Full wwPDB EM Validation Report

Aug 27, 2026 – 02:11 am BST

PDB ID	:	9FZY / pdb_00009fzy
EMDB ID	:	EMD-50897
Title	:	Structure of carbon monoxide dehydrogenase/acetyl-CoA synthase (CODH/ACS) in complex with corrinoid iron-sulfur protein (CoFeSP) from Clostridium autoethanogenum (composite structure, class 3A)
Authors	:	Yin, M.D.; Lemaire, O.N.; Wagner, T.; Murphy, B.J.
Deposited on	:	2024-07-06
Resolution	:	2.71 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 (i) symbol.

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

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

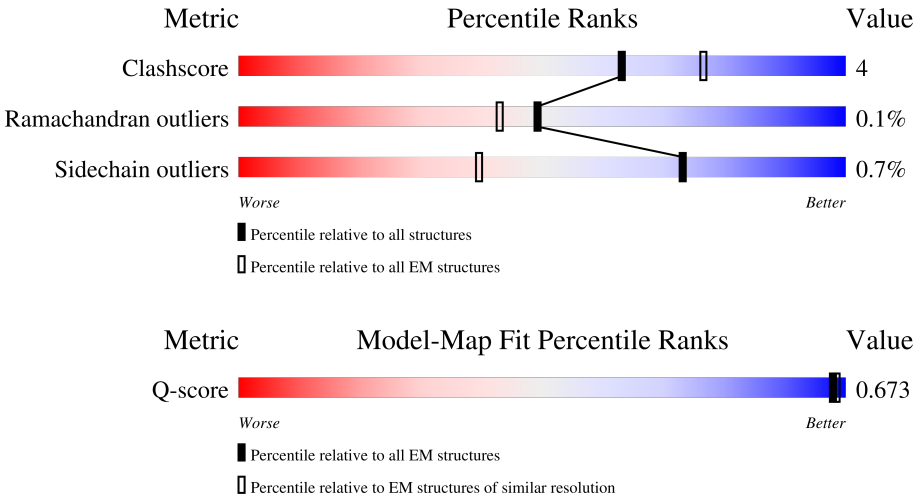
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.71 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.



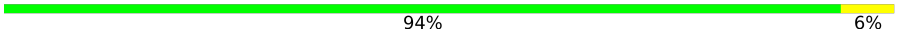
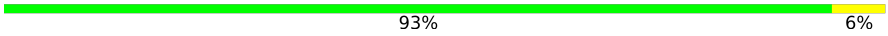
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10297 (2.21 - 3.21)

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	F	450	22% 81% 17%
2	A	708	39% 59%
2	D	708	12% 86% 14%
3	E	314	86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	630	
4	C	630	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 22924 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 Corrinoid iron-sulfur protein large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	442	3420	2198	557	645	20	0	0

- Molecule 2 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	708	5392	3449	884	1023	36	0	0
			Total	C	N	O	S		
2	A	290	2154	1391	347	409	7	0	0

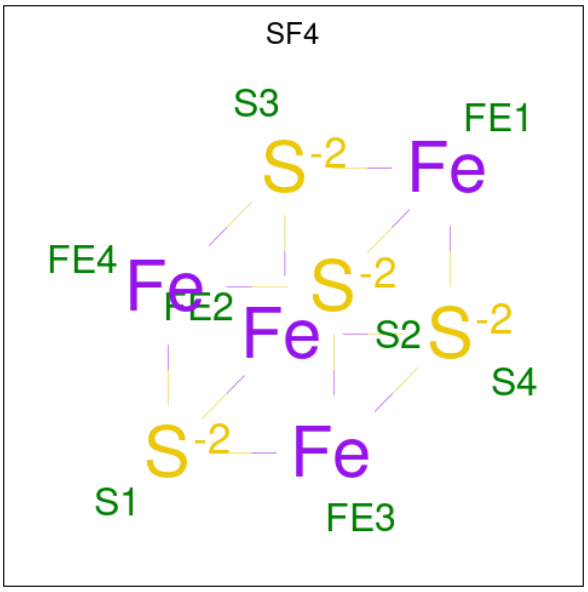
- Molecule 3 is a protein called Acetyl-CoA decarbonylase/synthase complex subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	313	2379	1506	386	477	10	0	0

- Molecule 4 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit.

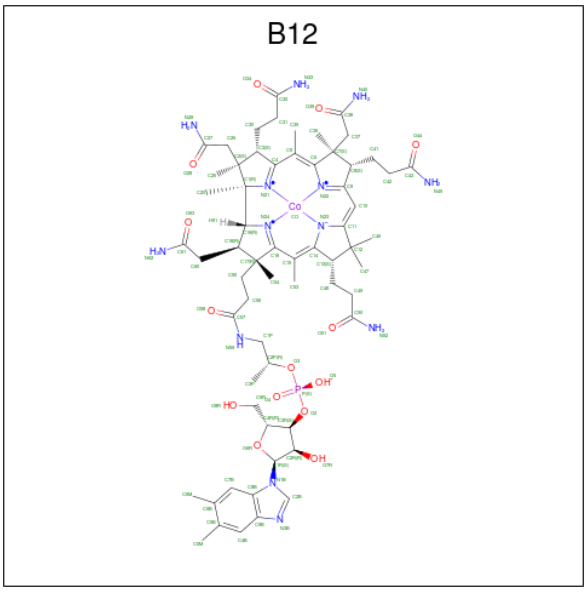
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	628	4714	2962	813	899	40	0	0
			Total	C	N	O	S		
4	C	628	4714	2962	813	899	40	0	0

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	F	1	Total Fe S 8 4 4	0
5	D	1	Total Fe S 8 4 4	0
5	B	1	Total Fe S 8 4 4	0
5	B	1	Total Fe S 8 4 4	0
5	C	1	Total Fe S 8 4 4	0

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).

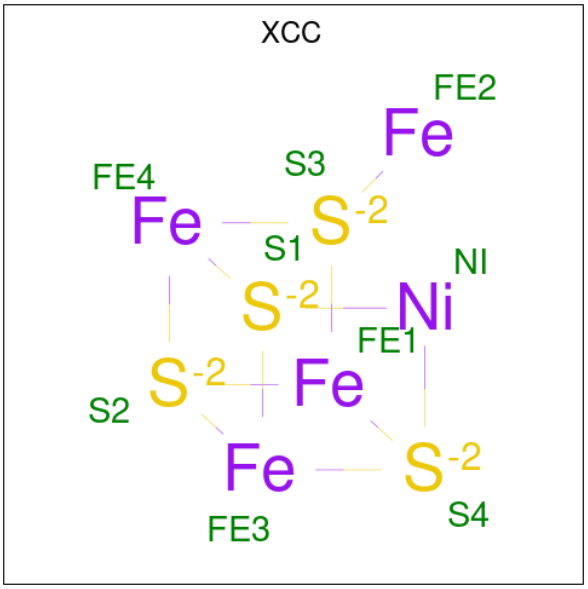


Mol	Chain	Residues	Atoms						AltConf
6	F	1	Total	C	Co	N	O	P	0
			91	62	1	13	14	1	

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Ni	0
			2	2	

- Molecule 8 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



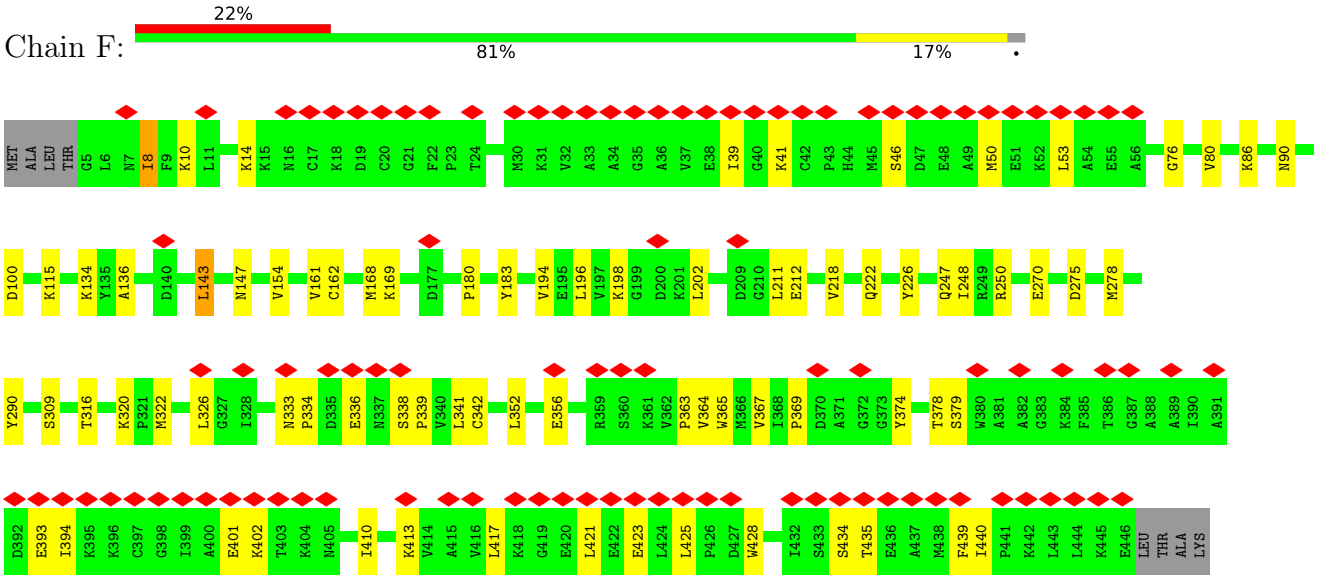
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total 9	Fe 4	Ni 1	S 4	0
8	C	1	Total 9	Fe 4	Ni 1	S 4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

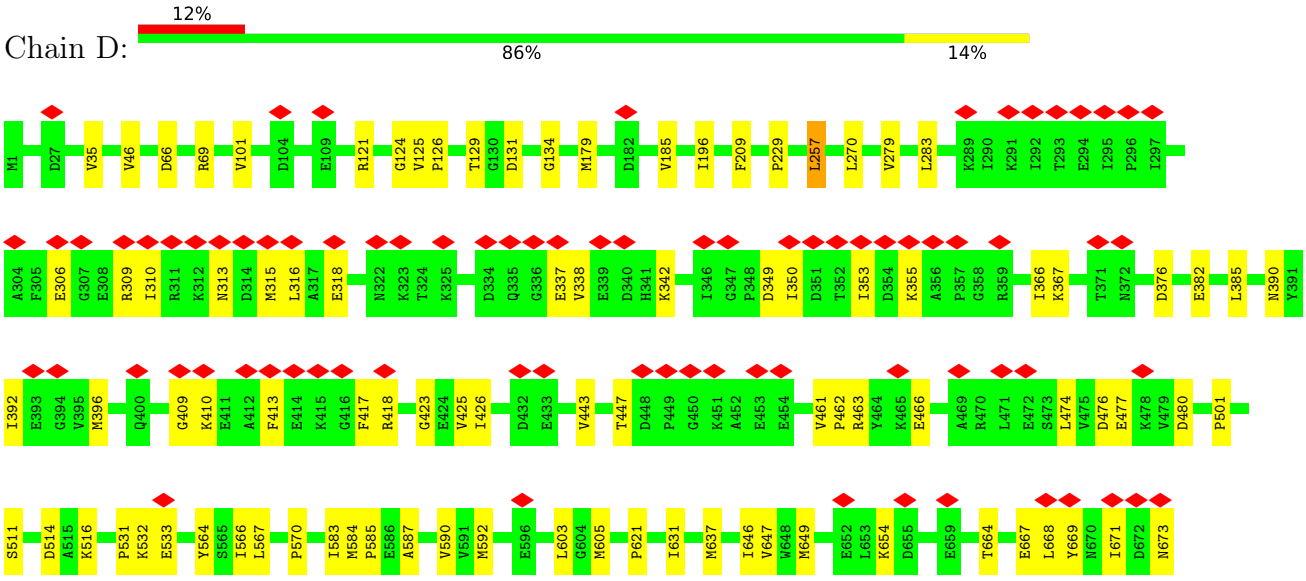
• Molecule 1: Corrinoid iron-sulfur protein large subunit

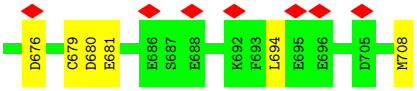
Chain F:



• Molecule 2: CO-methylating acetyl-CoA synthase

Chain D:

