Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 05:20 pm BST

PDB ID	:	9FZZ / pdb_00009fzz
EMDB ID	:	EMD-50900
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 3B)
Authors	:	Yin, M.D.; Lemaire, O.N.; Wagner, T.; Murphy, B.J.
Deposited on	:	2024-07-06
Resolution	:	2.65 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:

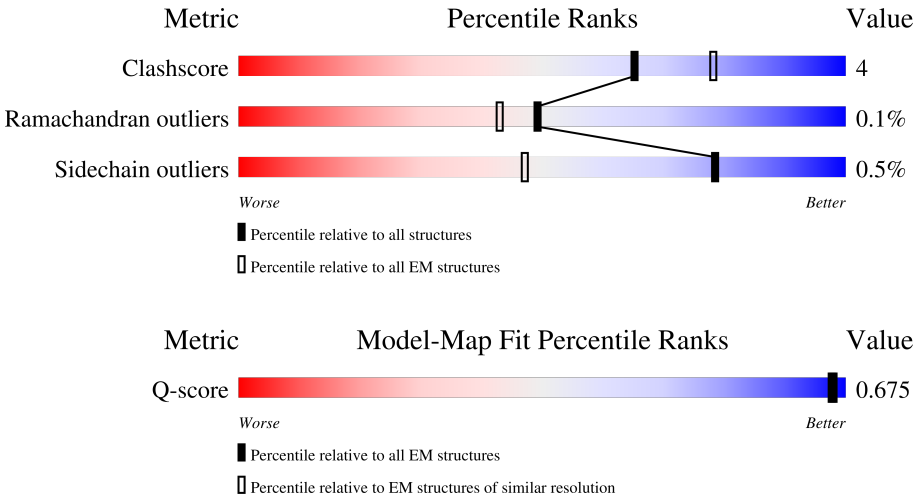
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.65 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.



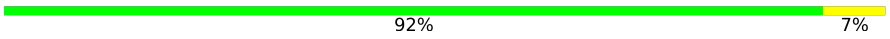
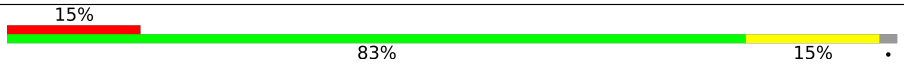
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9050 (2.15 - 3.15)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	708	39% 59%
1	D	708	11% 87% 13%
2	E	314	86% 13%
3	B	630	94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	630	
4	F	450	

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 CO-methylating acetyl-CoA synthase.

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

- Molecule 2 is a protein called Acetyl-CoA decarbonylase/synthase complex subunit delta.

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

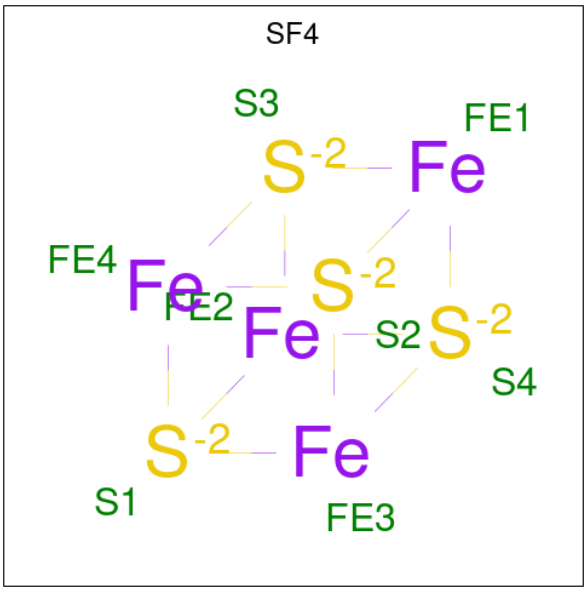
- Molecule 3 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit.

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

- Molecule 4 is a protein called Corrinoid iron-sulfur protein large subunit.

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

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

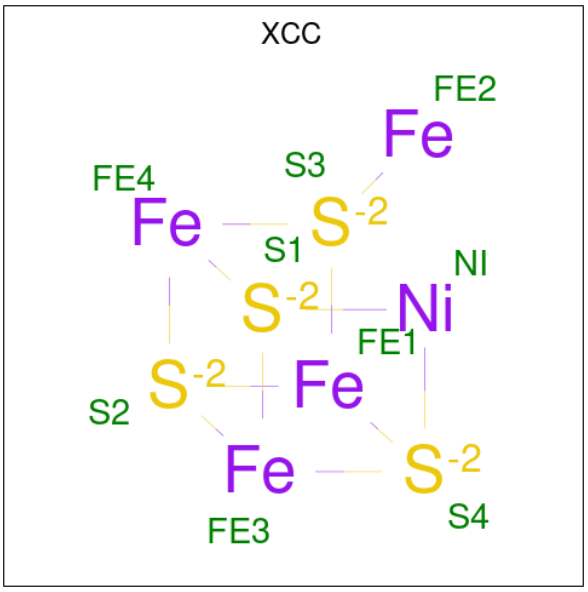


Mol	Chain	Residues	Atoms	AltConf
5	D	1	Total Fe S 8 4 4	0
5	B	1	Total Fe S 8 4 4	0
5	B	1	Total Fe S 8 4 4	0
5	C	1	Total Fe S 8 4 4	0
5	F	1	Total Fe S 8 4 4	0

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

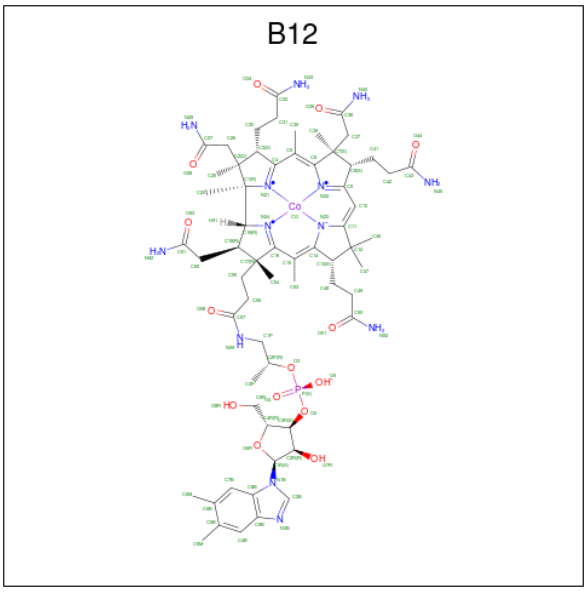
Mol	Chain	Residues	Atoms	AltConf
6	D	2	Total Ni 2 2	0

- Molecule 7 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
7	B	1	Total 9	Fe 4	Ni 1	S 4	0
7	C	1	Total 9	Fe 4	Ni 1	S 4	0

- Molecule 8 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).

