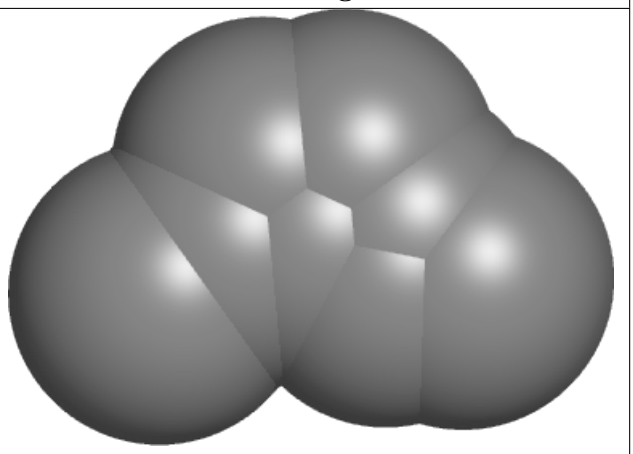
Bond lengths



Bond angles

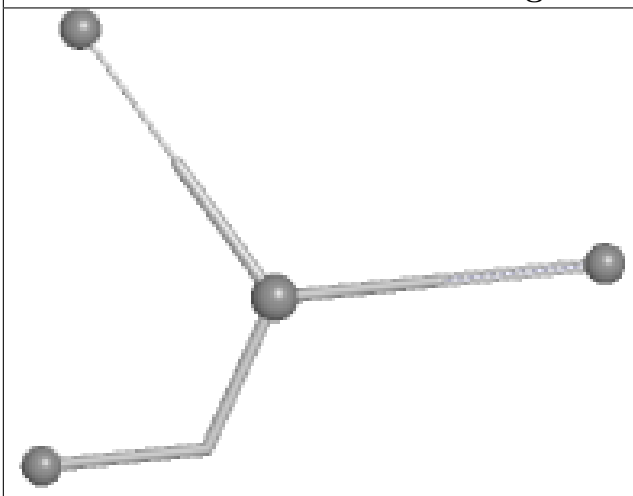


Torsions

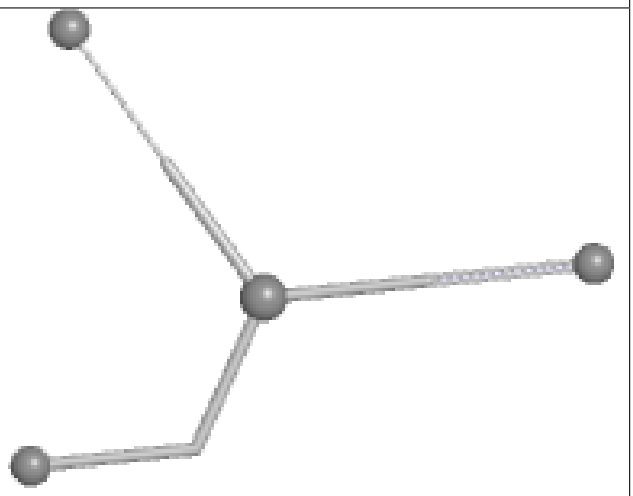


Rings

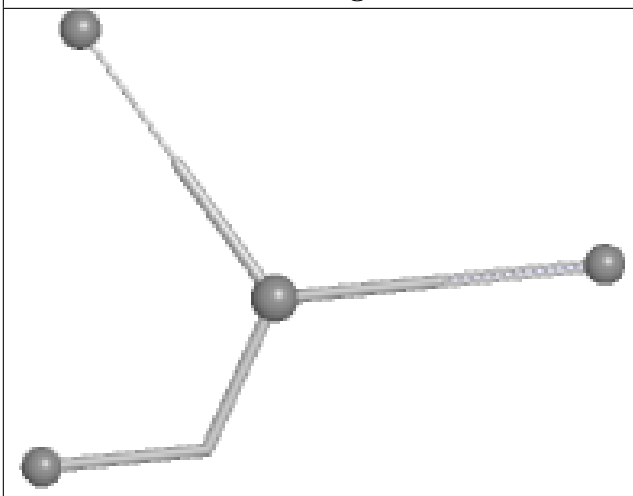
Ligand FCO E 602



Bond lengths



Bond angles



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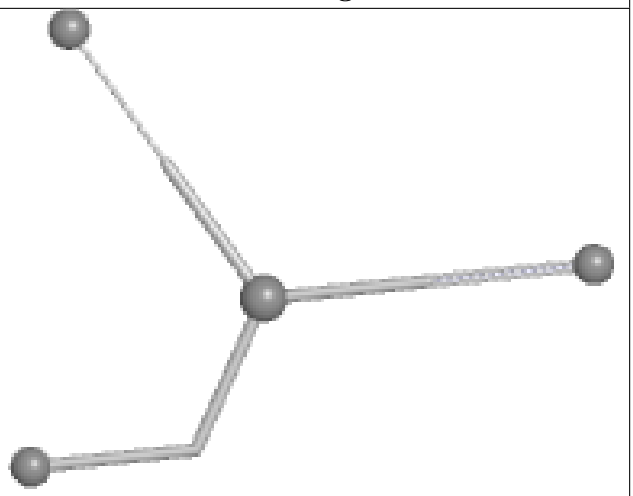
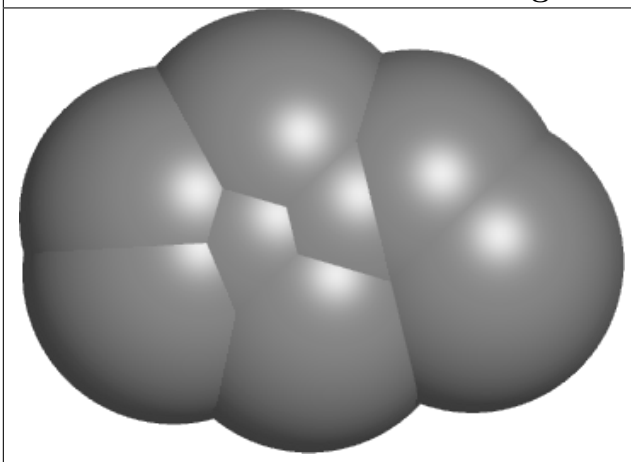
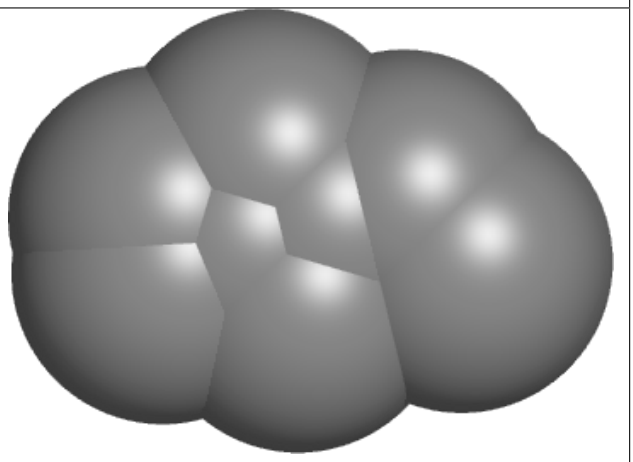