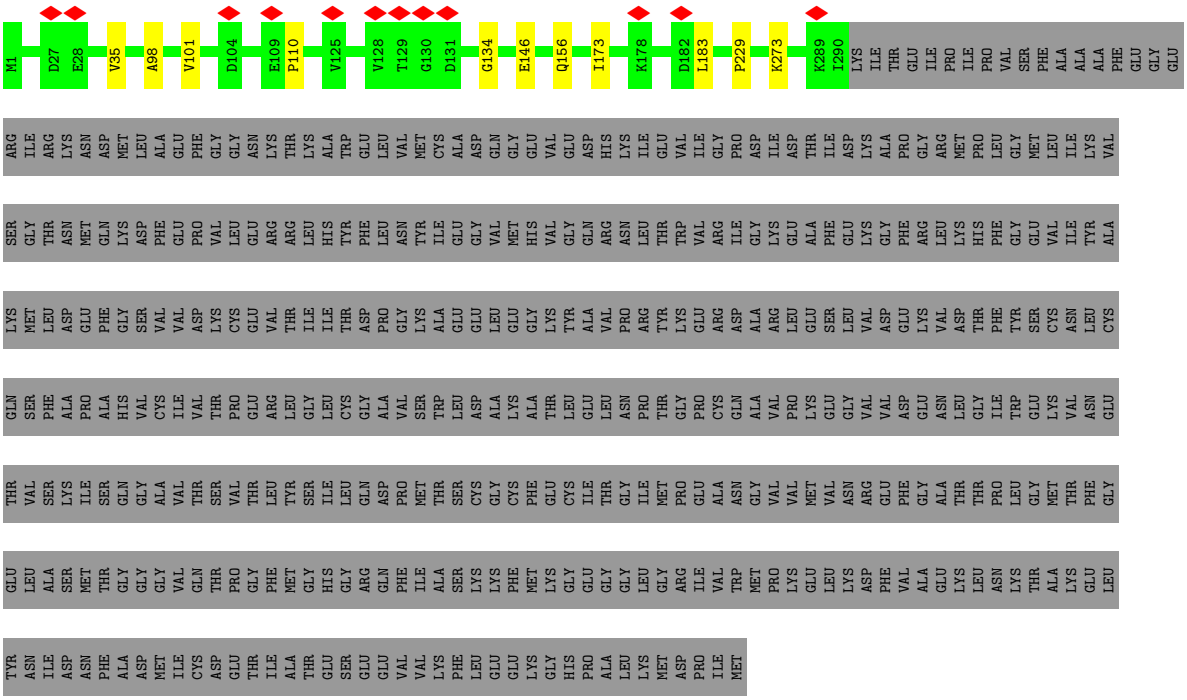




• Molecule 2: CO-methylating acetyl-CoA synthase

Chain A:

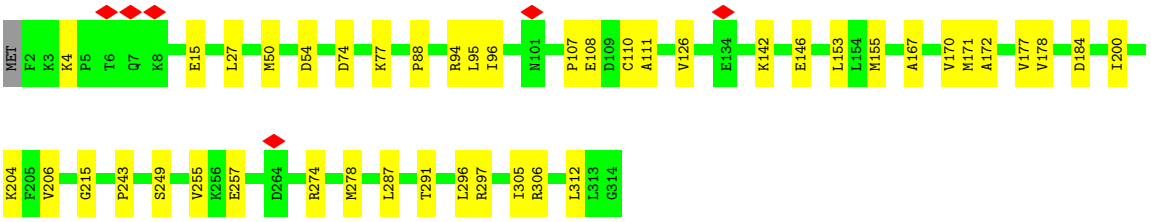




• Molecule 3: Acetyl-CoA decarbonylase/synthase complex subunit delta

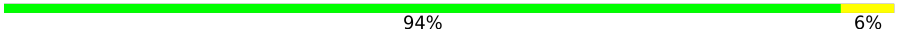
Chain E:

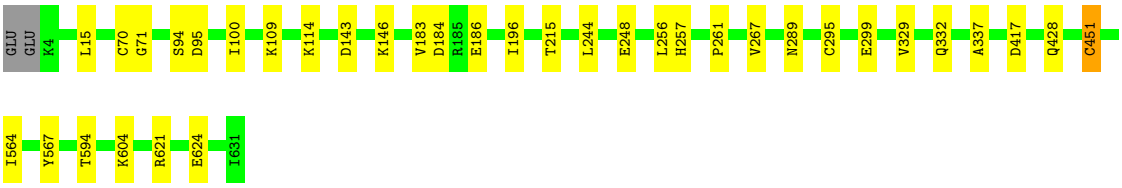




• Molecule 4: Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit

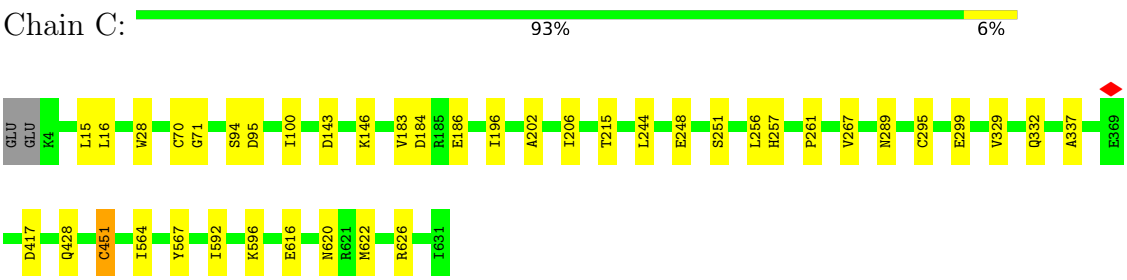
Chain B:





• Molecule 4: Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	649146	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	137.130	Depositor
Minimum map value	-128.571	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.052	Depositor
Recommended contour level	8	Depositor
Map size (Å)	490.56, 490.56, 490.56	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, XCC, NI, B12

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	F	0.17	0/3480	0.30	0/4698
2	A	0.23	0/2185	0.35	0/2970
2	D	0.20	0/5488	0.31	0/7428
3	E	0.17	0/2420	0.28	0/3279
4	B	0.32	0/4788	0.43	0/6476
4	C	0.31	0/4788	0.43	0/6476
All	All	0.25	0/23149	0.36	0/31327

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	F	3420	0	3503	52	0
2	A	2154	0	2264	6	0
2	D	5392	0	5489	56	0
3	E	2379	0	2368	29	0
4	B	4714	0	4797	22	0
4	C	4714	0	4797	25	0
5	B	16	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	8	0	0	1	0
5	D	8	0	0	0	0
5	F	8	0	0	0	0
6	F	91	0	88	17	0
7	D	2	0	0	0	0
8	B	9	0	0	1	0
8	C	9	0	0	1	0
All	All	22924	0	23306	193	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 4.