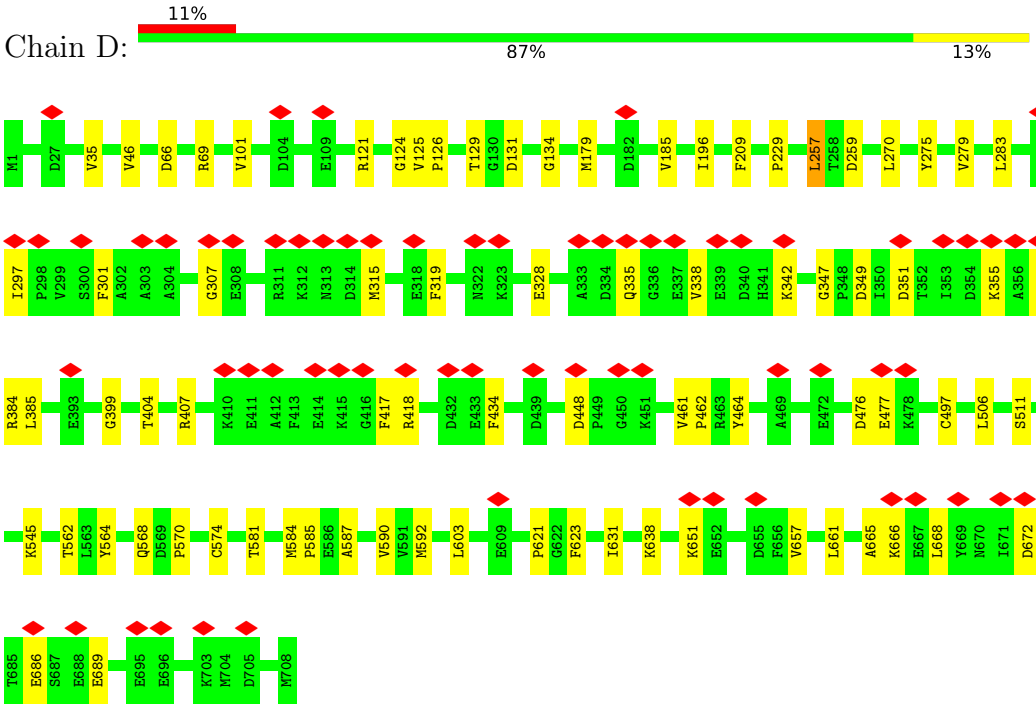


Mol	Chain	Residues	Atoms						AltConf
8	F	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0

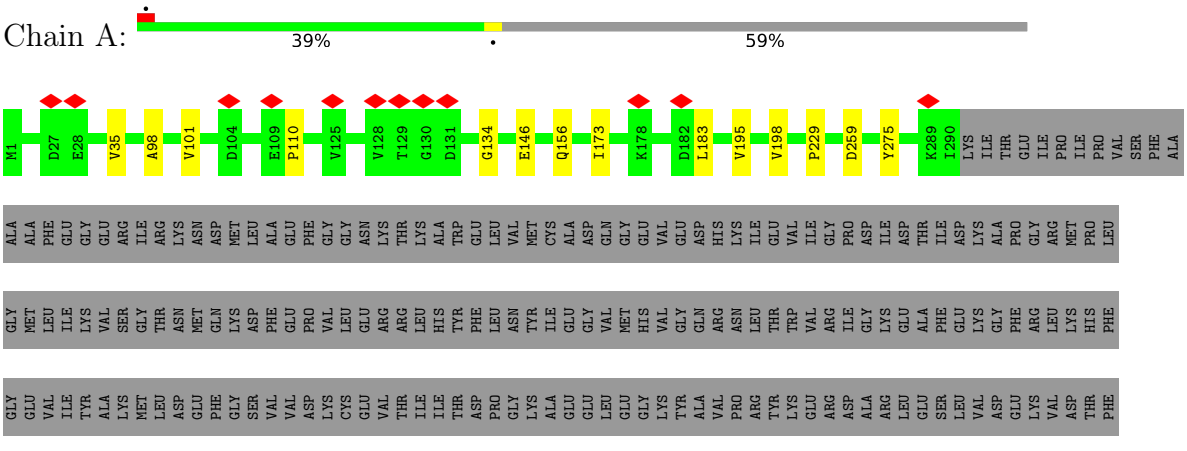
3 Residue-property plots (i)

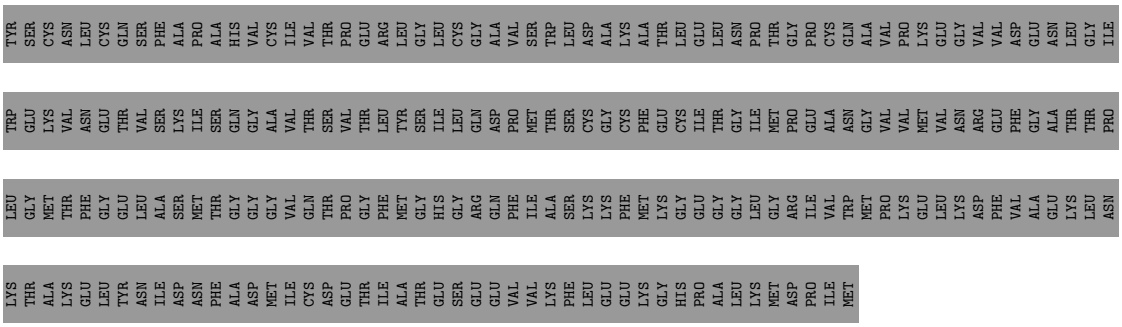
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



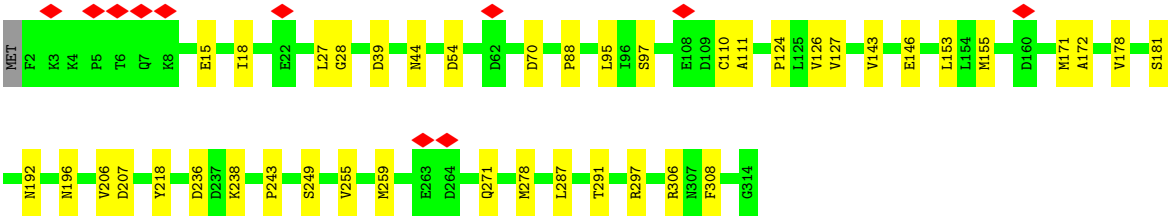
• Molecule 1: CO-methylating acetyl-CoA synthase