Rings

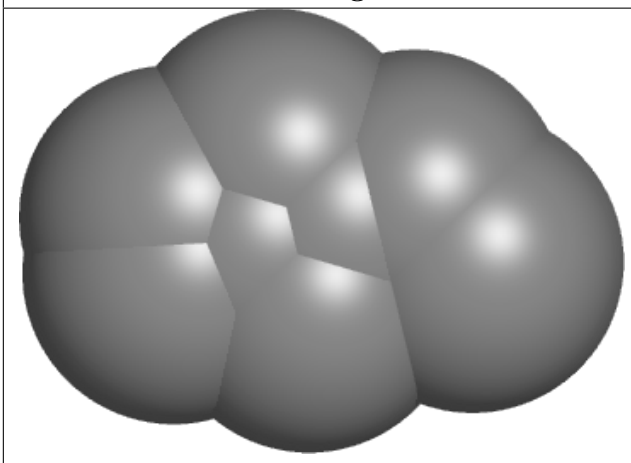
Ligand SF4 B 302



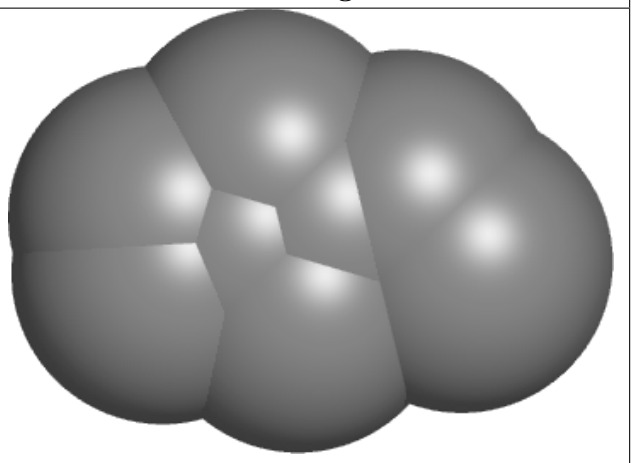
Bond lengths



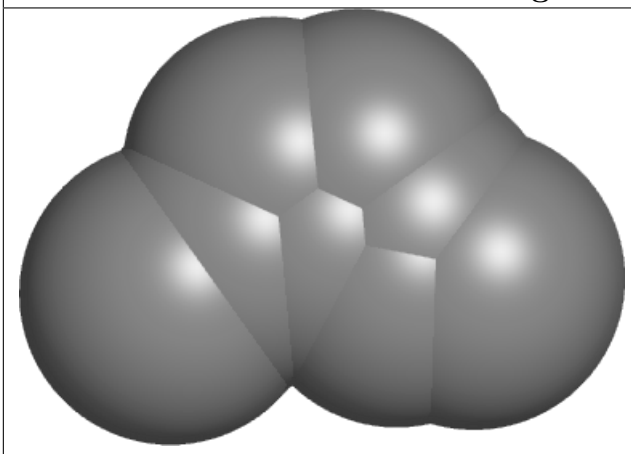
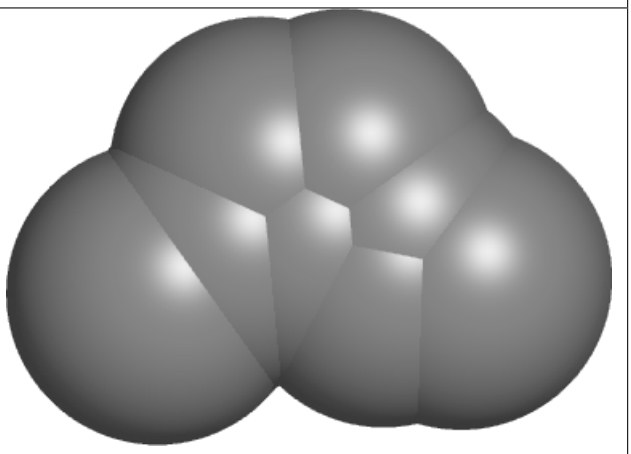
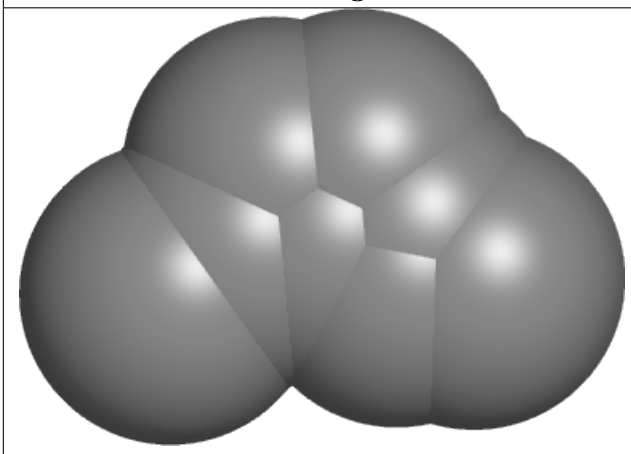
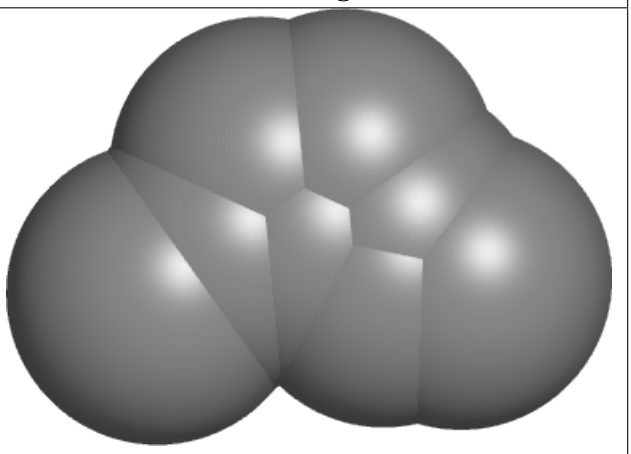
Bond angles