All (193) 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:D:673:ASN:ND2	2:D:676:ASP:OD2	2.19	0.75
6:F:502:B12:H481	6:F:502:B12:H533	1.69	0.73
4:C:451:CYS:HB3	8:C:702:XCC:S2	2.29	0.73
4:B:451:CYS:HB3	8:B:703:XCC:S2	2.29	0.72
1:F:410:ILE:HG21	1:F:417:LEU:HD11	1.76	0.68
1:F:336:GLU:HA	1:F:402:LYS:HD2	1.77	0.65
1:F:334:PRO:HA	1:F:363:PRO:HB3	1.80	0.63
1:F:39:ILE:HG12	1:F:53:LEU:HB3	1.79	0.63
4:B:196:ILE:HD13	5:B:702:SF4:S1	2.39	0.63
4:C:196:ILE:HD13	5:C:701:SF4:S3	2.40	0.62
2:D:664:THR:O	2:D:667:GLU:HG3	2.00	0.61
2:D:313:ASN:O	2:D:410:LYS:NZ	2.25	0.61
1:F:247:GLN:HE21	3:E:4:LYS:HE2	1.66	0.61
1:F:365:TRP:CZ2	1:F:402:LYS:HG3	2.36	0.61
1:F:334:PRO:HB2	1:F:365:TRP:CE2	2.36	0.60
3:E:206:VAL:HG12	3:E:243:PRO:HG2	1.83	0.59
3:E:287:LEU:HA	3:E:291:THR:HG22	1.85	0.59
3:E:257:GLU:O	3:E:274:ARG:NH1	2.32	0.59
1:F:425:LEU:HB3	1:F:428:TRP:HB2	1.84	0.58
4:B:257:HIS:HB3	4:B:329:VAL:HG12	1.85	0.58
2:D:337:GLU:N	2:D:337:GLU:OE1	2.37	0.57
2:D:654:LYS:NZ	2:D:680:ASP:OD2	2.34	0.57
2:D:349:ASP:OD1	2:D:350:ILE:N	2.34	0.57
2:D:129:THR:OG1	2:D:131:ASP:OD1	2.22	0.56
6:F:502:B12:H552	6:F:502:B12:H531	1.88	0.56
4:C:257:HIS:HB3	4:C:329:VAL:HG12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:88:PRO:HA	3:E:306:ARG:HH21	1.71	0.55
2:D:477:GLU:N	2:D:477:GLU:OE1	2.39	0.55
1:F:413:LYS:HG2	1:F:435:THR:HB	1.89	0.55
6:F:502:B12:H421	6:F:502:B12:H10	1.89	0.55
3:E:15:GLU:HA	3:E:27:LEU:O	2.06	0.55
2:A:110:PRO:HG3	2:A:173:ILE:HD11	1.89	0.55
1:F:194:VAL:O	1:F:198:LYS:HB2	2.09	0.53
4:C:417:ASP:OD2	4:C:428:GLN:NE2	2.40	0.53
2:D:376:ASP:OD2	2:D:516:LYS:NZ	2.35	0.53
4:C:15:LEU:HD12	4:C:244:LEU:HD13	1.91	0.53
2:D:476:ASP:OD2	2:D:564:TYR:OH	2.27	0.53
4:B:15:LEU:HD12	4:B:244:LEU:HD13	1.91	0.52
1:F:369:PRO:HA	1:F:393:GLU:HG2	1.92	0.52
2:A:146:GLU:OE1	2:A:146:GLU:N	2.39	0.52
2:D:316:LEU:HD22	2:D:413:PHE:HB2	1.92	0.52
1:F:162:CYS:HB3	1:F:168:MET:HE2	1.91	0.52
1:F:10:LYS:O	1:F:14:LYS:NZ	2.42	0.52
2:D:315:MET:HA	2:D:409:GLY:HA2	1.92	0.52
2:D:121:ARG:NH1	3:E:172:ALA:O	2.40	0.51
1:F:320:LYS:O	1:F:320:LYS:HG3	2.11	0.51
1:F:434:SER:HB3	1:F:439:PHE:HD2	1.76	0.51
1:F:202:LEU:O	1:F:226:TYR:OH	2.19	0.51
1:F:417:LEU:C	1:F:417:LEU:HD12	2.36	0.51
1:F:275:ASP:HB3	1:F:278:MET:HB2	1.93	0.50
2:D:134:GLY:HA2	2:D:229:PRO:HG2	1.93	0.50
1:F:413:LYS:HE2	6:F:502:B12:H2R	1.93	0.50
1:F:352:LEU:O	1:F:356:GLU:HG2	2.12	0.49
2:D:316:LEU:HB2	2:D:410:LYS:HG2	1.94	0.49
2:D:480:ASP:HA	2:D:532:LYS:HD3	1.94	0.49
2:D:306:GLU:HG2	2:D:390:ASN:HB3	1.94	0.49
4:B:100:ILE:HD11	4:B:261:PRO:HD2	1.94	0.49
1:F:410:ILE:HG21	1:F:417:LEU:CD1	2.42	0.49
4:B:295:CYS:O	4:B:299:GLU:HG2	2.13	0.49
3:E:95:LEU:HD13	3:E:110:CYS:HB3	1.94	0.49
1:F:115:LYS:HG3	1:F:154:VAL:HG12	1.94	0.49
4:B:184:ASP:HB3	4:C:184:ASP:HB3	1.94	0.49
4:B:417:ASP:OD2	4:B:428:GLN:NE2	2.44	0.49
1:F:316:THR:HG22	1:F:322:MET:HE3	1.95	0.48
2:D:209:PHE:HD1	3:E:171:MET:HB3	1.77	0.48
2:D:583:ILE:HA	2:D:590:VAL:HG12	1.95	0.48
6:F:502:B12:H301	6:F:502:B12:H203	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:461:VAL:HG22	2:D:462:PRO:HD3	1.95	0.48
3:E:255:VAL:HG21	3:E:278:MET:HE2	1.95	0.48
2:D:382:GLU:O	2:D:385:LEU:HB2	2.12	0.48
2:D:392:ILE:HD11	2:D:425:VAL:HG21	1.95	0.48
4:B:183:VAL:HG22	4:B:215:THR:HB	1.96	0.48
1:F:440:ILE:HD11	6:F:502:B12:HM63	1.96	0.47
4:B:621:ARG:O	4:B:624:GLU:HG3	2.14	0.47
1:F:410:ILE:C	6:F:502:B12:HM52	2.39	0.47
3:E:111:ALA:HB1	3:E:146:GLU:HG3	1.95	0.47
2:D:681:GLU:OE1	2:D:681:GLU:N	2.42	0.47
1:F:423:GLU:HG3	2:D:309:ARG:HB2	1.97	0.47
4:C:295:CYS:O	4:C:299:GLU:HG2	2.14	0.47
6:F:502:B12:H601	6:F:502:B12:H252	1.95	0.47
4:B:186:GLU:HG3	4:B:215:THR:HG21	1.96	0.47
1:F:134:LYS:NZ	1:F:270:GLU:OE2	2.43	0.47
4:C:183:VAL:HG22	4:C:215:THR:HB	1.97	0.46
4:C:186:GLU:HG3	4:C:215:THR:HG21	1.96	0.46
1:F:339:PRO:HG2	1:F:364:VAL:HG22	1.98	0.46
1:F:212:GLU:H	1:F:212:GLU:CD	2.23	0.46
2:D:310:ILE:HG12	2:D:396:MET:SD	2.56	0.46
3:E:177:VAL:HG12	3:E:178:VAL:N	2.31	0.46
2:D:511:SER:H	2:D:514:ASP:HB2	1.80	0.46
2:D:679:CYS:SG	2:D:680:ASP:N	2.89	0.45
2:A:156:GLN:NE2	2:A:183:LEU:O	2.41	0.45
3:E:74:ASP:HB3	3:E:77:LYS:HB2	1.98	0.45
1:F:333:ASN:O	1:F:333:ASN:ND2	2.49	0.45
2:D:423:GLY:HA2	2:D:443:VAL:HG11	1.97	0.45
2:D:66:ASP:OD1	2:D:69:ARG:NH1	2.50	0.45
2:D:315:MET:SD	2:D:318:GLU:OE2	2.74	0.45
3:E:155:MET:HA	3:E:178:VAL:HB	1.99	0.45
2:A:35:VAL:HG22	2:A:101:VAL:HG11	1.97	0.45
2:D:257:LEU:HD13	2:D:270:LEU:HB2	1.99	0.45
3:E:126:VAL:HG22	3:E:153:LEU:HB3	1.99	0.45
4:B:257:HIS:O	4:B:329:VAL:HA	2.16	0.45
1:F:211:LEU:HD11	1:F:248:ILE:HG13	1.98	0.45
2:D:124:GLY:HA3	2:D:209:PHE:CZ	2.52	0.45
3:E:50:MET:HA	3:E:296:LEU:O	2.17	0.45
2:D:592:MET:HE1	2:D:631:ILE:HG23	1.99	0.45
2:A:134:GLY:HA2	2:A:229:PRO:HG2	1.99	0.45
6:F:502:B12:H491	6:F:502:B12:H473	1.99	0.44
4:C:248:GLU:HG2	4:C:289:ASN:ND2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:257:HIS:O	4:C:329:VAL:HA	2.17	0.44
1:F:161:VAL:HG13	1:F:183:TYR:CD2	2.53	0.44
4:C:592:ILE:HA	4:C:596:LYS:HB2	1.99	0.44
6:F:502:B12:H361	6:F:502:B12:H411	1.71	0.44
4:B:71:GLY:HA3	4:C:337:ALA:HB2	1.99	0.44
2:D:566:ILE:HG23	2:D:567:LEU:HG	2.00	0.44
4:B:337:ALA:HB2	4:C:71:GLY:HA3	2.00	0.44
1:F:46:SER:O	1:F:50:MET:N	2.48	0.44
1:F:143:LEU:O	1:F:147:ASN:ND2	2.51	0.44
2:D:125:VAL:HB	2:D:126:PRO:HD3	2.00	0.44
1:F:367:VAL:HG21	1:F:394:ILE:HD11	1.98	0.43
2:D:366:ILE:HG12	2:D:426:ILE:HG21	1.99	0.43
1:F:247:GLN:OE1	1:F:250:ARG:NH2	2.44	0.43
1:F:309:SER:HB3	3:E:215:GLY:HA3	2.00	0.43
3:E:170:VAL:HG13	3:E:204:LYS:HD2	2.00	0.43
4:B:256:LEU:HD21	4:B:267:VAL:HG11	2.00	0.43
2:D:585:PRO:HB3	2:D:708:MET:HE2	2.00	0.43
1:F:374:TYR:HB2	1:F:379:SER:HB2	2.01	0.43
2:D:647:VAL:HB	2:D:694:LEU:HD11	2.00	0.43
1:F:378:THR:HG21	6:F:502:B12:H491	2.00	0.43
6:F:502:B12:H203	6:F:502:B12:C30	2.49	0.43
2:D:592:MET:HE3	2:D:592:MET:HB2	1.91	0.43
3:E:108:GLU:HG3	3:E:142:LYS:HE2	2.00	0.43
2:A:98:ALA:HA	2:A:101:VAL:HG22	2.01	0.43
4:C:70:CYS:CB	4:C:196:ILE:HD11	2.49	0.42
2:D:125:VAL:HG13	3:E:167:ALA:HB3	2.01	0.42
4:B:564:ILE:HA	4:B:567:TYR:CE2	2.54	0.42
1:F:100:ASP:OD2	1:F:136:ALA:N	2.40	0.42
6:F:502:B12:H531	6:F:502:B12:C55	2.49	0.42
4:B:94:SER:HB2	4:B:183:VAL:HG11	2.01	0.42
4:B:143:ASP:HA	4:B:146:LYS:HD2	2.01	0.42
4:B:594:THR:O	4:B:604:LYS:HD2	2.20	0.42
4:C:622:MET:O	4:C:626:ARG:HG3	2.20	0.42
1:F:76:GLY:O	1:F:90:ASN:ND2	2.38	0.42
4:B:109:LYS:O	4:B:114:LYS:NZ	2.49	0.42
6:F:502:B12:H481	6:F:502:B12:C53	2.45	0.42
2:D:474:LEU:HB3	2:D:501:PRO:HB3	2.01	0.42
1:F:338:SER:HB2	1:F:365:TRP:CD1	2.55	0.42
4:C:564:ILE:HA	4:C:567:TYR:CE2	2.55	0.42
2:D:353:ILE:HG22	2:D:355:LYS:H	1.84	0.42
3:E:50:MET:HG3	3:E:88:PRO:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:155:MET:HG2	3:E:178:VAL:HG21	2.01	0.42
3:E:312:LEU:HD23	3:E:312:LEU:HA	1.92	0.42
1:F:342:CYS:SG	1:F:367:VAL:HG23	2.60	0.42
2:D:417:PHE:O	2:D:418:ARG:NE	2.44	0.42
3:E:54:ASP:OD1	3:E:54:ASP:N	2.45	0.42
3:E:170:VAL:HG11	3:E:200:ILE:HG23	2.02	0.42
4:C:100:ILE:HD11	4:C:261:PRO:HD2	2.01	0.42
4:C:616:GLU:OE2	4:C:620:ASN:ND2	2.53	0.42
1:F:169:LYS:HG2	1:F:196:LEU:HD21	2.00	0.41
4:C:94:SER:HB2	4:C:183:VAL:HG11	2.02	0.41
2:D:463:ARG:HA	2:D:466:GLU:HG2	2.03	0.41
3:E:107:PRO:HB2	3:E:142:LYS:HG3	2.02	0.41
2:D:35:VAL:HG22	2:D:101:VAL:HG21	2.02	0.41
2:D:179:MET:HA	2:D:185:VAL:HB	2.03	0.41
2:D:637:MET:HE2	2:D:637:MET:HB3	1.97	0.41
1:F:401:GLU:OE2	1:F:402:LYS:NZ	2.52	0.41
2:D:338:VAL:HG12	2:D:367:LYS:HB3	2.03	0.41
2:D:646:ILE:HG21	2:D:649:MET:HE2	2.03	0.41
3:E:296:LEU:HD21	3:E:305:ILE:HG13	2.02	0.41
4:C:202:ALA:O	4:C:206:ILE:HG12	2.20	0.41
1:F:39:ILE:O	1:F:39:ILE:HG13	2.21	0.41
6:F:502:B12:H353	6:F:502:B12:H302	2.03	0.41
2:D:46:VAL:HG21	2:D:196:ILE:HD11	2.01	0.41
1:F:180:PRO:HD2	1:F:202:LEU:HD22	2.02	0.41
4:B:70:CYS:CB	4:B:196:ILE:HD11	2.51	0.41
1:F:341:LEU:HD11	6:F:502:B12:C5M	2.51	0.41
1:F:421:LEU:HD23	1:F:421:LEU:HA	1.92	0.41
6:F:502:B12:H531	6:F:502:B12:H543	2.03	0.41
2:D:531:PRO:HB2	2:D:533:GLU:HG2	2.03	0.41
2:D:584:MET:HE2	2:D:587:ALA:HB2	2.02	0.41
4:C:143:ASP:HA	4:C:146:LYS:HD2	2.03	0.41
4:C:248:GLU:HB2	4:C:251:SER:HB2	2.03	0.41
1:F:80:VAL:HG21	1:F:86:LYS:H	1.86	0.41
3:E:249:SER:HB2	3:E:297:ARG:HB2	2.03	0.41
1:F:8:ILE:HB	1:F:53:LEU:HD21	2.02	0.40
4:C:256:LEU:HD21	4:C:267:VAL:HG11	2.02	0.40
1:F:218:VAL:HG12	1:F:222:GLN:NE2	2.36	0.40
2:D:279:VAL:O	2:D:283:LEU:HG	2.21	0.40
4:B:248:GLU:HG2	4:B:289:ASN:ND2	2.36	0.40
2:D:592:MET:HB3	2:D:649:MET:HG3	2.03	0.40
2:D:605:MET:SD	2:D:605:MET:N	2.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:94:ARG:HG2	3:E:96:ILE:HG22	2.03	0.40
4:C:16:LEU:HD21	4:C:28:TRP:CE3	2.57	0.40
2:D:570:PRO:HG3	2:D:621:PRO:HA	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	F	440/450 (98%)	418 (95%)	22 (5%)	0	100	100
2	A	288/708 (41%)	284 (99%)	4 (1%)	0	100	100
2	D	706/708 (100%)	688 (98%)	18 (2%)	0	100	100
3	E	311/314 (99%)	300 (96%)	11 (4%)	0	100	100
4	B	626/630 (99%)	608 (97%)	17 (3%)	1 (0%)	43	66
4	C	626/630 (99%)	608 (97%)	17 (3%)	1 (0%)	43	66
All	All	2997/3440 (87%)	2906 (97%)	89 (3%)	2 (0%)	49	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	332	GLN
4	B	332	GLN

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	F	371/377 (98%)	366 (99%)	5 (1%)	61 81
2	A	232/583 (40%)	231 (100%)	1 (0%)	84 92
2	D	583/583 (100%)	576 (99%)	7 (1%)	63 82
3	E	259/260 (100%)	258 (100%)	1 (0%)	84 92
4	B	517/519 (100%)	515 (100%)	2 (0%)	84 92
4	C	517/519 (100%)	515 (100%)	2 (0%)	84 92
All	All	2479/2841 (87%)	2461 (99%)	18 (1%)	73 89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	8	ILE
1	F	41	LYS
1	F	143	LEU
1	F	290	TYR
1	F	326	LEU
2	D	257	LEU
2	D	342	LYS
2	D	447	THR
2	D	603	LEU
2	D	668	LEU
2	D	669	TYR
2	D	671	ILE
3	E	184	ASP
2	A	273	LYS
4	B	95	ASP
4	B	451	CYS
4	C	95	ASP
4	C	451	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	71	ASN
1	F	222	GLN
2	D	594	ASN
2	D	670	ASN
3	E	307	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	233	ASN
2	A	287	ASN
4	B	14	GLN
4	C	10	GLN
4	C	357	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
8	XCC	C	702	4	0,12,12	-	-	-		
5	SF4	B	702	4	0,12,12	-	-	-		
6	B12	F	502	-	93,101,101	0.86	2 (2%)	146,166,166	0.97	3 (2%)
5	SF4	C	701	4	0,12,12	-	-	-		
5	SF4	F	501	1	0,12,12	-	-	-		
5	SF4	B	701	4	0,12,12	-	-	-		
5	SF4	D	801	2,7	0,12,12	-	-	-		
8	XCC	B	703	4	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
8	XCC	C	702	4	-	-	0/4/4/4
5	SF4	B	702	4	-	-	0/6/5/5
6	B12	F	502	-	-	9/56/223/223	0/3/11/11
5	SF4	C	701	4	-	-	0/6/5/5
5	SF4	F	501	1	-	-	0/6/5/5
5	SF4	B	701	4	-	-	0/6/5/5
5	SF4	D	801	2,7	-	-	0/6/5/5
8	XCC	B	703	4	-	-	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	502	B12	C2B-N1B	-2.40	1.33	1.37
6	F	502	B12	C14-N23	2.17	1.37	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	502	B12	C9B-C8B-N1B	4.15	107.10	105.35
6	F	502	B12	C8B-C9B-N3B	-2.19	107.55	109.97
6	F	502	B12	C3R-C2R-C1R	2.01	104.34	99.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	502	B12	O6R-C4R-C5R-O8R
6	F	502	B12	C3R-C4R-C5R-O8R
6	F	502	B12	C2R-C1R-N1B-C8B
6	F	502	B12	O6R-C1R-N1B-C8B
6	F	502	B12	C1P-C2P-O3-P
6	F	502	B12	C3P-C2P-O3-P
6	F	502	B12	C4-C3-C30-C31
6	F	502	B12	C42-C41-C8-C9
6	F	502	B12	C2P-O3-P-O2

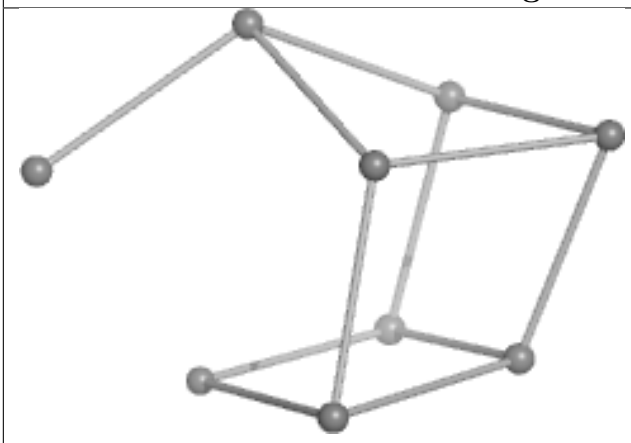
There are no ring outliers.