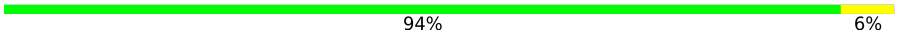
• Molecule 2: Acetyl-CoA decarbonylase/synthase complex subunit delta

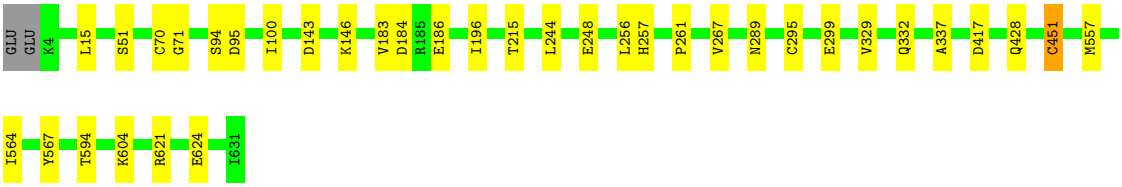
Chain E:



• Molecule 3: Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit

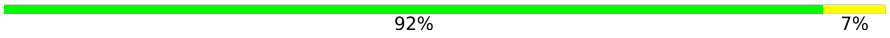
Chain B:

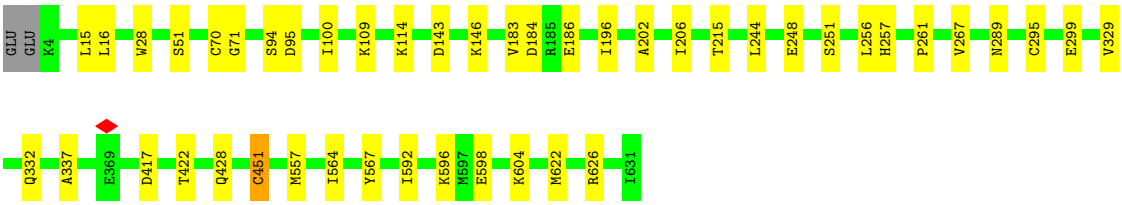




• Molecule 3: Carbon monoxide dehydrogenase/acetyl-CoA synthase beta subunit

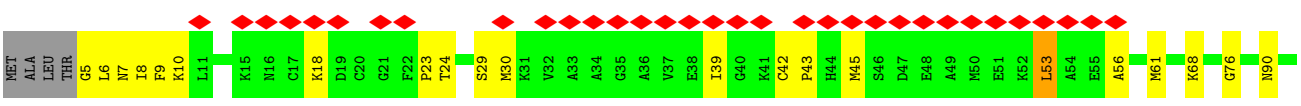
Chain C:

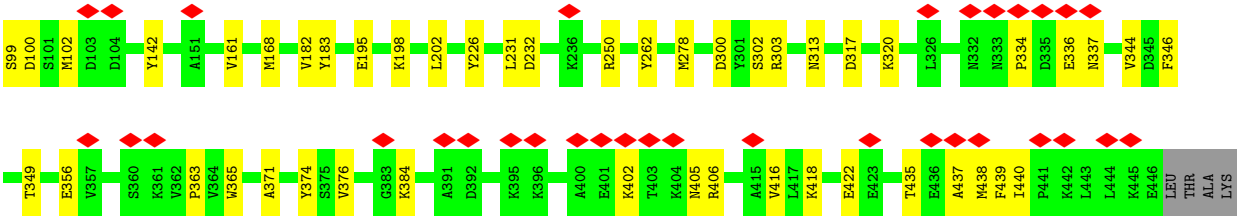




• Molecule 4: Corrinoid iron-sulfur protein large subunit

Chain F:




S99
D100
S101
M102
D103
D104
Y142
A151
V161
M168
V182
Y183
E195
K198
L202
Y226
L231
D232
K236
R250
Y262
M278
D300
Y301
S302
R303
N313
D317
K320
L326
N332
N333
P334
D335
E336
N337
V344
D345
F346
T349
E356
V357
S360
K361
V362
P363
V364
W365
A371
Y374
S375
V376
G383
K384
A391
D392
K395
K396
A400
E401
K402
T403
K404
N405
R406
A415
V416
L417
K418
E422
E423
T435
E436
A437
M438
F439
I440
P441
K442
L443
L444
K445
E446
LEU
THR
ALA
LYS