Torsions



Rings

Ligand SF4 B 303	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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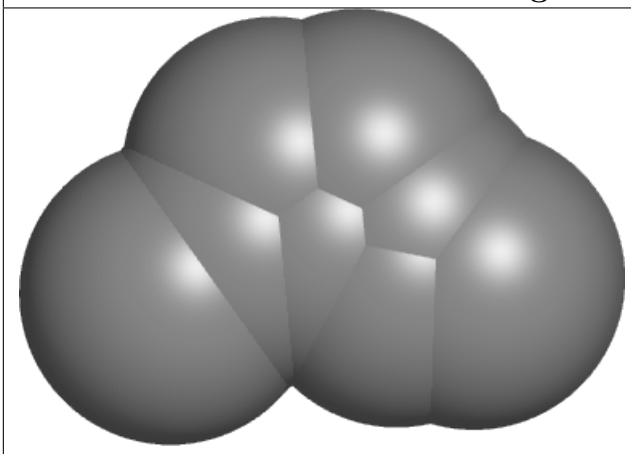
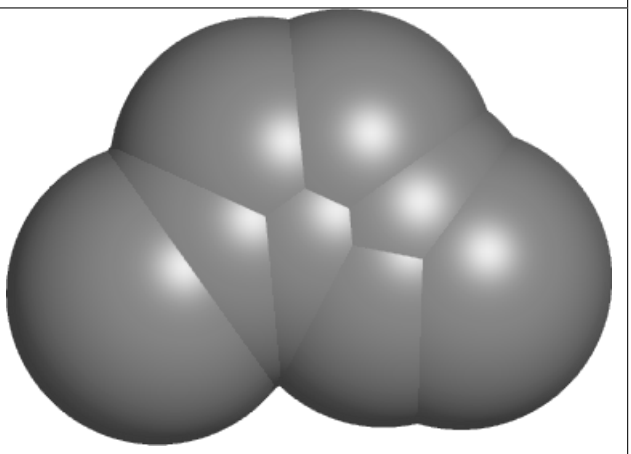
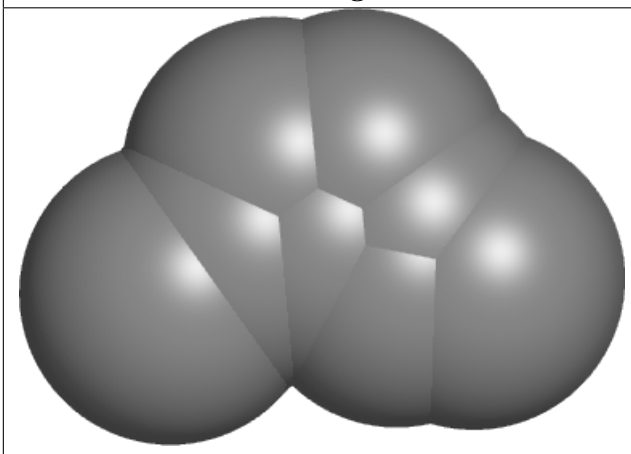
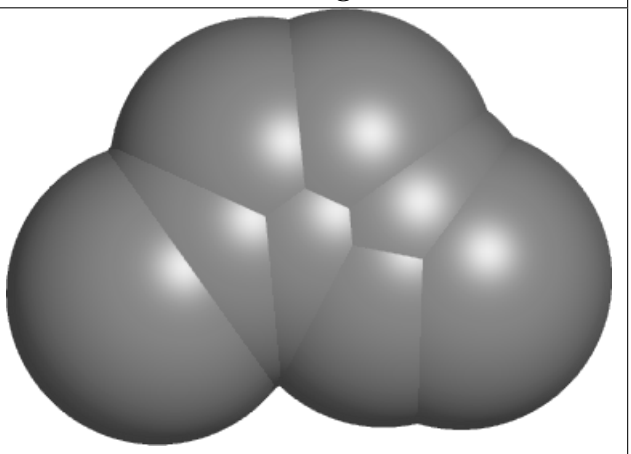
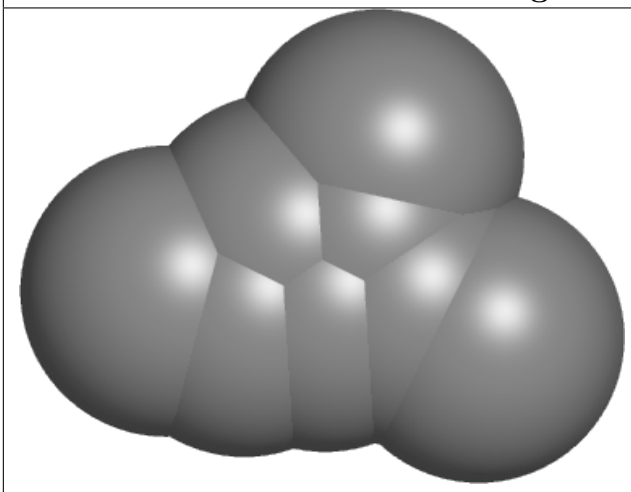
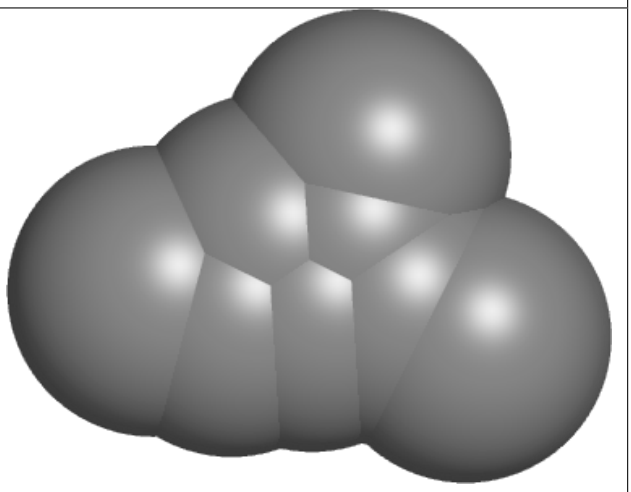
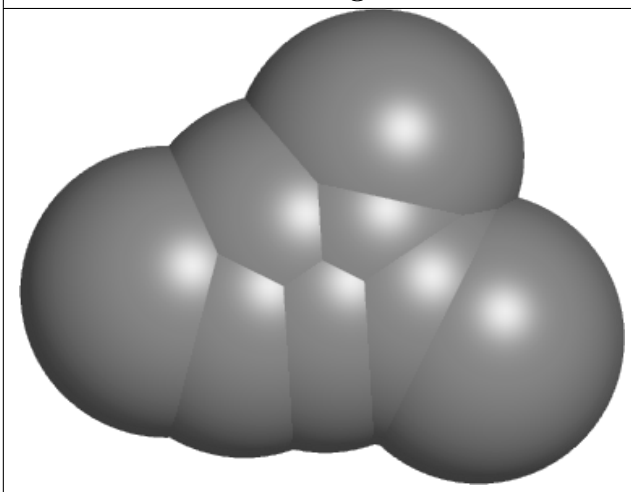
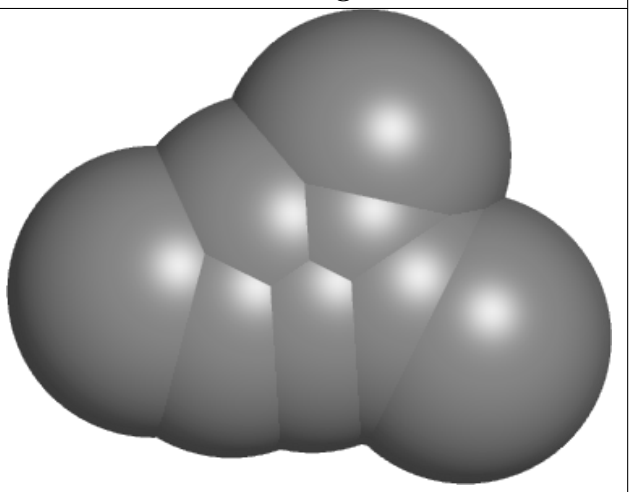
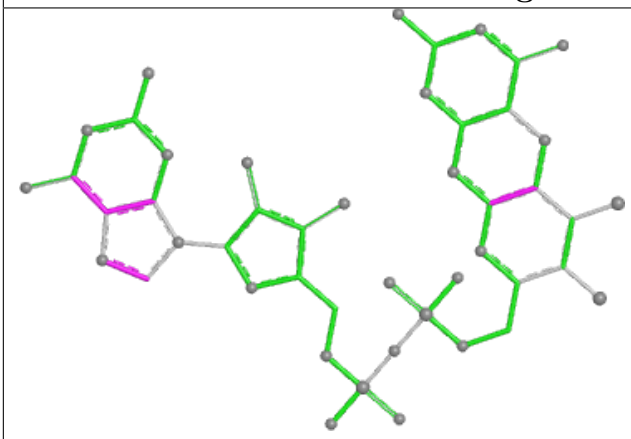
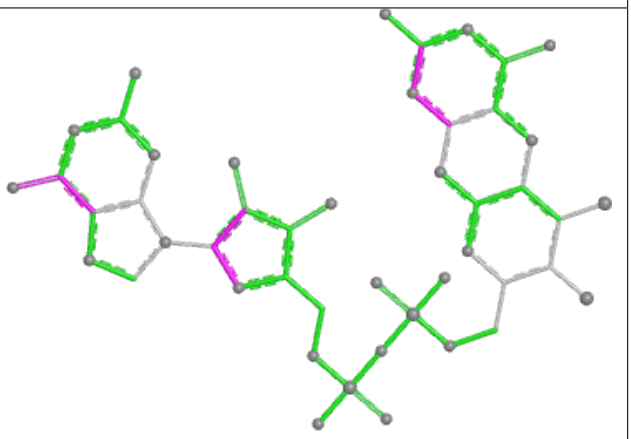
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand SF4 A 800	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