5 monomers are involved in 21 short contacts:

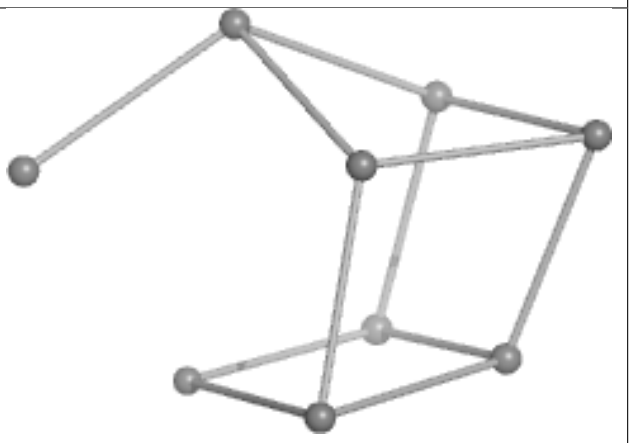
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	702	XCC	1	0
5	B	702	SF4	1	0
6	F	502	B12	17	0
5	C	701	SF4	1	0
8	B	703	XCC	1	0

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.

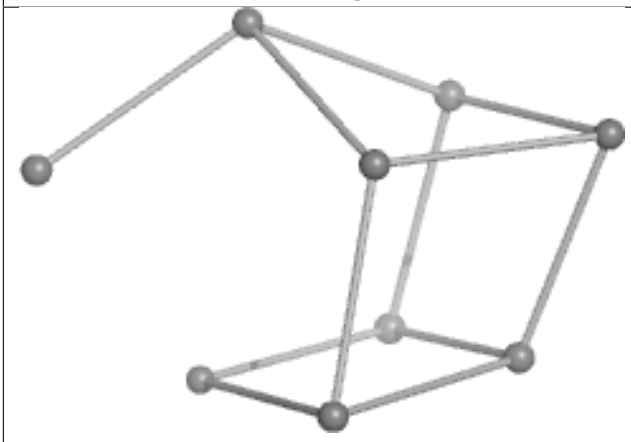
Ligand XCC C 702



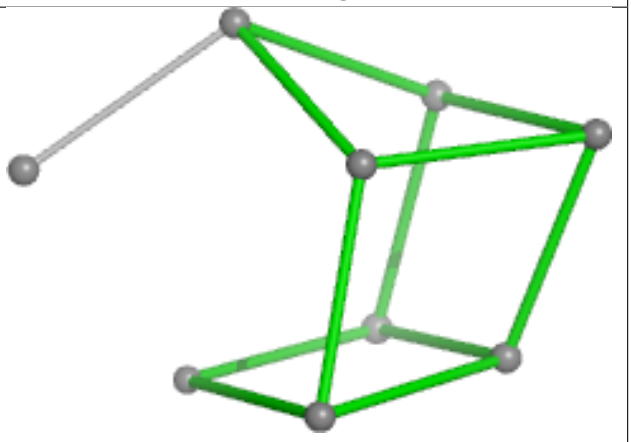
Bond lengths



Bond angles

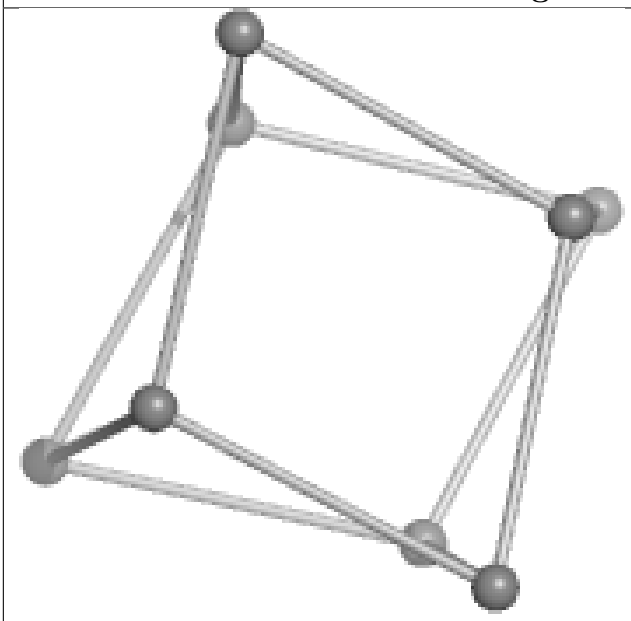


Torsions

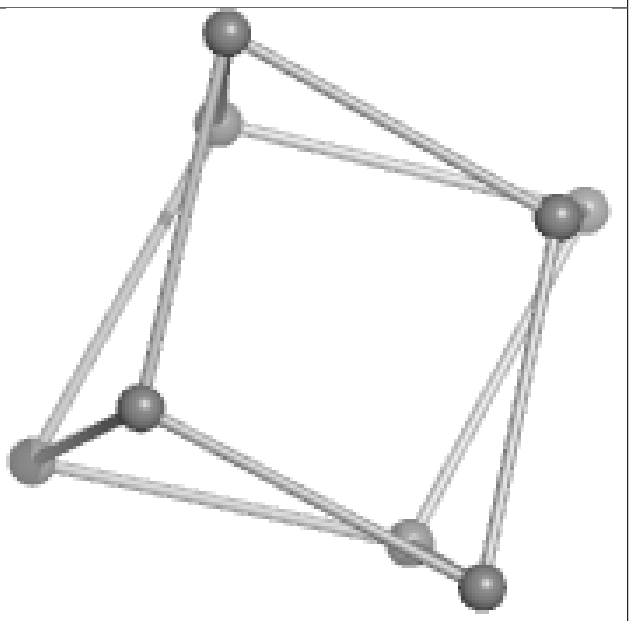


Rings

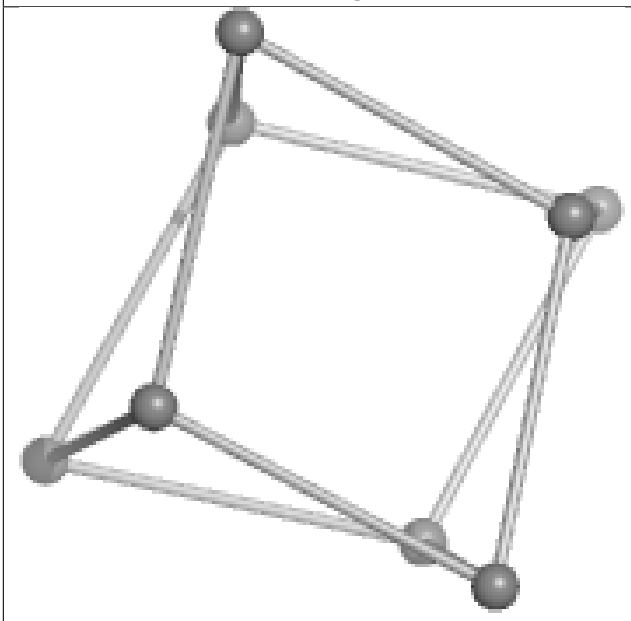
Ligand SF4 B 702



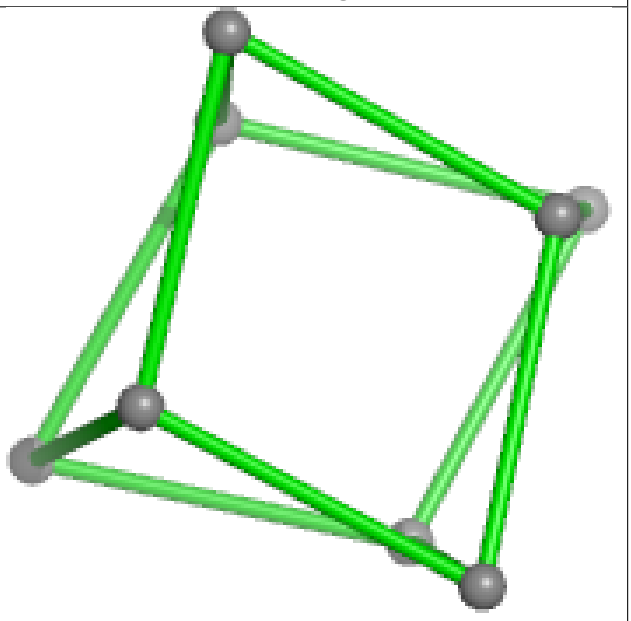
Bond lengths



Bond angles

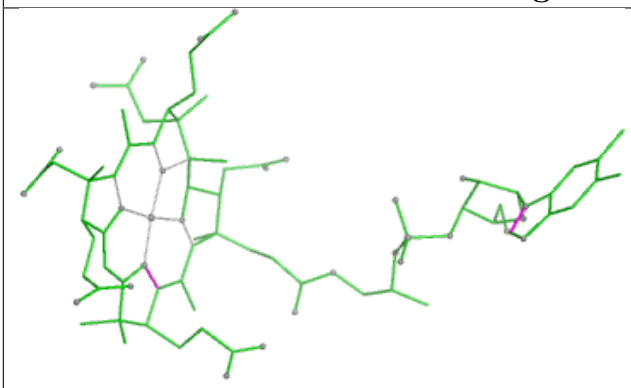


Torsions

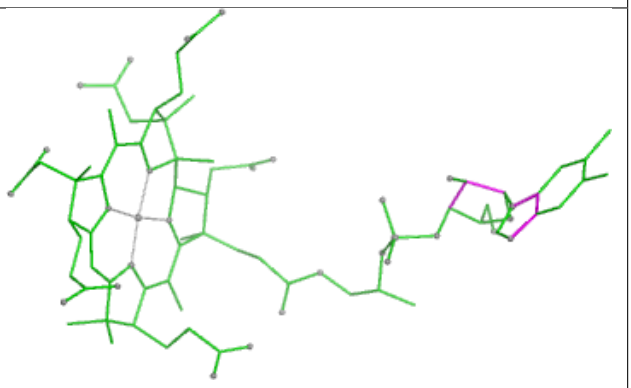


Rings

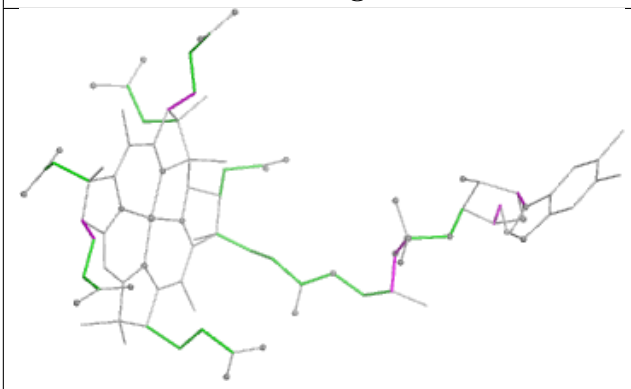
Ligand B12 F 502