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	1.050	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: NI, B12, SF4, XCC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/2185	0.36	0/2970
1	D	0.29	0/5488	0.34	0/7428
2	E	0.25	0/2420	0.33	0/3279
3	B	0.37	0/4788	0.45	0/6476
3	C	0.37	0/4788	0.44	0/6476
4	F	0.29	0/3480	0.38	0/4698
All	All	0.32	0/23149	0.39	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	A	2154	0	2264	8	0
1	D	5392	0	5489	57	0
2	E	2379	0	2368	23	0
3	B	4714	0	4797	23	0
3	C	4714	0	4797	29	0
4	F	3420	0	3503	49	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	1	0
6	D	2	0	0	0	0
7	B	9	0	0	1	0
7	C	9	0	0	1	0
8	F	91	0	88	11	0
All	All	22924	0	23306	183	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 (183) 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)
3:C:451:CYS:HB3	7:C:702:XCC:S2	2.29	0.73
3:B:451:CYS:HB3	7:B:703:XCC:S2	2.29	0.72
8:F:502:B12:H301	8:F:502:B12:H203	1.73	0.71
2:E:259:MET:O	2:E:271:GLN:NE2	2.28	0.67
8:F:502:B12:H203	8:F:502:B12:C30	2.25	0.66
3:B:196:ILE:HD13	5:B:702:SF4:S1	2.36	0.65
3:C:196:ILE:HD13	5:C:701:SF4:S3	2.37	0.65
4:F:202:LEU:O	4:F:226:TYR:OH	2.12	0.65
4:F:183:TYR:OH	4:F:232:ASP:OD2	2.14	0.65
4:F:334:PRO:HA	4:F:363:PRO:HB3	1.78	0.64
2:E:192:ASN:O	2:E:196:ASN:ND2	2.30	0.63
4:F:39:ILE:HD12	4:F:53:LEU:HD12	1.82	0.62
1:D:657:VAL:HG12	1:D:661:LEU:HB2	1.84	0.60
4:F:344:VAL:HG21	4:F:376:VAL:HA	1.82	0.59
1:D:121:ARG:NH1	2:E:172:ALA:O	2.36	0.59
4:F:61:MET:HE2	4:F:76:GLY:HA2	1.84	0.59
4:F:365:TRP:CD1	4:F:402:LYS:HD2	2.38	0.59
3:B:257:HIS:HB3	3:B:329:VAL:HG12	1.85	0.59
4:F:8:ILE:HD11	4:F:29:SER:O	2.02	0.58
1:D:476:ASP:OD2	1:D:564:TYR:OH	2.21	0.58
1:D:581:THR:HG23	1:D:590:VAL:CG2	2.33	0.57
4:F:300:ASP:OD2	4:F:303:ARG:NH1	2.38	0.57
8:F:502:B12:H361	8:F:502:B12:H422	1.87	0.57
1:D:399:GLY:HA3	1:D:404:THR:HA	1.86	0.56
1:A:110:PRO:HG3	1:A:173:ILE:HD11	1.87	0.56
3:C:257:HIS:HB3	3:C:329:VAL:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:236:ASP:OD2	2:E:238:LYS:NZ	2.40	0.55
1:D:666:LYS:NZ	1:D:672:ASP:OD1	2.37	0.55
4:F:418:LYS:NZ	4:F:422:GLU:OE2	2.40	0.55
1:D:417:PHE:O	1:D:418:ARG:NE	2.37	0.54
1:D:542:ILE:HG12	1:D:562:THR:HG22	1.90	0.54
1:D:129:THR:OG1	1:D:131:ASP:OD1	2.24	0.54
3:C:15:LEU:HD12	3:C:244:LEU:HD13	1.90	0.53
3:B:15:LEU:HD12	3:B:244:LEU:HD13	1.90	0.53
4:F:8:ILE:HG22	4:F:53:LEU:HD11	1.90	0.53
4:F:337:ASN:HA	4:F:405:ASN:HB2	1.91	0.53
4:F:8:ILE:CG2	4:F:53:LEU:HD11	2.39	0.53
1:D:686:GLU:HB3	1:D:689:GLU:HG2	1.90	0.53
4:F:99:SER:HB3	4:F:102:MET:HG3	1.91	0.53
4:F:438:MET:HE2	4:F:439:PHE:CZ	2.44	0.53
1:D:511:SER:H	1:D:514:ASP:HB2	1.73	0.52
3:C:417:ASP:OD2	3:C:428:GLN:NE2	2.41	0.52
1:D:134:GLY:HA2	1:D:229:PRO:HG2	1.92	0.52
4:F:43:PRO:HD2	5:F:501:SF4:S2	2.50	0.52
8:F:502:B12:H533	8:F:502:B12:H482	1.91	0.52
1:A:146:GLU:OE1	1:A:146:GLU:N	2.40	0.52
4:F:231:LEU:HG	4:F:262:TYR:HB2	1.92	0.52
1:D:374:GLN:OE1	1:D:516:LYS:NZ	2.44	0.51
2:E:18:ILE:HG22	2:E:124:PRO:HB3	1.93	0.51
4:F:300:ASP:OD1	4:F:302:SER:OG	2.20	0.50
2:E:206:VAL:HG12	2:E:243:PRO:HG2	1.92	0.50
1:D:564:TYR:HB3	1:D:638:LYS:HB3	1.93	0.50
2:E:111:ALA:HB1	2:E:146:GLU:HG3	1.93	0.50
4:F:76:GLY:O	4:F:90:ASN:ND2	2.35	0.49
3:B:100:ILE:HD11	3:B:261:PRO:HD2	1.94	0.49
1:D:209:PHE:HD1	2:E:171:MET:HB3	1.77	0.49
2:E:15:GLU:HA	2:E:27:LEU:O	2.12	0.48
2:E:95:LEU:HD13	2:E:110:CYS:HB3	1.94	0.48
3:B:183:VAL:HG22	3:B:215:THR:HB	1.95	0.48
3:B:295:CYS:O	3:B:299:GLU:HG2	2.14	0.48
2:E:287:LEU:HA	2:E:291:THR:HG22	1.94	0.48
3:B:417:ASP:OD2	3:B:428:GLN:NE2	2.45	0.48
1:D:581:THR:HG23	1:D:590:VAL:HG21	1.95	0.48
1:D:477:GLU:OE1	1:D:477:GLU:N	2.37	0.48
1:D:584:MET:HE2	1:D:587:ALA:HB2	1.95	0.48
4:F:42:CYS:SG	4:F:45:MET:HG2	2.54	0.48
3:B:621:ARG:O	3:B:624:GLU:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:5:GLY:O	4:F:8:ILE:HG12	2.13	0.48
2:E:308:PHE:HA	4:F:278:MET:HE1	1.96	0.47
1:D:355:LYS:HD2	1:D:357:PRO:HD2	1.95	0.47
4:F:349:THR:OG1	8:F:502:B12:H3P1	2.14	0.47
1:D:461:VAL:HG22	1:D:462:PRO:HD3	1.96	0.47
1:D:581:THR:CG2	1:D:590:VAL:HG21	2.45	0.47
3:C:183:VAL:HG22	3:C:215:THR:HB	1.96	0.47
3:B:184:ASP:HB3	3:C:184:ASP:HB3	1.96	0.47
8:F:502:B12:H361	8:F:502:B12:C42	2.44	0.47
1:D:531:PRO:HG2	1:D:545:LYS:HG2	1.97	0.47
3:C:295:CYS:O	3:C:299:GLU:HG2	2.14	0.47
4:F:344:VAL:HG12	4:F:346:PHE:H	1.80	0.46
1:D:66:ASP:OD1	1:D:69:ARG:NH1	2.48	0.46
1:A:134:GLY:HA2	1:A:229:PRO:HG2	1.98	0.46
4:F:8:ILE:HG13	4:F:29:SER:OG	2.16	0.46
2:E:39:ASP:OD2	4:F:250:ARG:NH1	2.41	0.46
1:A:35:VAL:HG22	1:A:101:VAL:HG11	1.97	0.46
3:B:186:GLU:HG3	3:B:215:THR:HG21	1.97	0.46
2:E:28:GLY:O	2:E:44:ASN:ND2	2.36	0.46
4:F:18:LYS:HG2	4:F:23:PRO:HA	1.98	0.46
4:F:53:LEU:HD22	4:F:56:ALA:HB3	1.98	0.46
1:D:257:LEU:HD13	1:D:270:LEU:HB2	1.98	0.46
2:E:218:TYR:H	4:F:313:ASN:HD22	1.64	0.46
1:D:124:GLY:HA3	1:D:209:PHE:CZ	2.51	0.45
3:B:257:HIS:O	3:B:329:VAL:HA	2.16	0.45
4:F:168:MET:HE3	4:F:182:VAL:HG13	1.98	0.45
3:C:186:GLU:HG3	3:C:215:THR:HG21	1.97	0.45
4:F:100:ASP:OD1	4:F:142:TYR:N	2.50	0.45
4:F:356:GLU:HG3	4:F:437:ALA:HB1	1.99	0.45