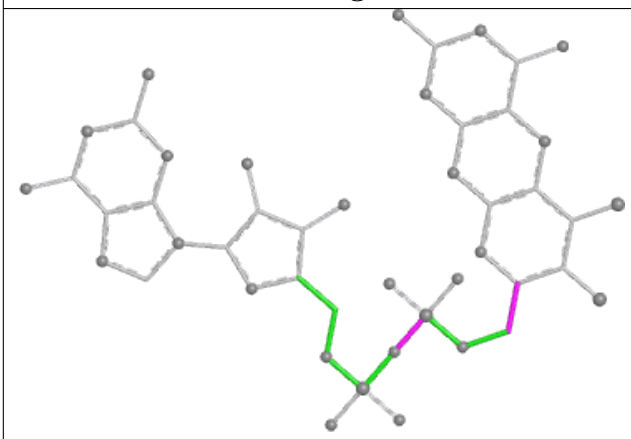
Ligand MGD A 802



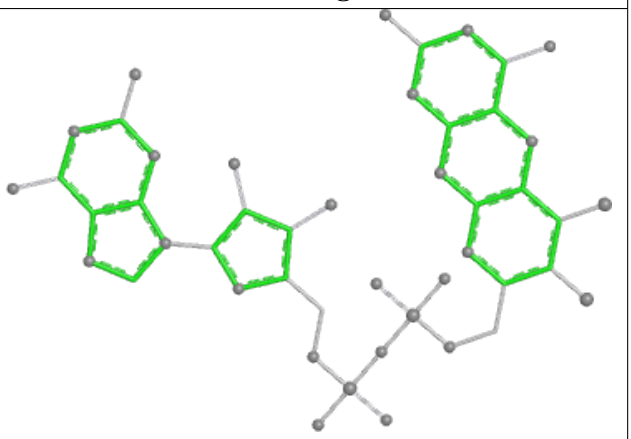
Bond lengths



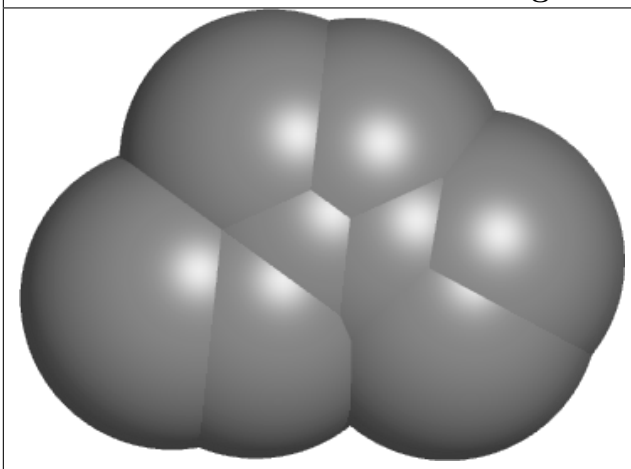
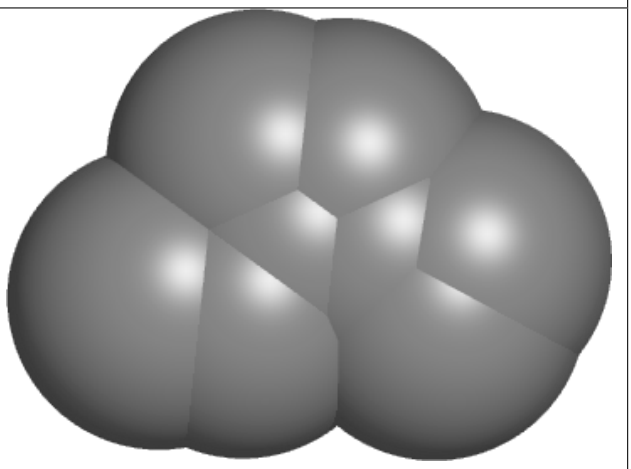
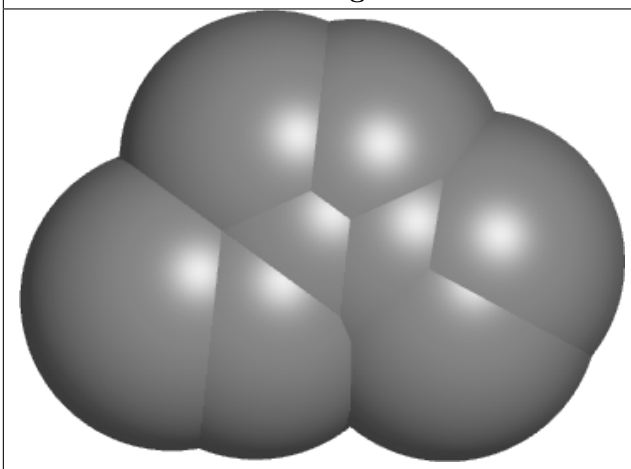
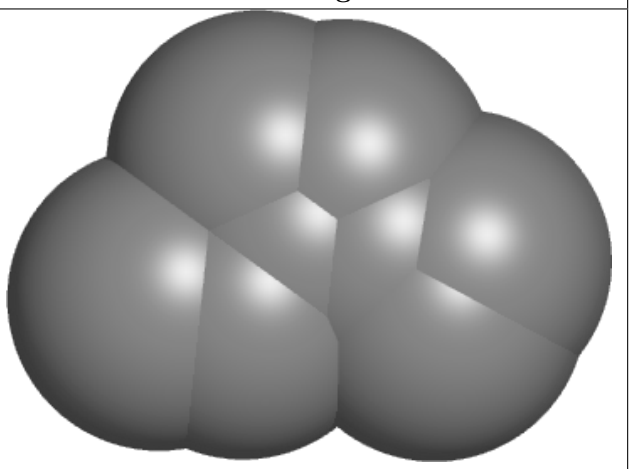
Bond angles

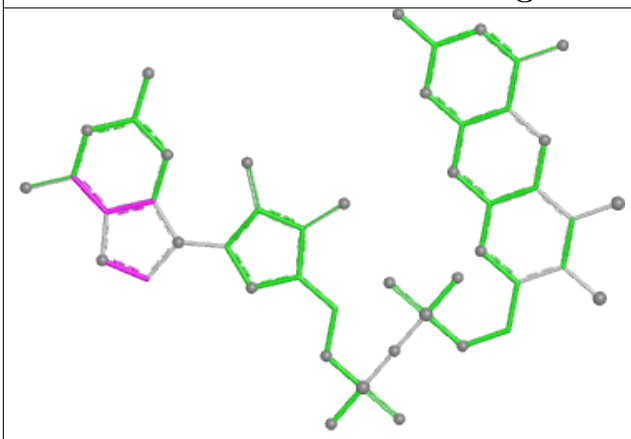
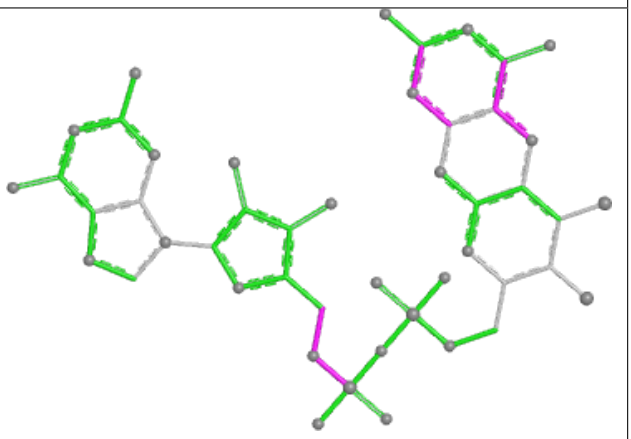
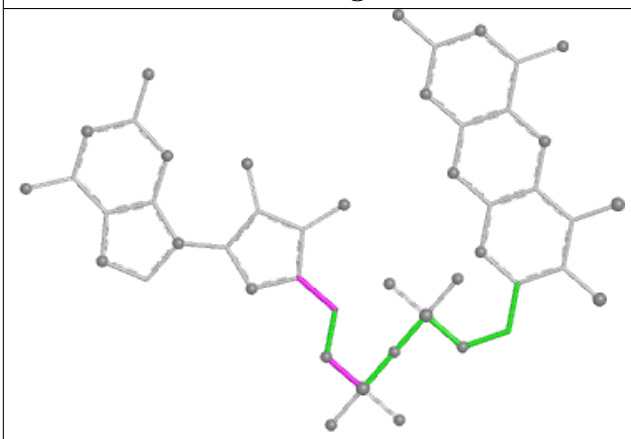
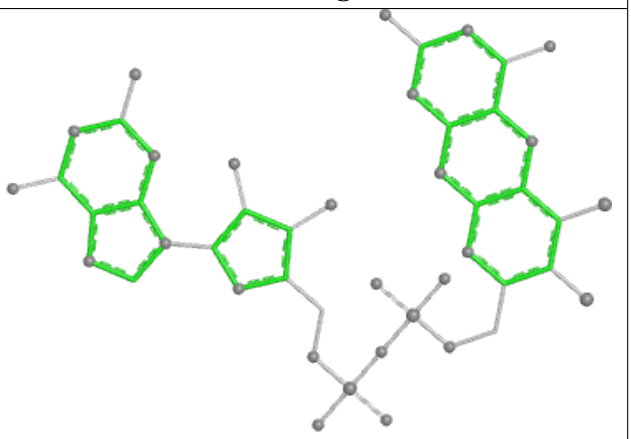