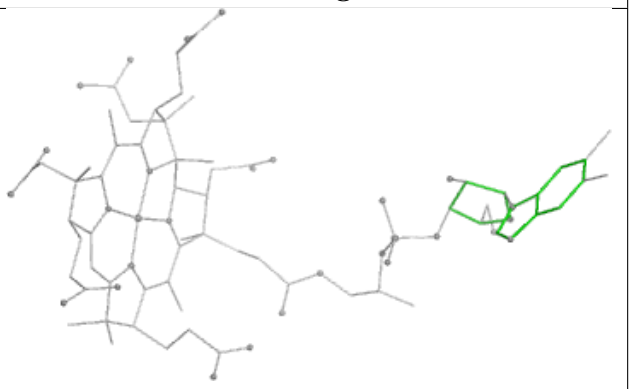
Bond lengths



Bond angles

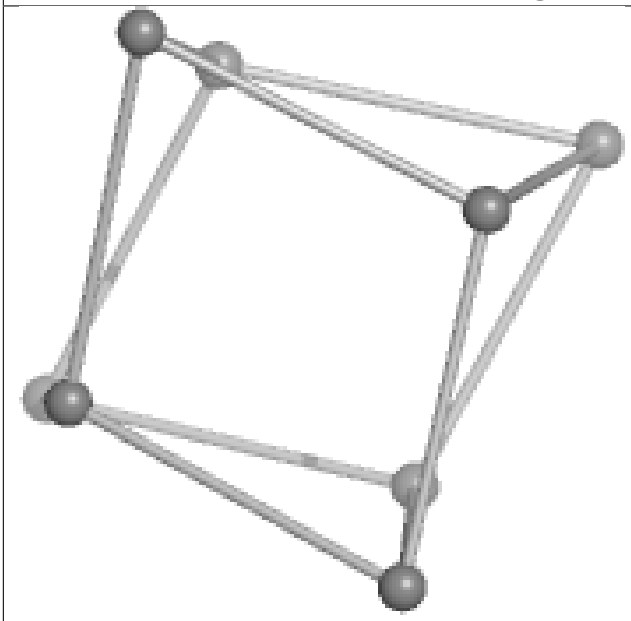


Torsions

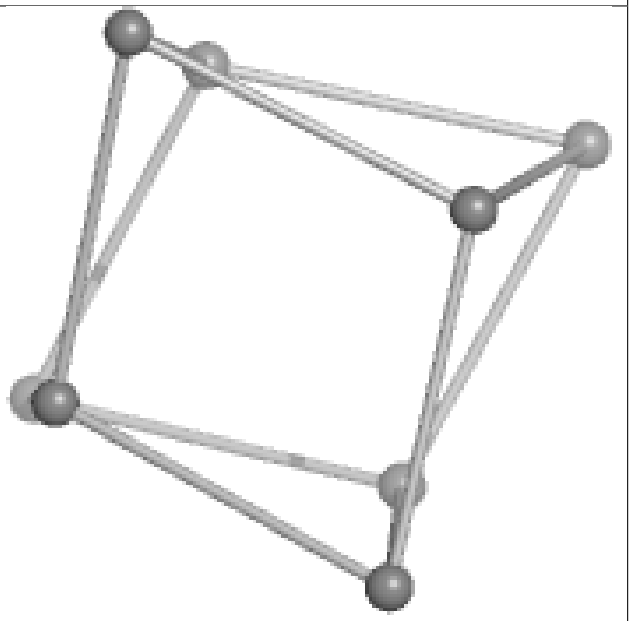


Rings

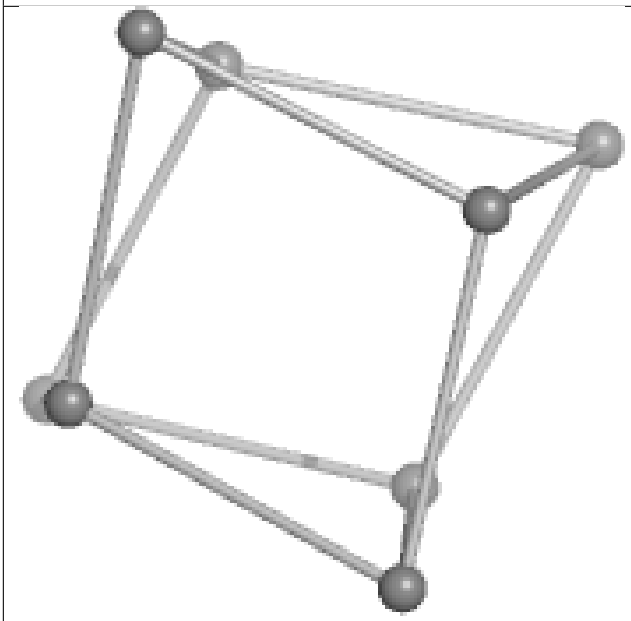
Ligand SF4 C 701



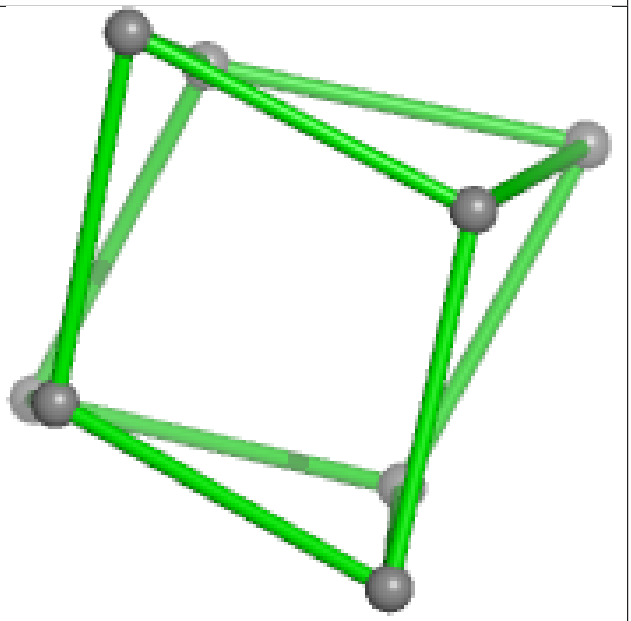
Bond lengths



Bond angles

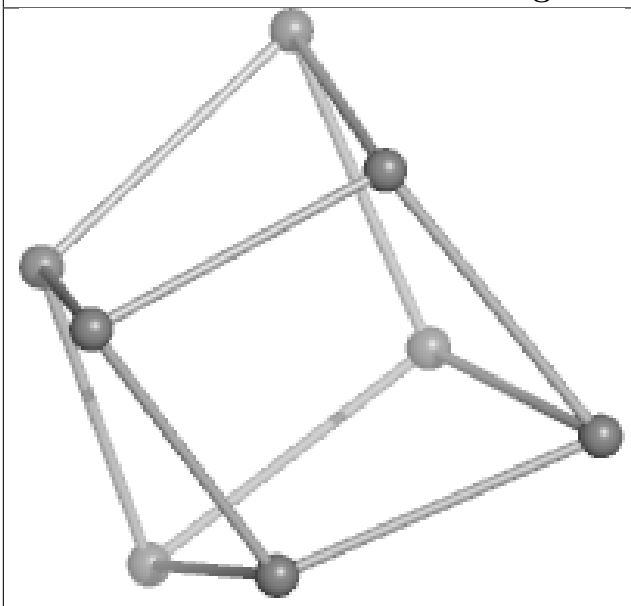


Torsions

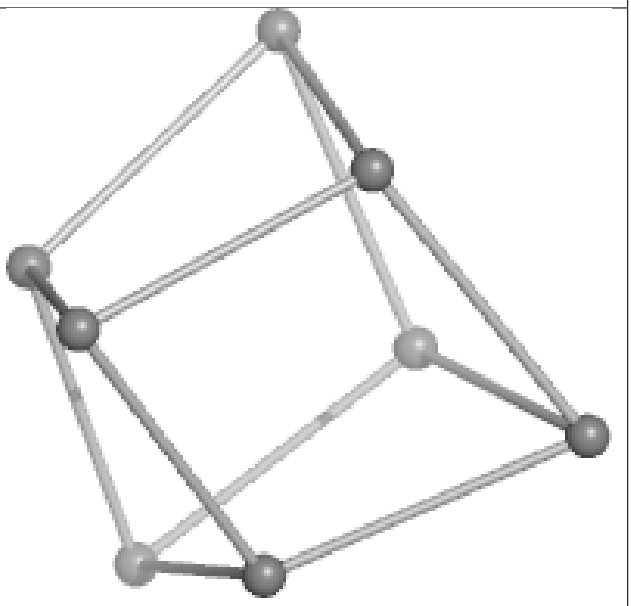


Rings

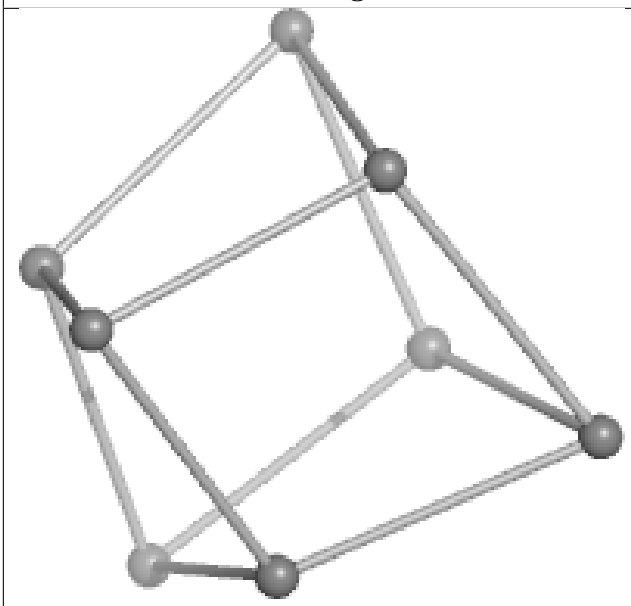
Ligand SF4 F 501



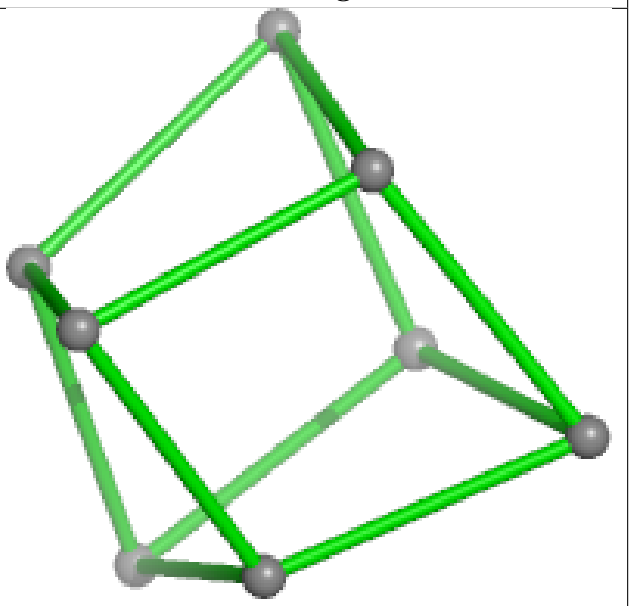
Bond lengths



Bond angles

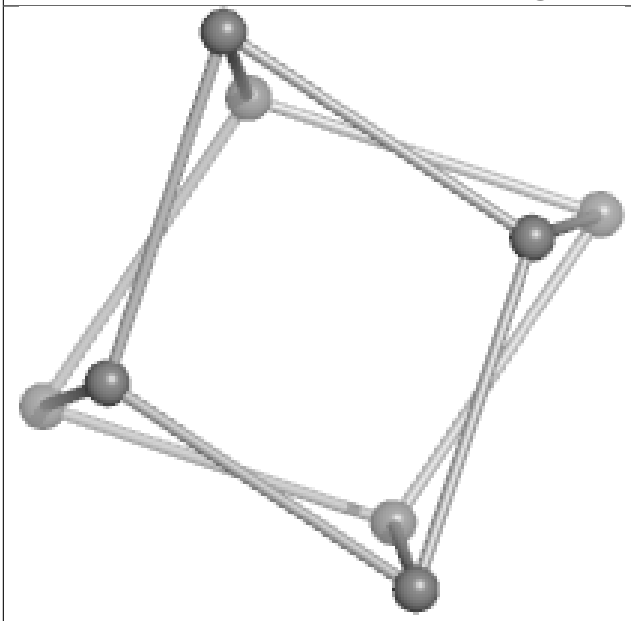


Torsions

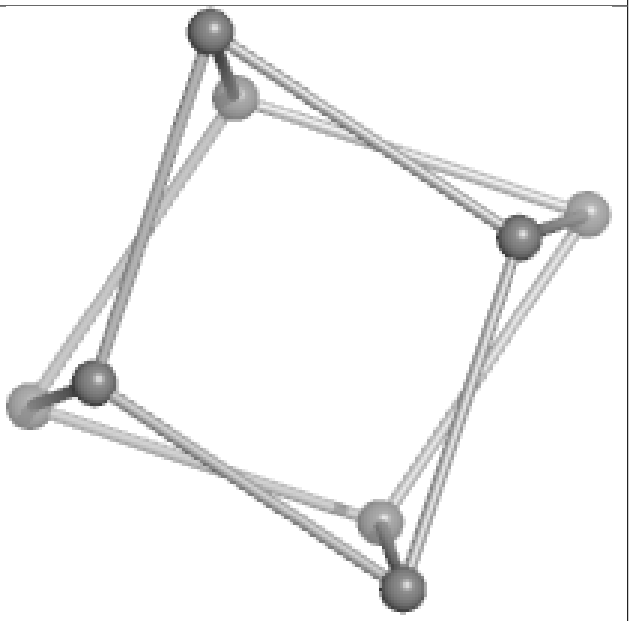


Rings

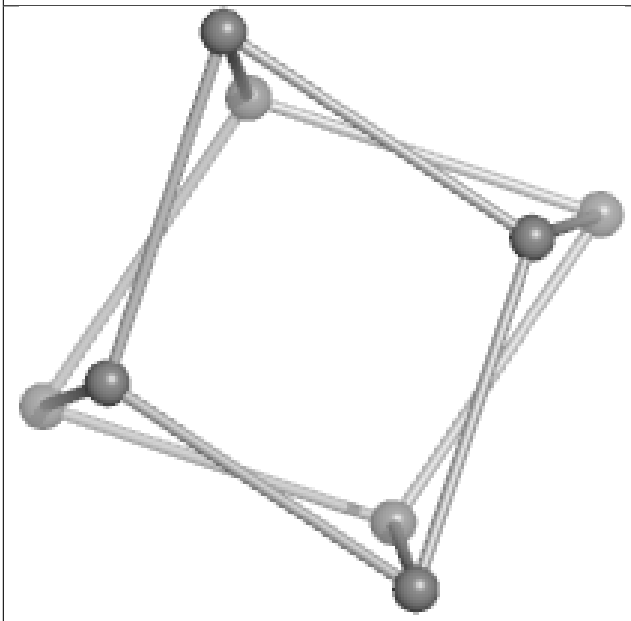
Ligand SF4 B 701



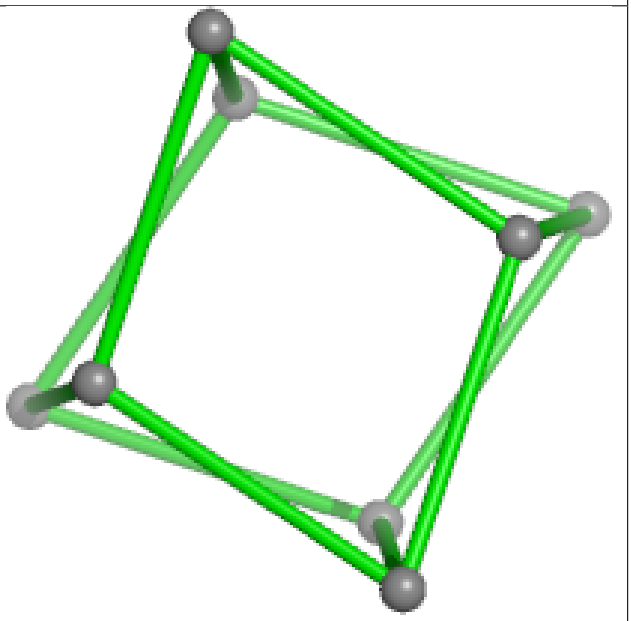
Bond lengths



Bond angles

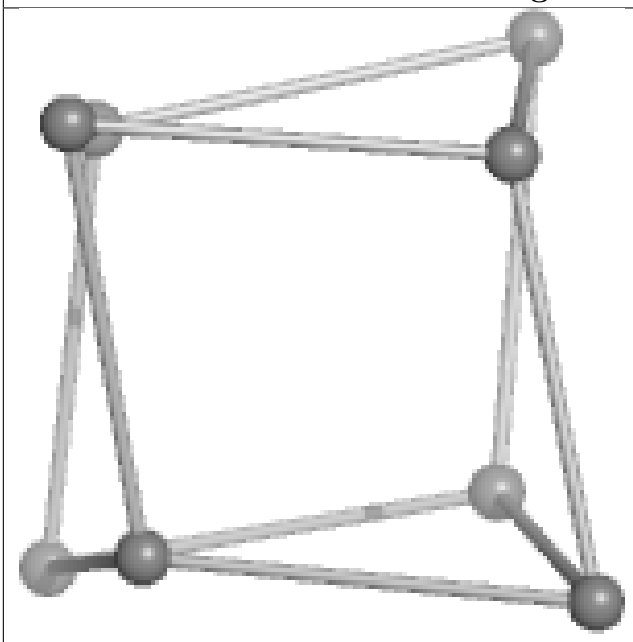


Torsions