8:F:502:B12:H531	8:F:502:B12:H543	1.98	0.45
1:D:373:MET:HE3	1:D:377:PHE:HB2	1.99	0.45
1:D:384:ARG:HG3	1:D:434:PHE:HZ	1.80	0.45
3:C:248:GLU:HG2	3:C:289:ASN:ND2	2.32	0.45
4:F:344:VAL:HG11	4:F:374:TYR:O	2.17	0.45
1:D:651:LYS:NZ	1:D:682:THR:OG1	2.44	0.45
4:F:438:MET:HE2	4:F:439:PHE:CE1	2.52	0.45
4:F:371:ALA:HA	4:F:384:LYS:HB3	1.99	0.44
1:D:342:LYS:C	1:D:342:LYS:HD2	2.42	0.44
1:D:125:VAL:HB	1:D:126:PRO:HD3	1.99	0.44
1:D:315:MET:SD	1:D:407:ARG:HB3	2.57	0.44
3:C:257:HIS:O	3:C:329:VAL:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:337:ALA:HB2	3:C:71:GLY:HA3	2.00	0.44
3:B:71:GLY:HA3	3:C:337:ALA:HB2	1.99	0.44
3:B:143:ASP:HA	3:B:146:LYS:HD2	2.00	0.44
3:C:592:ILE:HA	3:C:596:LYS:HB2	2.00	0.44
4:F:376:VAL:HG23	8:F:502:B12:O4	2.17	0.44
1:D:307:GLY:HA3	4:F:416:VAL:HG23	2.00	0.44
1:D:382:GLU:O	1:D:385:LEU:HB2	2.18	0.44
1:D:297:ILE:HD11	1:D:301:PHE:HB2	1.99	0.43
3:B:256:LEU:HD21	3:B:267:VAL:HG11	2.00	0.43
4:F:439:PHE:O	4:F:440:ILE:C	2.60	0.43
1:D:665:ALA:O	1:D:668:LEU:HB3	2.18	0.43
1:A:156:GLN:NE2	1:A:183:LEU:O	2.43	0.43
4:F:7:ASN:HA	4:F:10:LYS:HD3	2.00	0.43
1:D:461:VAL:CG2	1:D:462:PRO:HD3	2.48	0.43
2:E:54:ASP:OD2	2:E:97:SER:OG	2.29	0.43
3:C:109:LYS:O	3:C:114:LYS:NZ	2.46	0.43
8:F:502:B12:H362	8:F:502:B12:H351	2.01	0.43
1:D:506:LEU:HD11	1:D:574:CYS:SG	2.59	0.43
1:A:98:ALA:HA	1:A:101:VAL:HG22	2.01	0.43
2:E:126:VAL:HG22	2:E:153:LEU:HB3	2.00	0.43
1:D:315:MET:HA	1:D:315:MET:HE2	2.00	0.43
1:D:585:PRO:HG2	4:F:9:PHE:CE2	2.54	0.43
1:D:603:LEU:O	4:F:24:THR:OG1	2.30	0.43
1:D:623:PHE:HE1	4:F:30:MET:HE3	1.84	0.43
2:E:127:VAL:HG11	2:E:143:VAL:HG11	2.00	0.43
1:D:666:LYS:HE2	1:D:672:ASP:HA	1.99	0.43
3:C:70:CYS:CB	3:C:196:ILE:HD11	2.49	0.43
4:F:195:GLU:HA	4:F:198:LYS:HE2	2.01	0.43
1:D:592:MET:HE1	1:D:631:ILE:HG12	2.00	0.42
3:B:564:ILE:HA	3:B:567:TYR:CE2	2.54	0.42
4:F:68:LYS:HA	4:F:68:LYS:HD3	1.83	0.42
2:E:255:VAL:HG21	2:E:278:MET:HE2	2.00	0.42
4:F:317:ASP:HB3	4:F:320:LYS:HB2	2.01	0.42
8:F:502:B12:H473	8:F:502:B12:H481	1.87	0.42
2:E:70:ASP:OD1	2:E:70:ASP:N	2.46	0.42
2:E:88:PRO:HA	2:E:306:ARG:HH12	1.84	0.42
3:B:594:THR:O	3:B:604:LYS:HD2	2.20	0.42
1:D:328:GLU:O	1:D:464:TYR:OH	2.37	0.42
4:F:39:ILE:HG12	4:F:39:ILE:O	2.19	0.42
8:F:502:B12:H533	8:F:502:B12:C48	2.50	0.42
1:D:259:ASP:OD2	1:D:275:TYR:OH	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:562:THR:OG1	1:D:568:GLN:O	2.35	0.42
1:D:570:PRO:HG3	1:D:621:PRO:HA	2.02	0.42
3:C:143:ASP:HA	3:C:146:LYS:HD2	2.02	0.42
3:C:564:ILE:HA	3:C:567:TYR:CE2	2.55	0.42
3:C:622:MET:O	3:C:626:ARG:HG3	2.20	0.42
3:B:94:SER:HB2	3:B:183:VAL:HG11	2.01	0.42
1:D:35:VAL:HG22	1:D:101:VAL:HG21	2.02	0.42
1:D:347:GLY:HA2	1:D:448:ASP:OD1	2.20	0.42
3:C:100:ILE:HD11	3:C:261:PRO:HD2	2.01	0.42
1:D:179:MET:HA	1:D:185:VAL:HB	2.02	0.41
3:C:202:ALA:O	3:C:206:ILE:HG12	2.20	0.41
3:B:70:CYS:CB	3:B:196:ILE:HD11	2.51	0.41
4:F:161:VAL:HG13	4:F:183:TYR:CD1	2.56	0.41
3:C:598:GLU:HB2	3:C:604:LYS:HD3	2.02	0.41
1:D:684:ALA:HB1	1:D:689:GLU:HB2	2.03	0.41
2:E:249:SER:HB2	2:E:297:ARG:HB2	2.03	0.41
1:D:335:GLN:OE1	3:C:422:THR:OG1	2.39	0.41
3:C:94:SER:HB2	3:C:183:VAL:HG11	2.02	0.41
1:D:279:VAL:O	1:D:283:LEU:HG	2.21	0.41
1:D:399:GLY:C	1:D:404:THR:HG22	2.46	0.41
2:E:155:MET:HA	2:E:178:VAL:HB	2.03	0.41
3:C:16:LEU:HD21	3:C:28:TRP:CE3	2.56	0.41
4:F:406:ARG:HD2	4:F:406:ARG:HA	1.92	0.41
3:C:256:LEU:HD21	3:C:267:VAL:HG11	2.02	0.41
1:D:358:GLY:O	1:D:359:ARG:NE	2.51	0.40
1:D:349:ASP:HB3	1:D:351:ASP:OD1	2.21	0.40
3:B:51:SER:OG	3:C:557:MET:HA	2.21	0.40
3:B:248:GLU:HG2	3:B:289:ASN:ND2	2.36	0.40
4:F:334:PRO:O	4:F:365:TRP:NE1	2.55	0.40
1:A:259:ASP:OD2	1:A:275:TYR:OH	2.33	0.40
1:A:195:VAL:O	1:A:198:VAL:HG12	2.22	0.40
3:B:557:MET:HA	3:C:51:SER:OG	2.21	0.40
3:C:248:GLU:HB2	3:C:251:SER:HB2	2.03	0.40
1:D:46:VAL:HG21	1:D:196:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/708 (41%)	284 (99%)	4 (1%)	0	100	100
1	D	706/708 (100%)	692 (98%)	14 (2%)	0	100	100
2	E	311/314 (99%)	300 (96%)	11 (4%)	0	100	100
3	B	626/630 (99%)	608 (97%)	17 (3%)	1 (0%)	43	60
3	C	626/630 (99%)	608 (97%)	17 (3%)	1 (0%)	43	60
4	F	440/450 (98%)	424 (96%)	15 (3%)	1 (0%)	43	60
All	All	2997/3440 (87%)	2916 (97%)	78 (3%)	3 (0%)	49	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	332	GLN
4	F	336	GLU
3	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	A	232/583 (40%)	232 (100%)	0	100	100
1	D	583/583 (100%)	579 (99%)	4 (1%)	76	86
2	E	259/260 (100%)	257 (99%)	2 (1%)	73	85
3	B	517/519 (100%)	515 (100%)	2 (0%)	84	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	517/519 (100%)	515 (100%)	2 (0%)	84 93
4	F	371/377 (98%)	368 (99%)	3 (1%)	73 85
All	All	2479/2841 (87%)	2466 (100%)	13 (0%)	78 91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	257	LEU
1	D	319	PHE
1	D	338	VAL
1	D	497	CYS
2	E	181	SER
2	E	207	ASP
3	B	95	ASP
3	B	451	CYS
3	C	95	ASP
3	C	451	CYS
4	F	6	LEU
4	F	53	LEU
4	F	435	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	341	HIS
1	D	386	HIS
1	D	390	ASN
2	E	186	ASN
1	A	233	ASN
1	A	287	ASN
3	B	388	ASN
3	C	357	HIS
3	C	388	ASN
4	F	71	ASN
4	F	125	GLN
4	F	222	GLN