Torsions

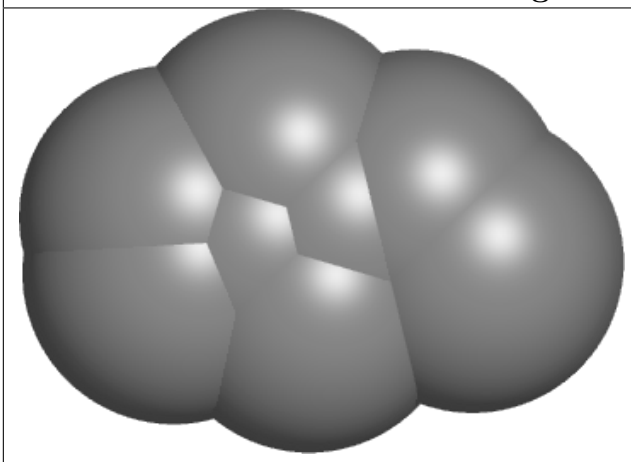


Rings

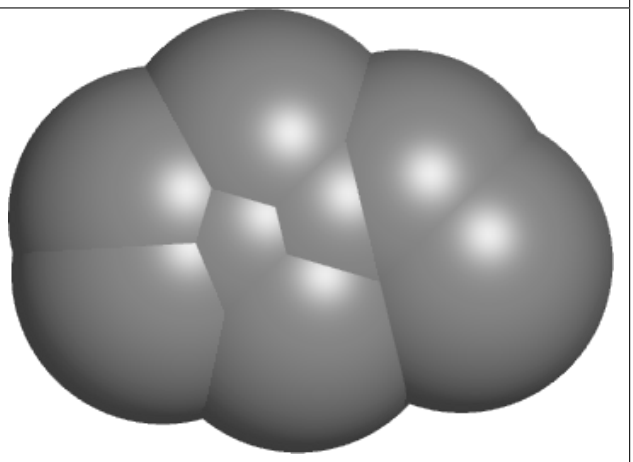
Ligand SF4 B 304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand MGD A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

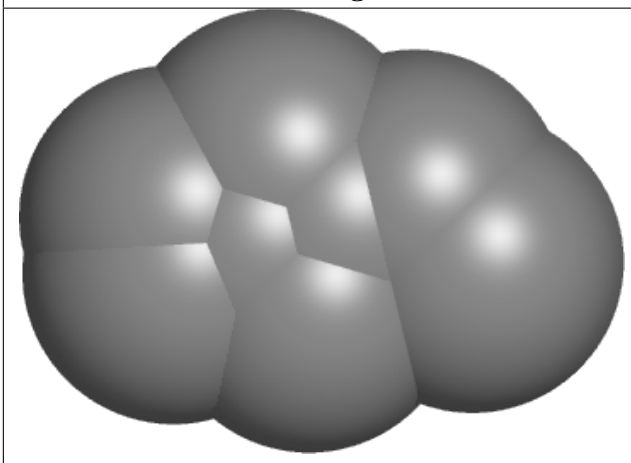
Ligand SF4 B 301



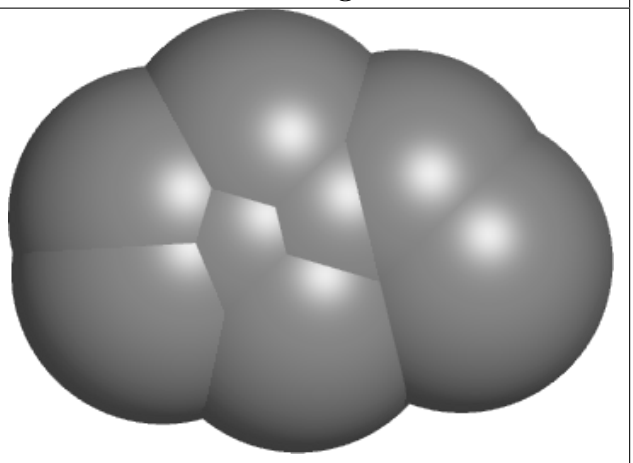
Bond lengths



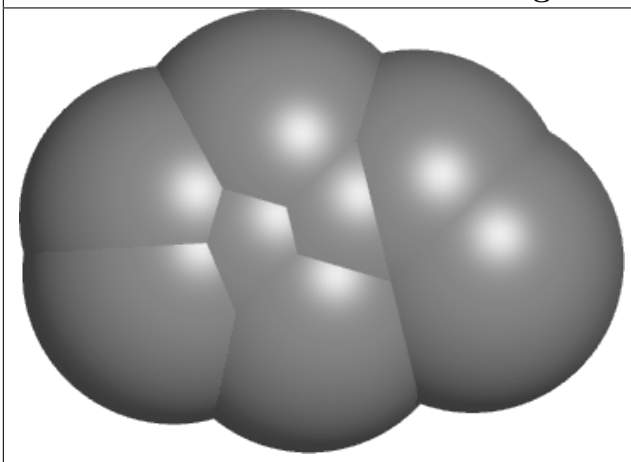
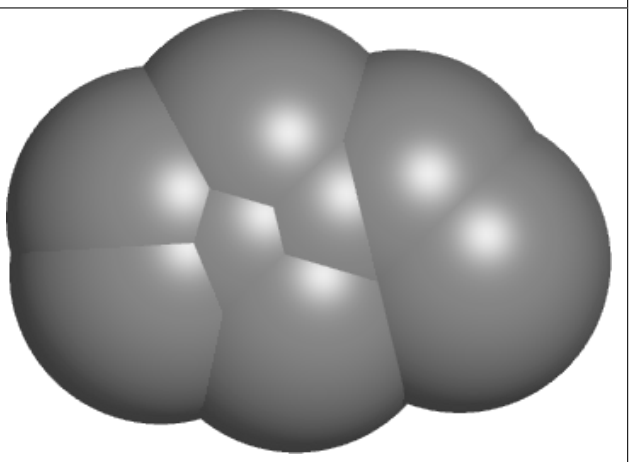
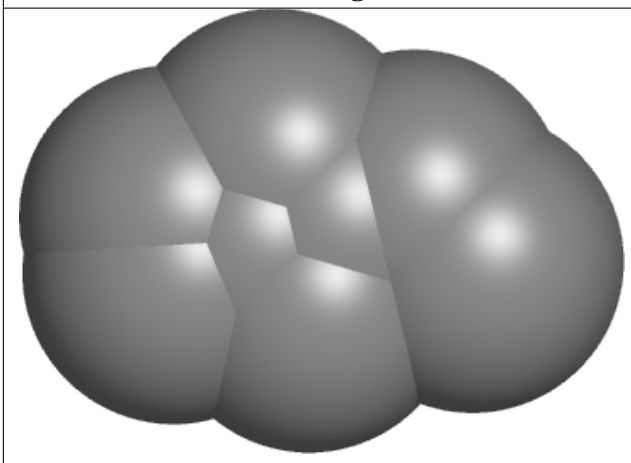
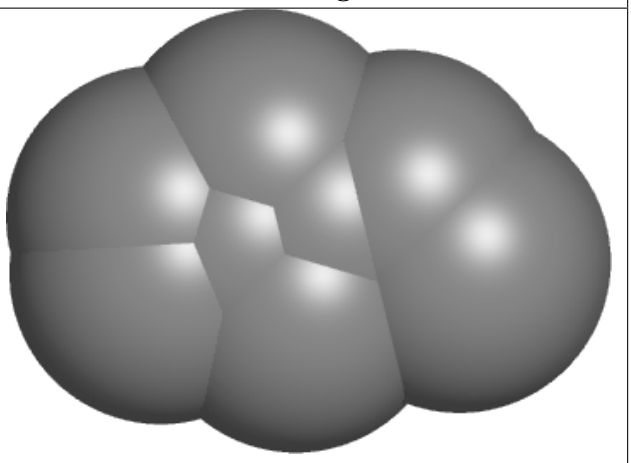
Bond angles



Torsions



Rings

Ligand SF4 F 202	
 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.