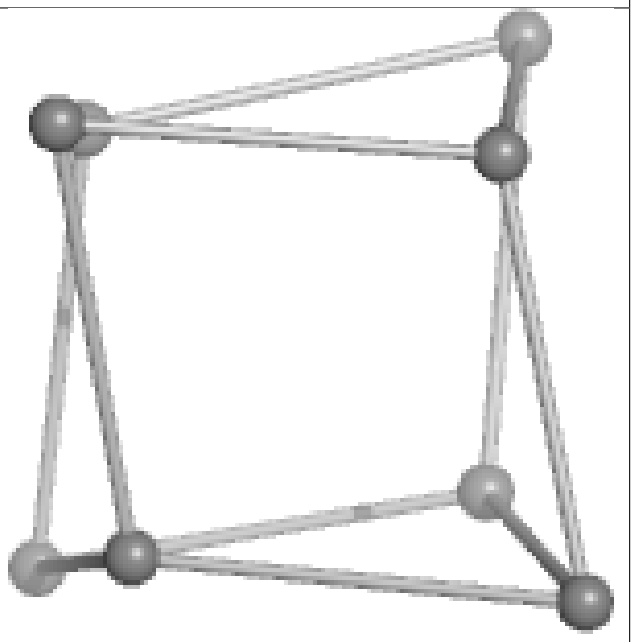


Rings

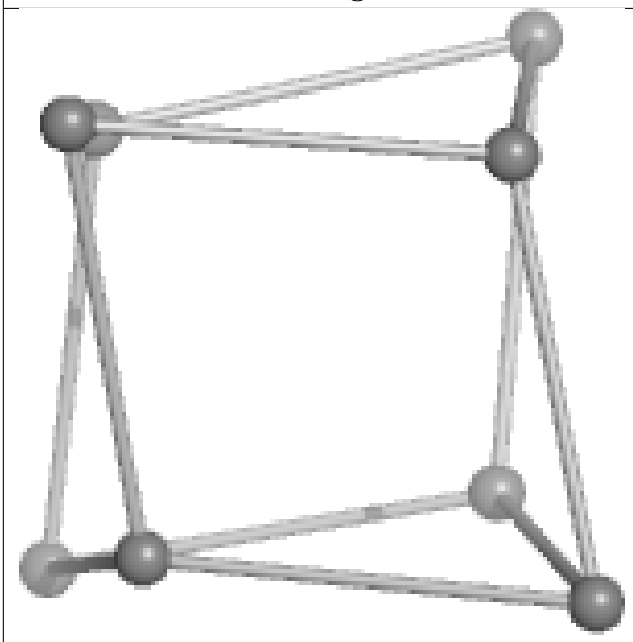
Ligand SF4 D 801



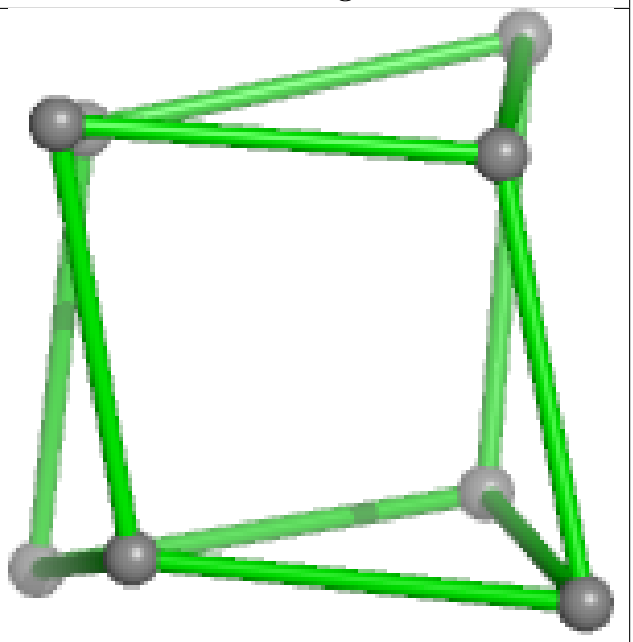
Bond lengths



Bond angles

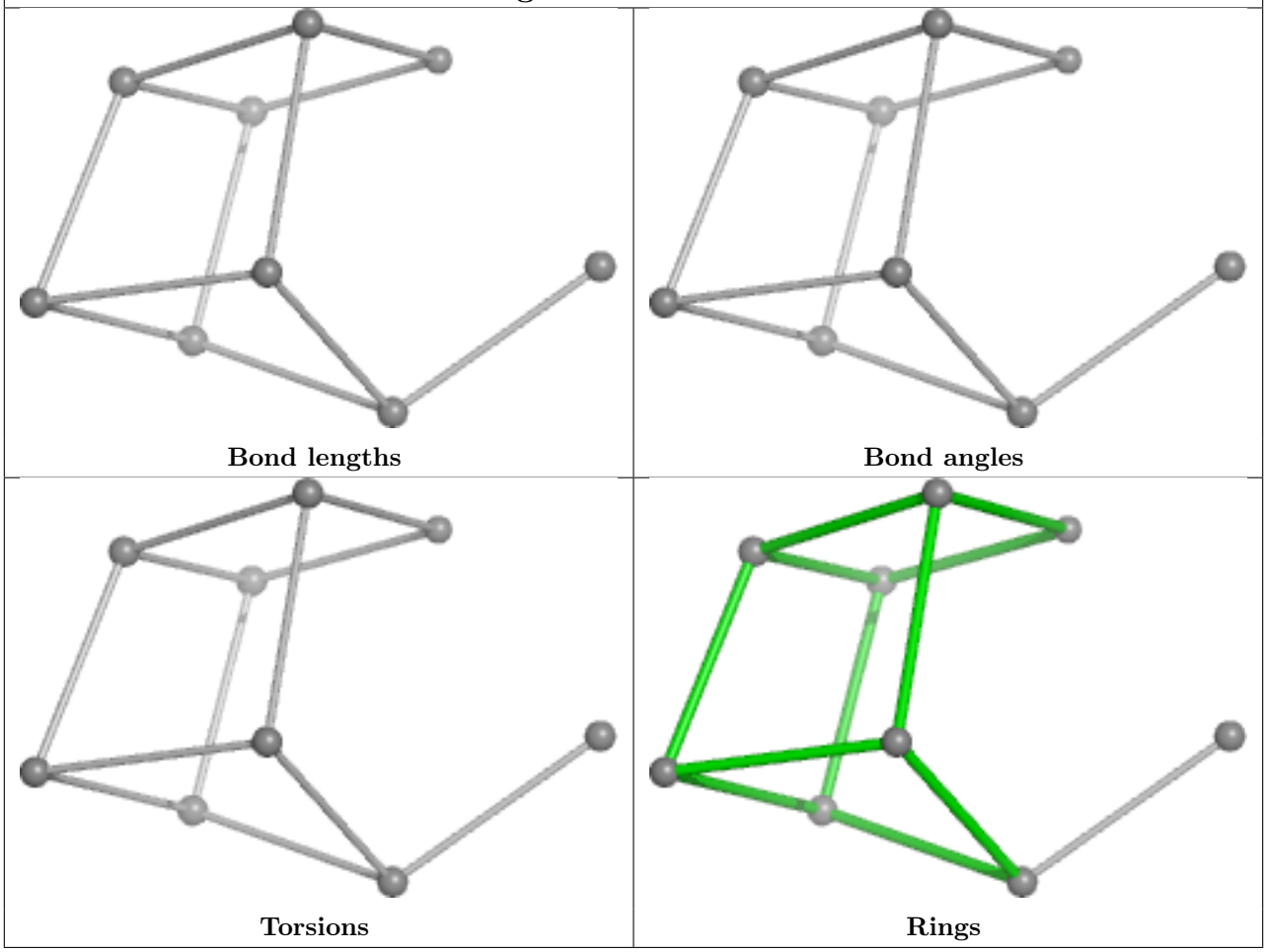


Torsions



Rings

Ligand XCC B 703



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.

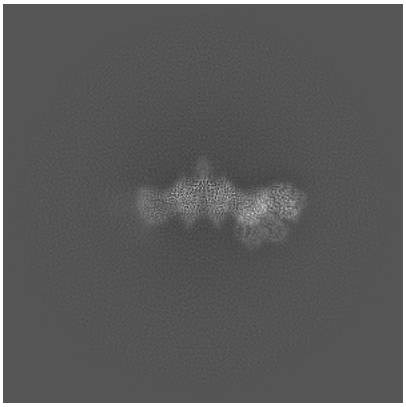
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50897. These allow visual inspection of the internal detail of the map and identification of artifacts.

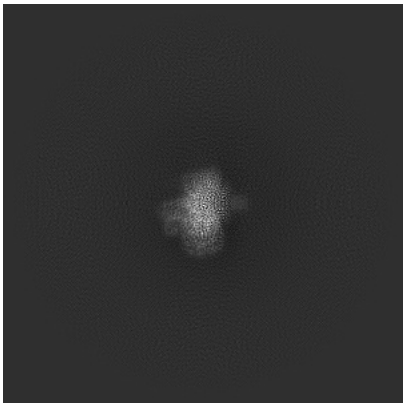
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

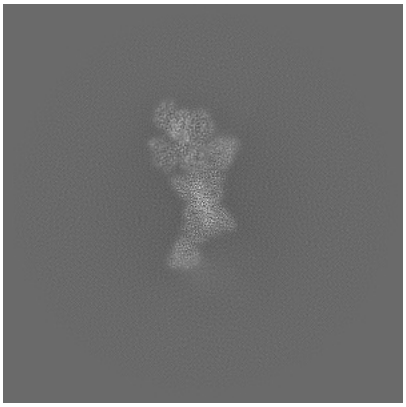
6.1.1 Primary map



X



Y

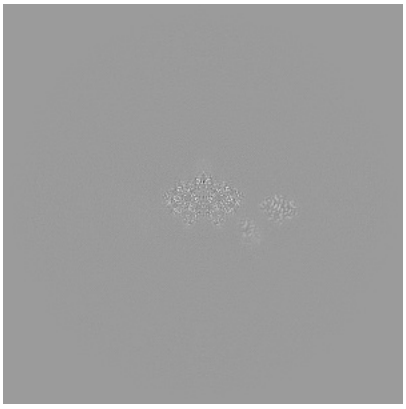


Z

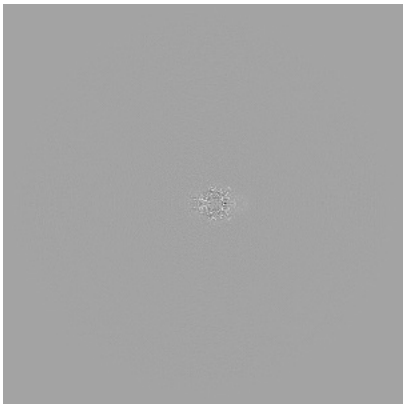
The images above show the map projected in three orthogonal directions.