5.3.3 RNA

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	$\#\|Z\| > 2$
5	SF4	B	701	3	0,12,12	-	-	-		
7	XCC	B	703	3	0,12,12	-	-	-		
7	XCC	C	702	3	0,12,12	-	-	-		
8	B12	F	502	-	93,101,101	0.82	1 (1%)	146,166,166	1.10	8 (5%)
5	SF4	F	501	4	0,12,12	-	-	-		
5	SF4	C	701	3	0,12,12	-	-	-		
5	SF4	B	702	3	0,12,12	-	-	-		
5	SF4	D	801	1,6	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
5	SF4	B	701	3	-	-	0/6/5/5
7	XCC	B	703	3	-	-	0/4/4/4
7	XCC	C	702	3	-	-	0/4/4/4
8	B12	F	502	-	-	10/56/223/223	0/3/11/11
5	SF4	F	501	4	-	-	0/6/5/5
5	SF4	C	701	3	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	B	702	3	-	-	0/6/5/5
5	SF4	D	801	1,6	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	502	B12	C2B-N1B	-2.29	1.33	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	502	B12	C9B-C8B-N1B	6.23	107.98	105.35
8	F	502	B12	C8B-C9B-N3B	-2.92	106.75	109.97
8	F	502	B12	C20-C1-C19	-2.49	106.96	109.36
8	F	502	B12	C1-C2-C3	-2.20	98.79	101.60
8	F	502	B12	C35-C5-C4	-2.14	112.43	116.79
8	F	502	B12	C4B-C9B-N3B	2.14	134.18	130.51
8	F	502	B12	C60-C18-C19	-2.11	109.13	114.62
8	F	502	B12	C10-C9-N22	-2.08	123.34	125.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	502	B12	C1P-C2P-O3-P
8	F	502	B12	C3P-C2P-O3-P
8	F	502	B12	C54-C17-C55-C56
8	F	502	B12	C18-C17-C55-C56
8	F	502	B12	N59-C1P-C2P-O3
8	F	502	B12	C2-C3-C30-C31
8	F	502	B12	C4-C3-C30-C31
8	F	502	B12	C2R-C1R-N1B-C8B
8	F	502	B12	O6R-C1R-N1B-C8B
8	F	502	B12	C16-C17-C55-C56

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	703	XCC	1	0
7	C	702	XCC	1	0

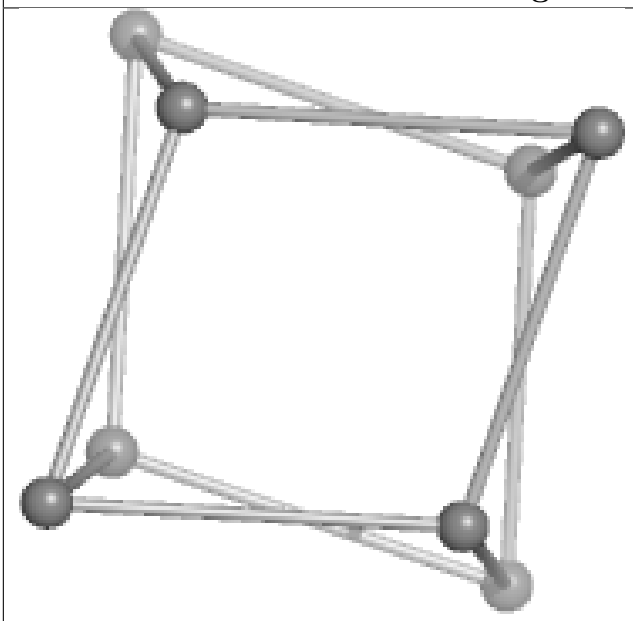
Continued on next page...

Continued from previous page...