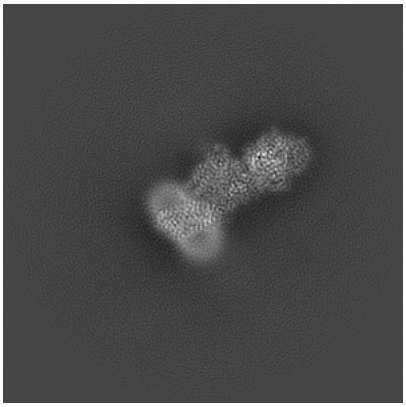
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14430. These allow visual inspection of the internal detail of the map and identification of artifacts.

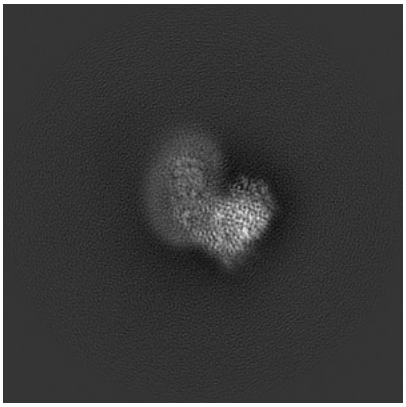
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

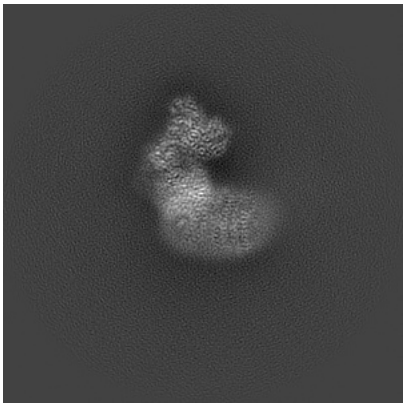
6.1.1 Primary map



X



Y

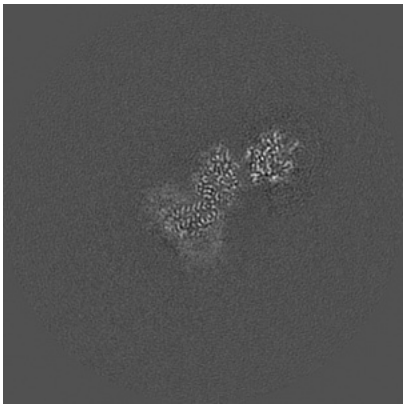


Z

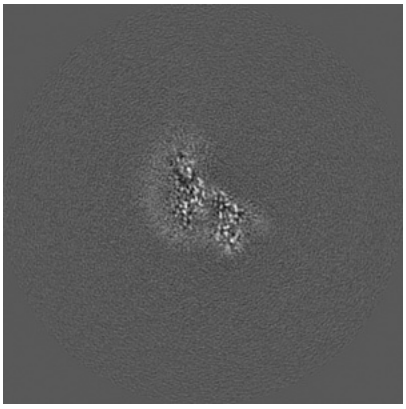
The images above show the map projected in three orthogonal directions.

6.2 Central slices

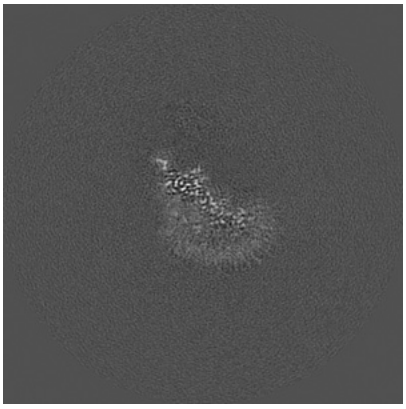
6.2.1 Primary map



X Index: 240



Y Index: 240

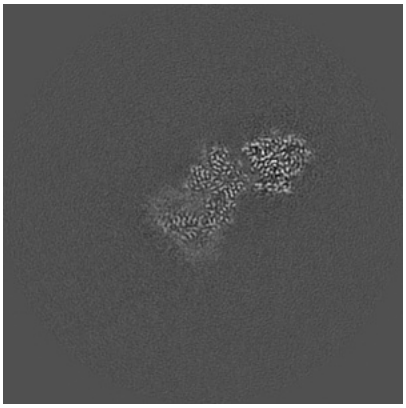


Z Index: 240

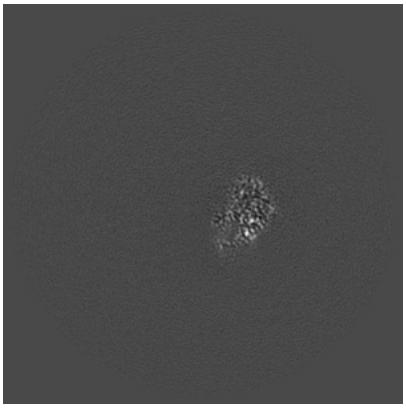
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

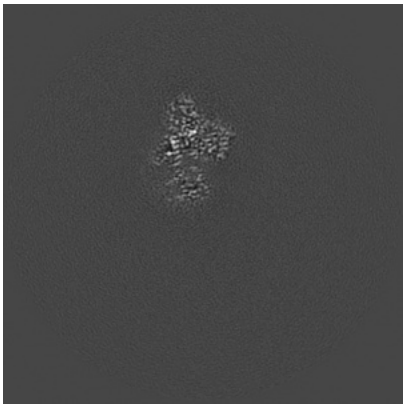
6.3.1 Primary map



X Index: 225



Y Index: 314



Z Index: 291

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 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