6.2 Central slices

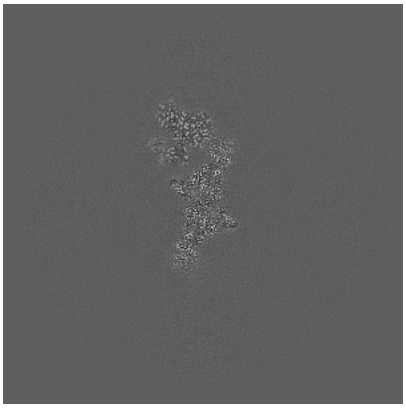
6.2.1 Primary map



X Index: 280



Y Index: 280



Z Index: 280

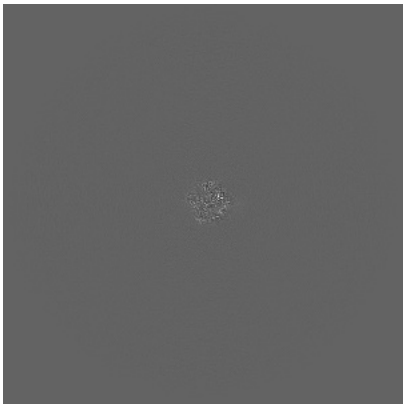
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

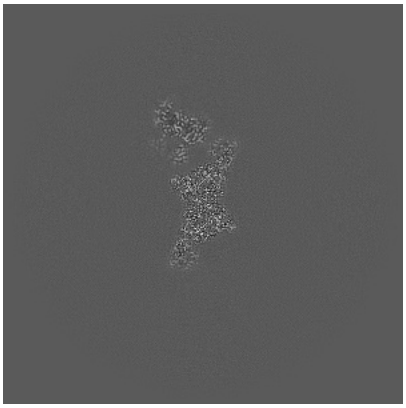
6.3.1 Primary map



X Index: 272



Y Index: 270

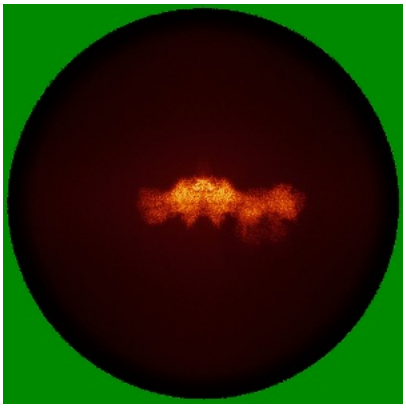


Z Index: 287

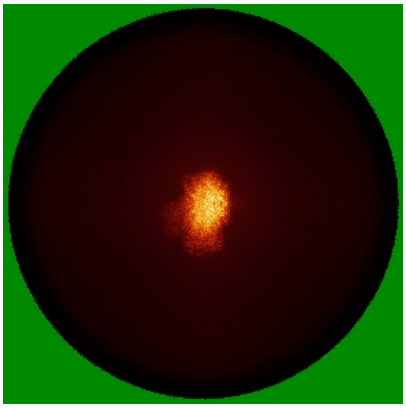
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

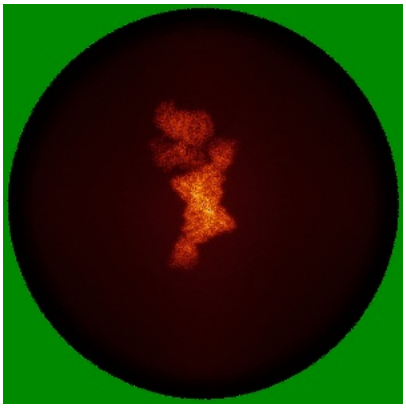
6.4.1 Primary map



X



Y

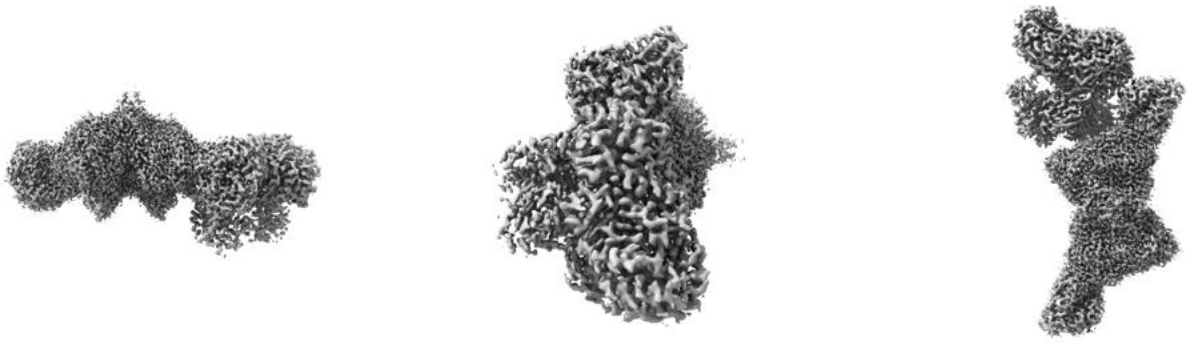


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 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.

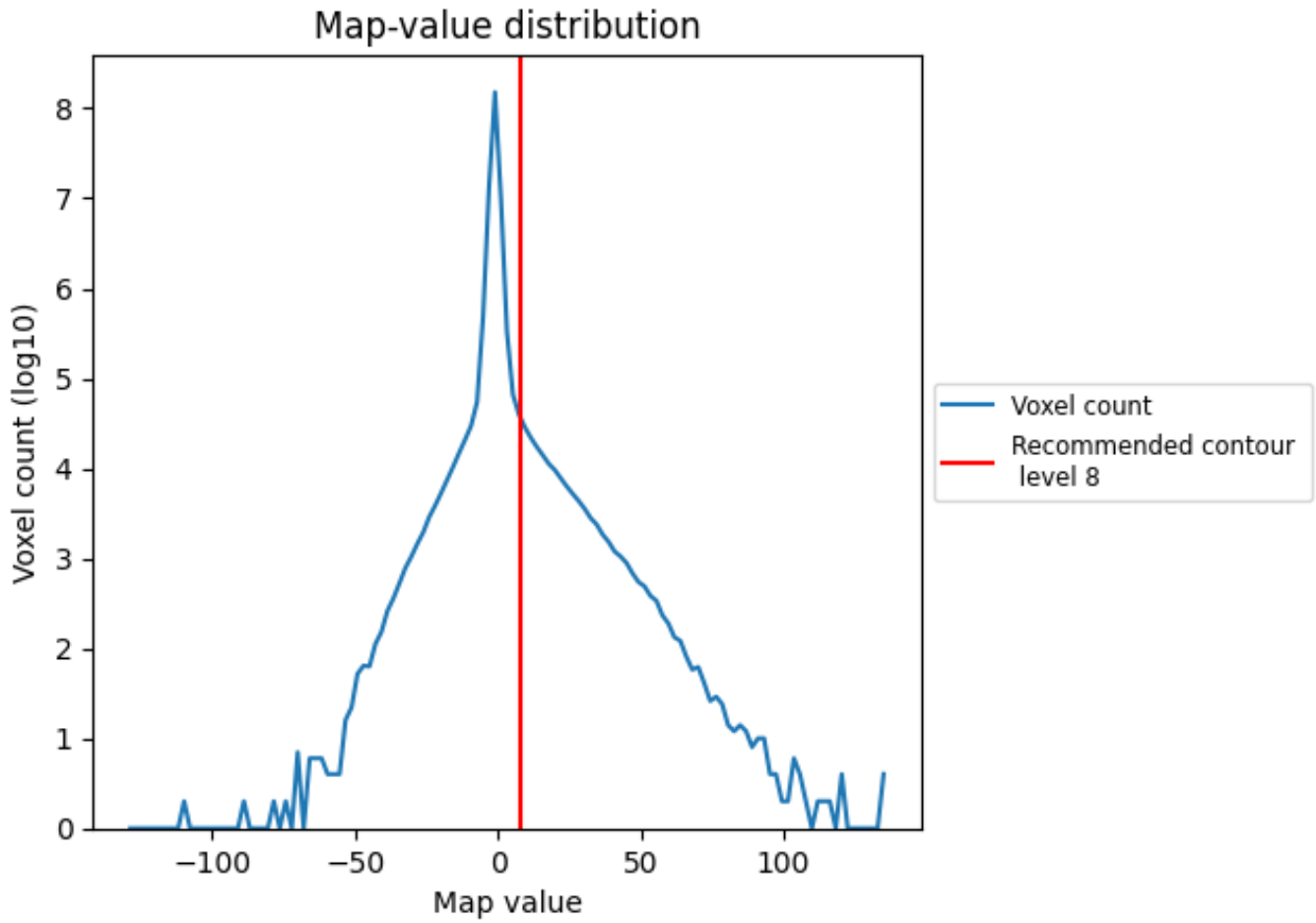
6.6 Mask visualisation (i)

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

7 Map analysis

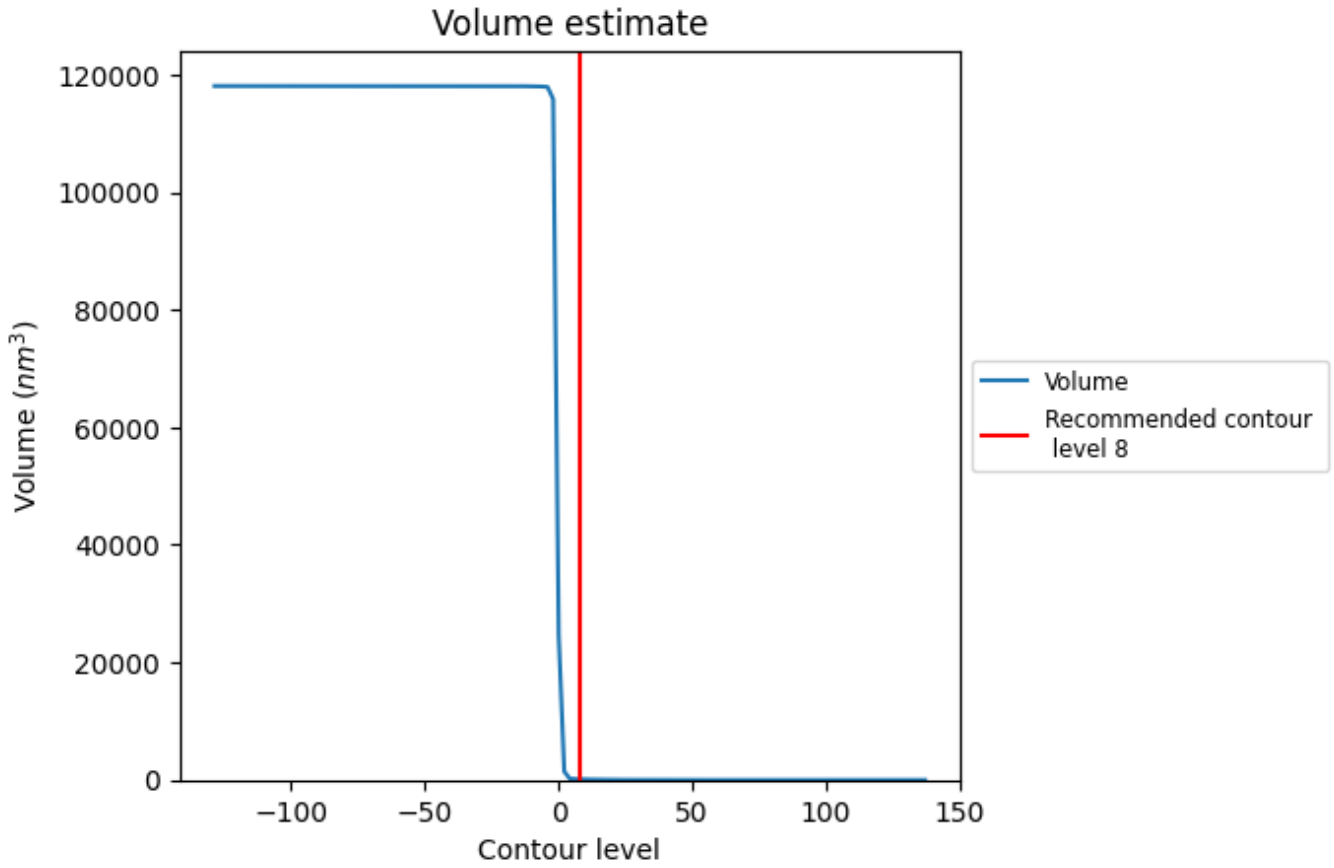
This section contains the results of statistical analysis of the map.