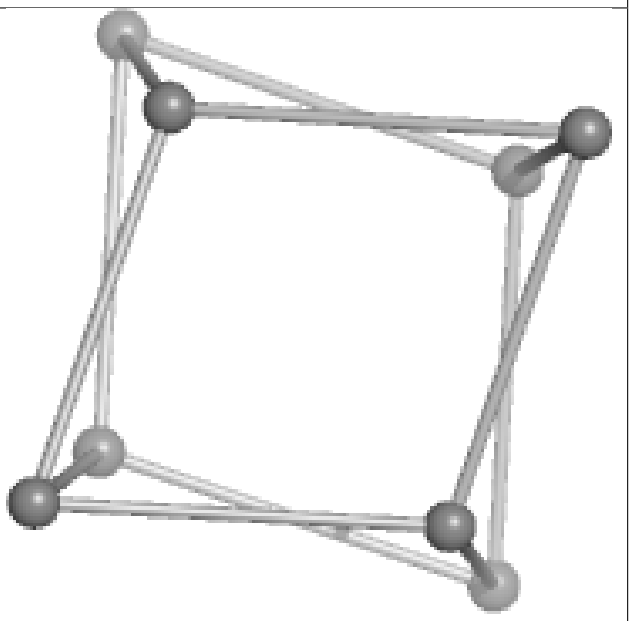
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	502	B12	11	0
5	F	501	SF4	1	0
5	C	701	SF4	1	0
5	B	702	SF4	1	0

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.