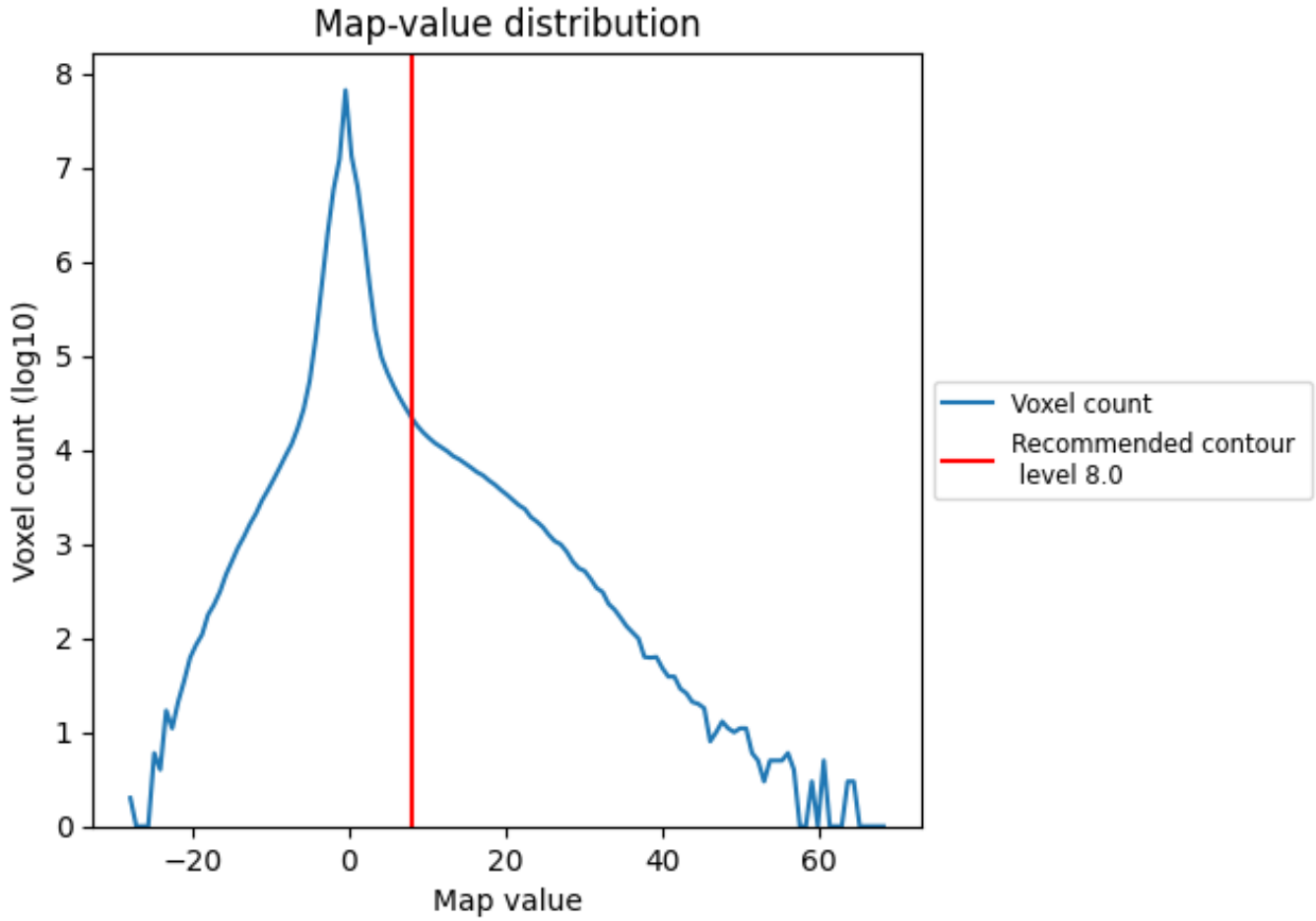
6.5 Mask visualisation (i)

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

7 Map analysis

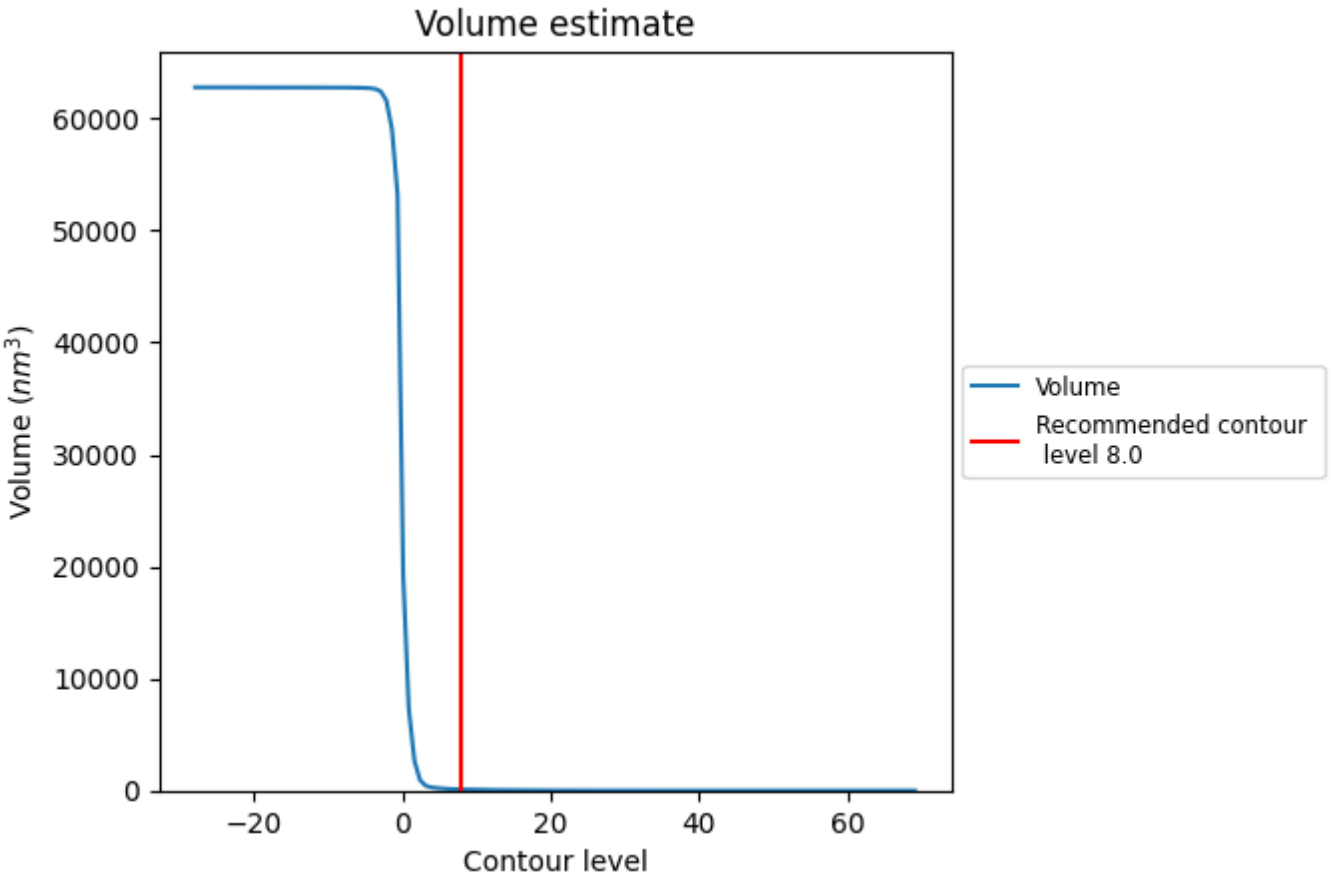
This section contains the results of statistical analysis of the map.

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.