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.

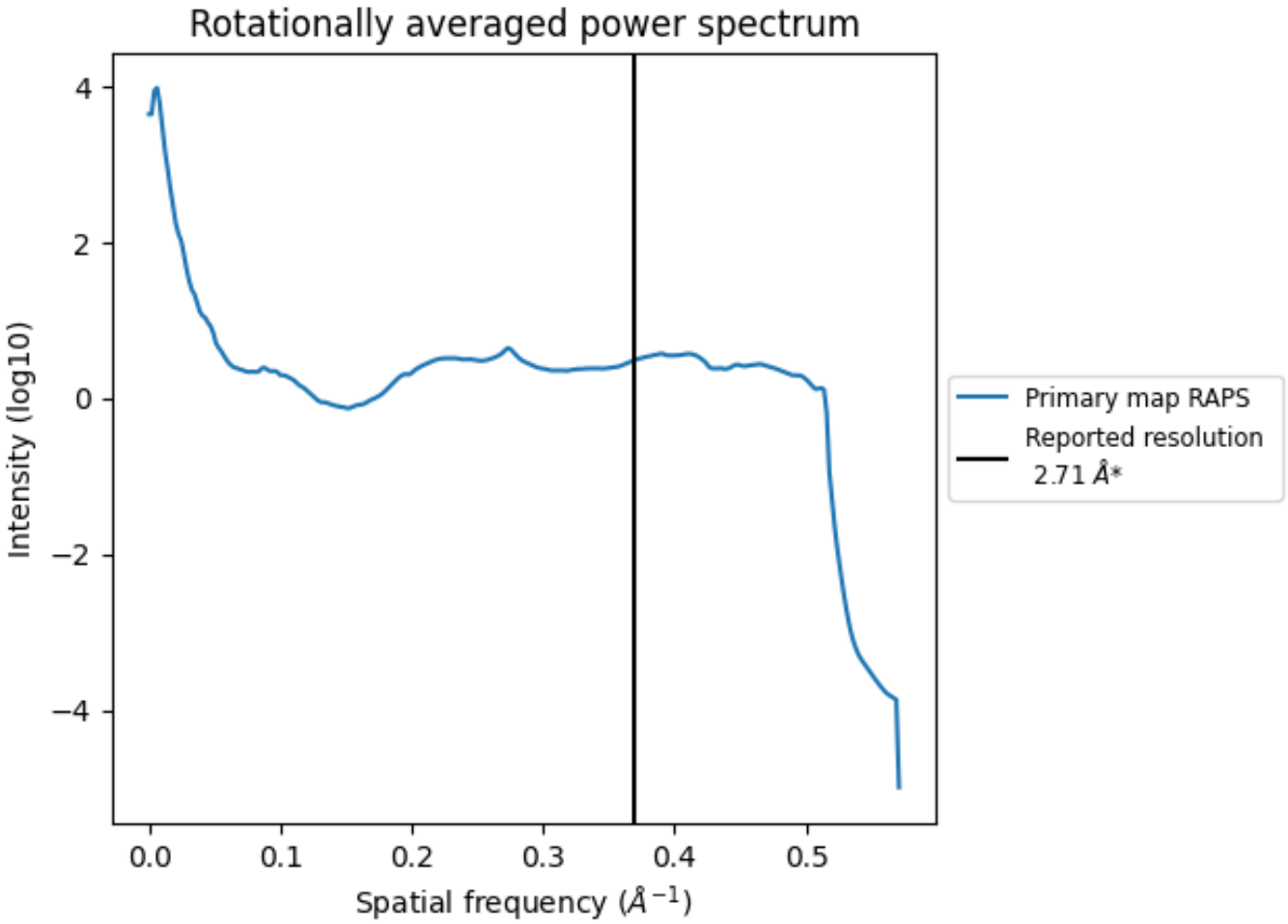
7.2 Volume estimate



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 105 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 0.369 Å^{-1}

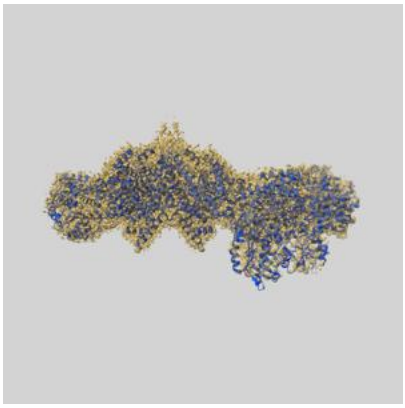
8 Fourier-Shell correlation

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

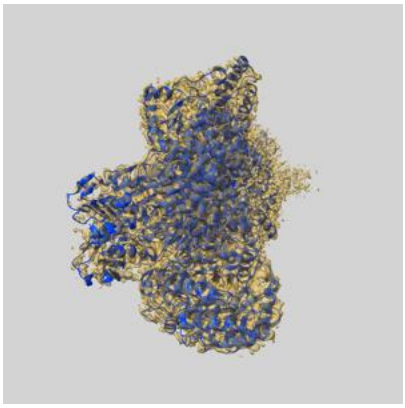
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50897 and PDB model 9FZY. Per-residue inclusion information can be found in section 3 on page 8.

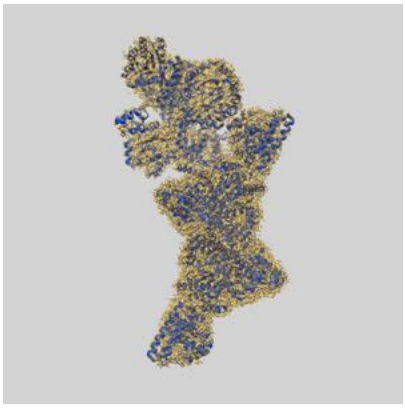
9.1 Map-model overlay



X



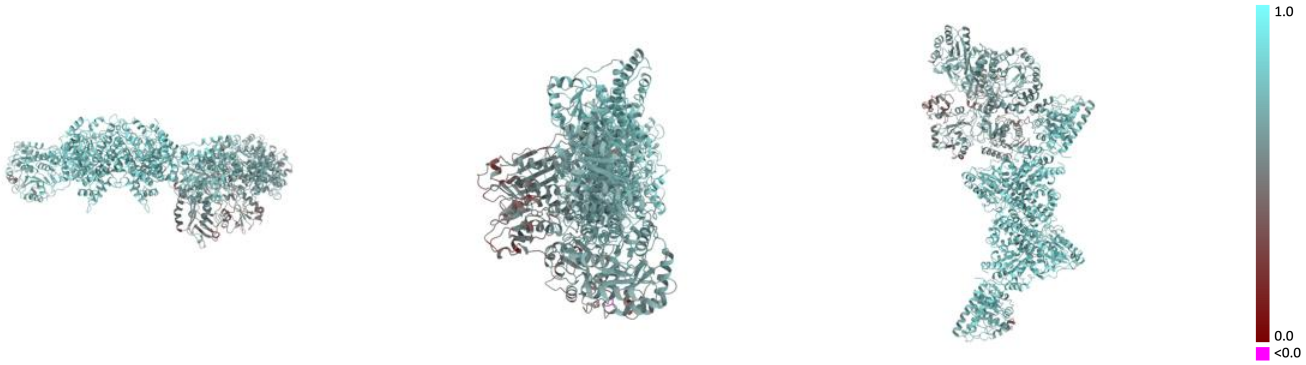
Y



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.

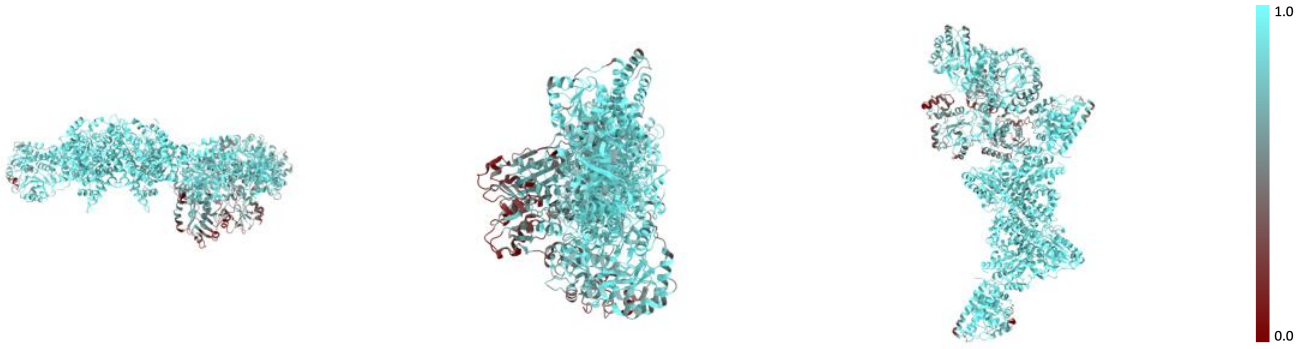
9.2 Q-score mapped to coordinate model (i)



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.

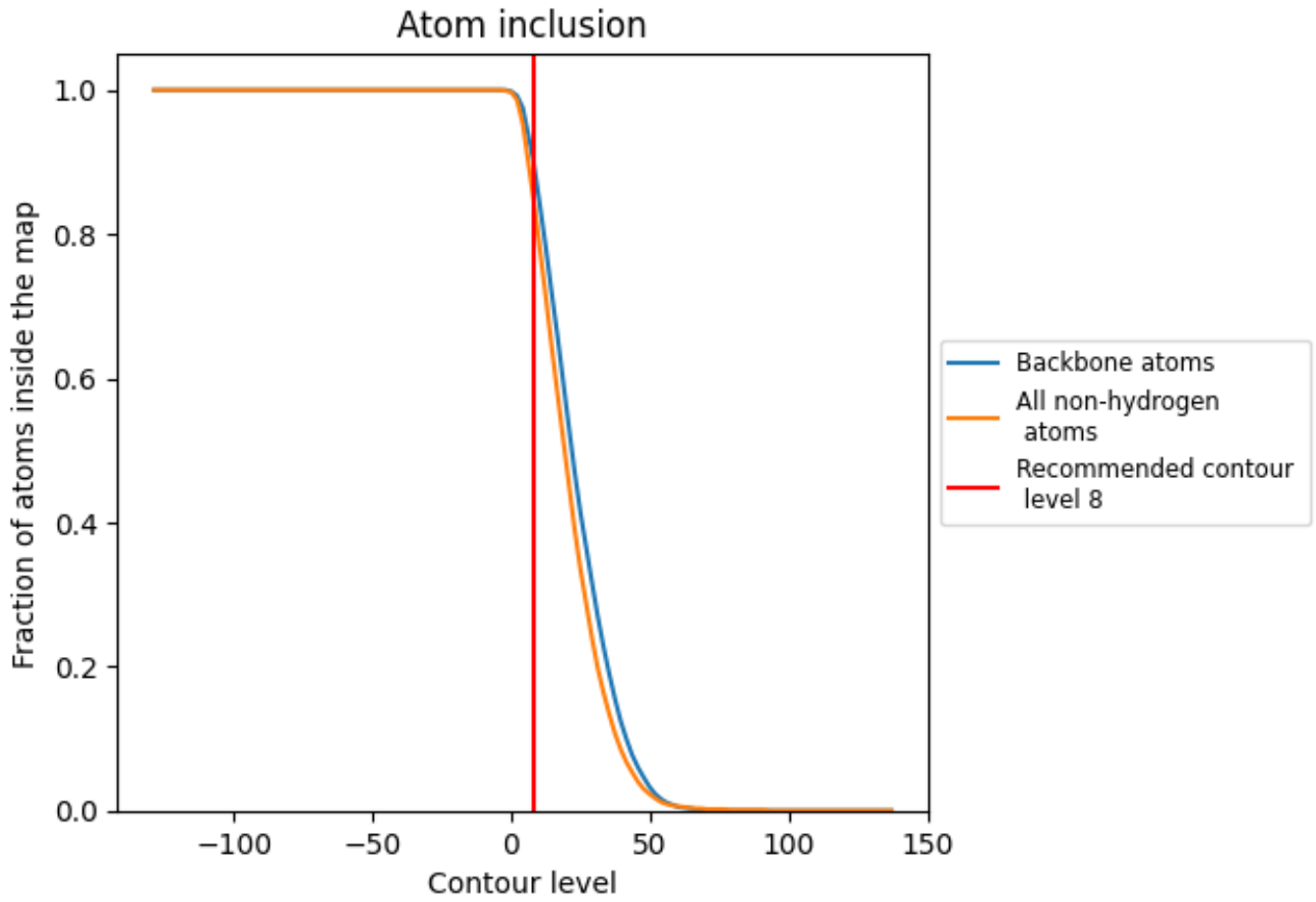
9.3 Atom inclusion mapped to coordinate model (i)



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 (8).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.6730
A	0.8840	0.6970
B	0.9690	0.7610
C	0.9670	0.7610
D	0.7490	0.6120
E	0.8480	0.6200
F	0.6840	0.5540