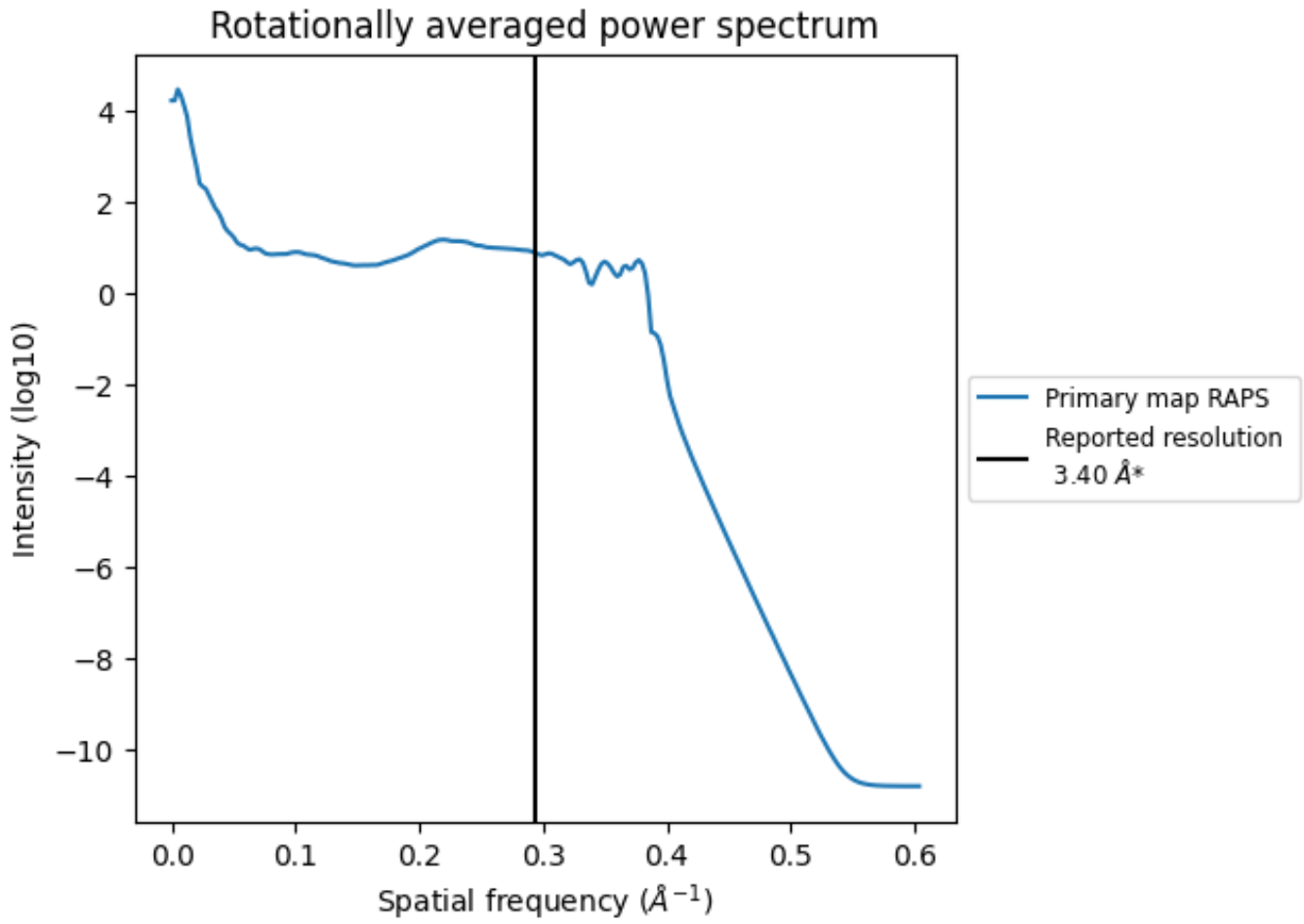
7.2 Volume estimate



The volume at the recommended contour level is 102 nm^3; this corresponds to an approximate mass of 92 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 0.294 Å^{-1}

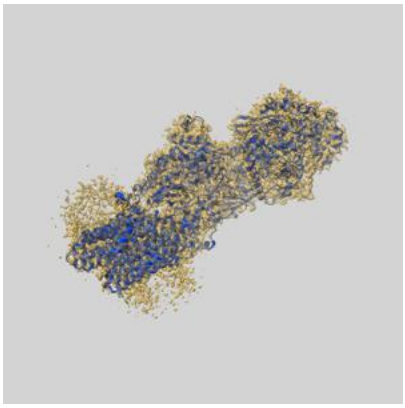
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

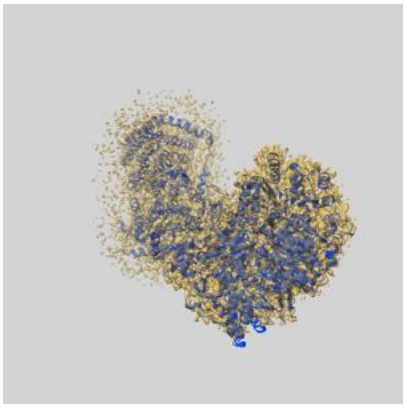
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14430 and PDB model 7Z0T. Per-residue inclusion information can be found in section 3 on page 9.

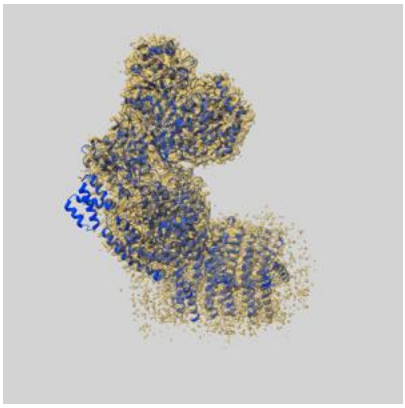
9.1 Map-model overlay



X



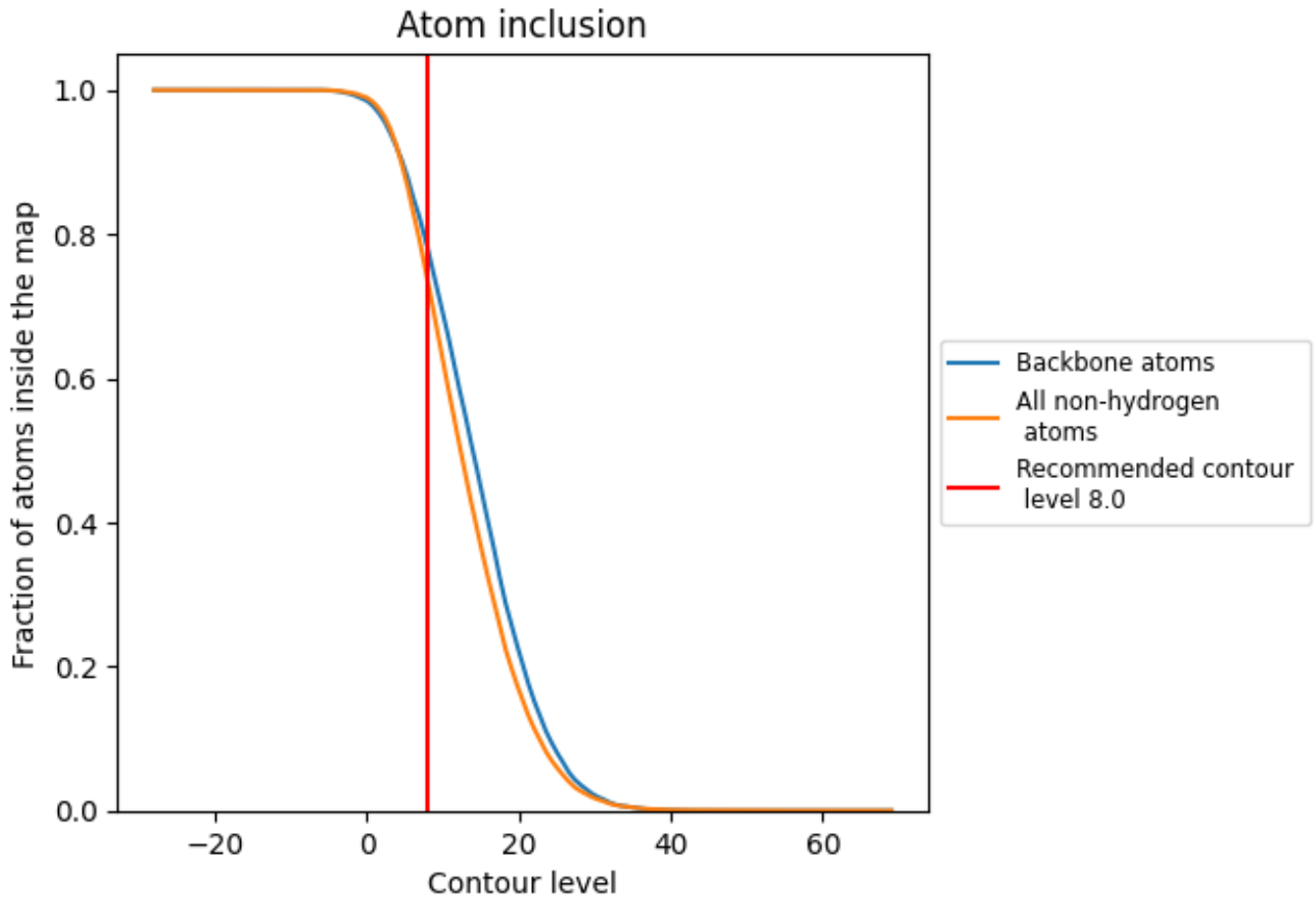
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.