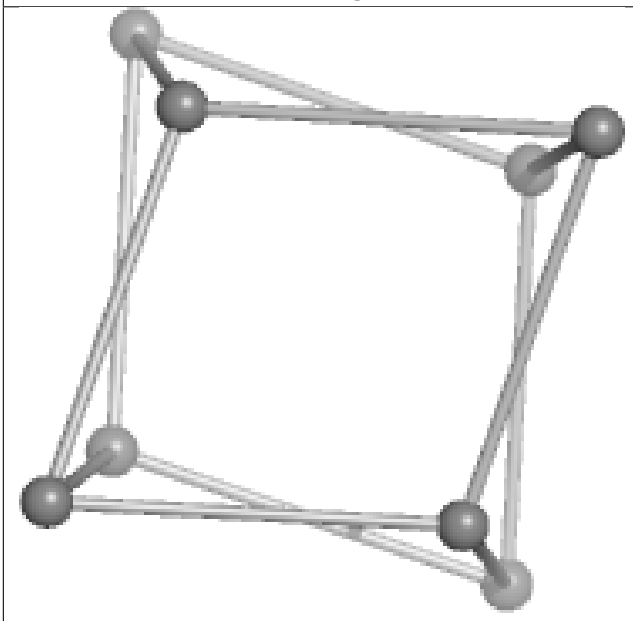
Ligand SF4 B 701



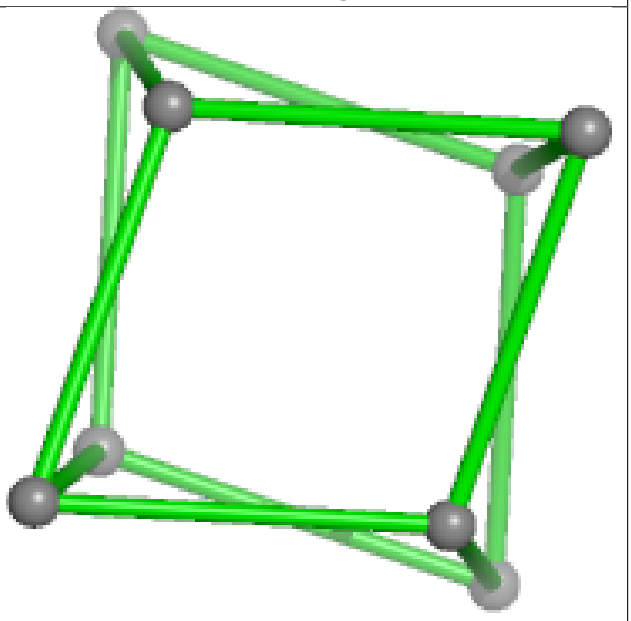
Bond lengths



Bond angles

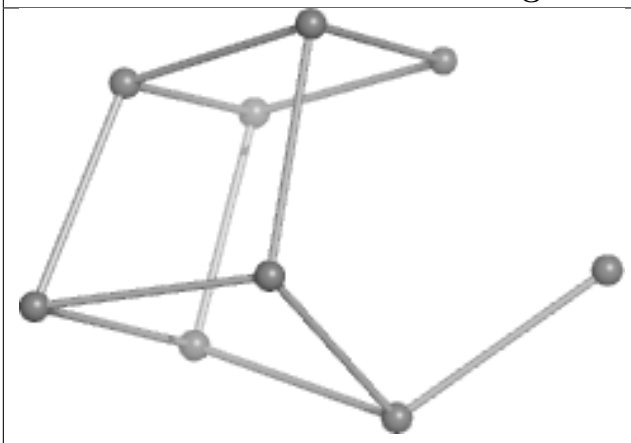


Torsions

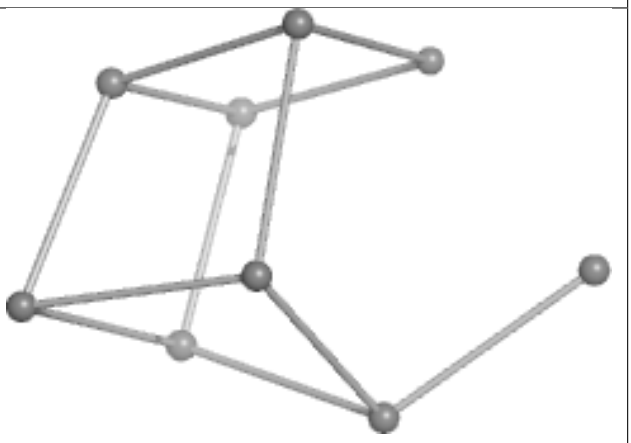


Rings

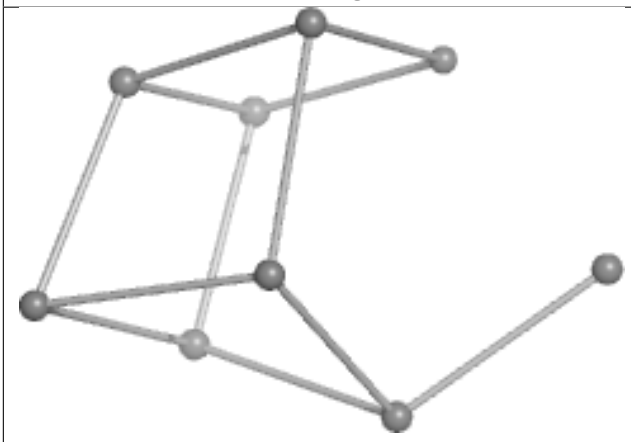
Ligand XCC B 703



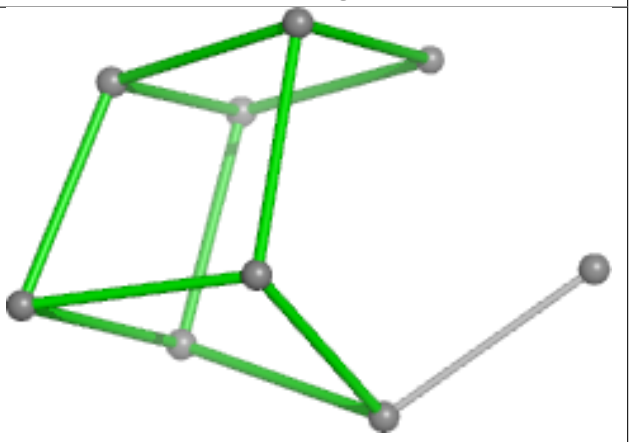
Bond lengths



Bond angles

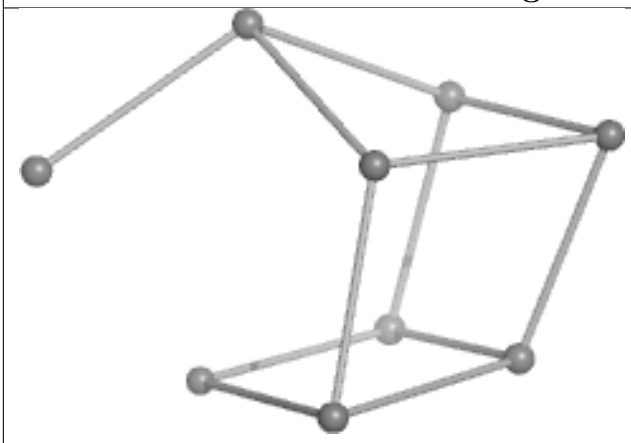


Torsions

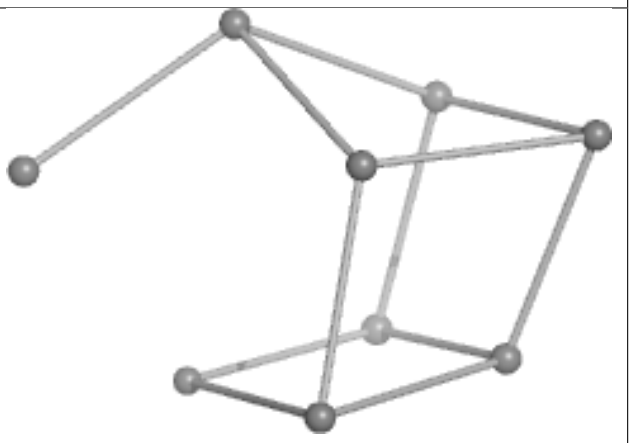


Rings

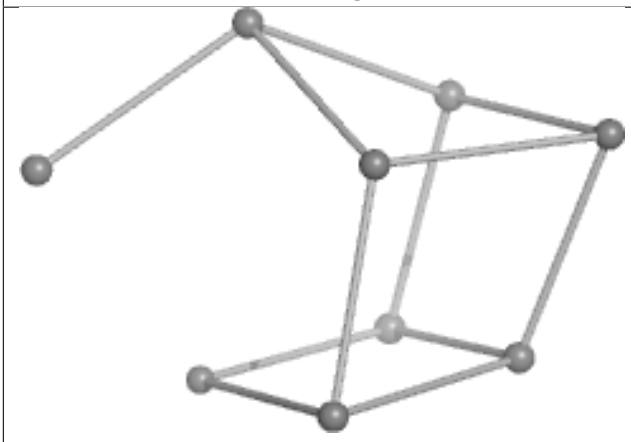
Ligand XCC C 702



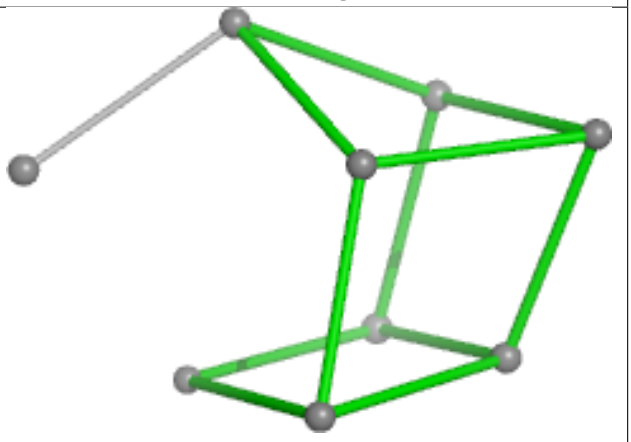
Bond lengths



Bond angles

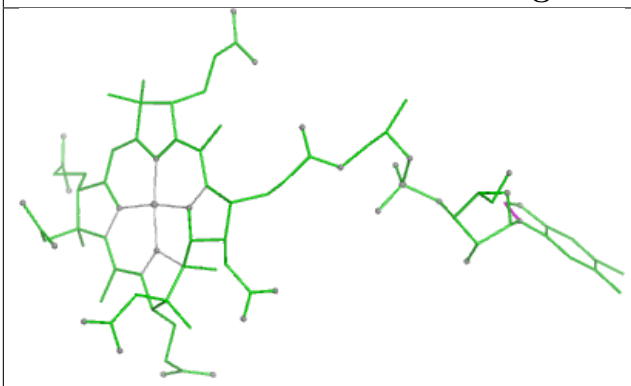


Torsions

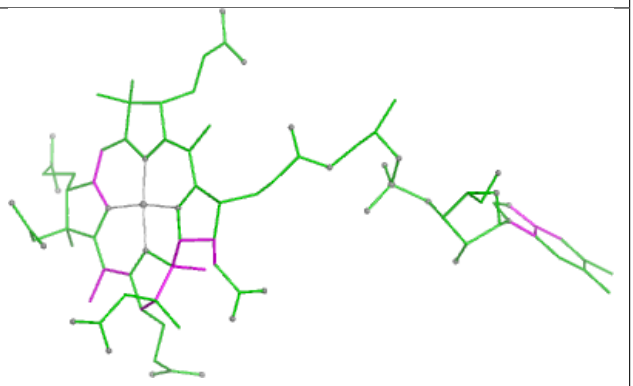


Rings

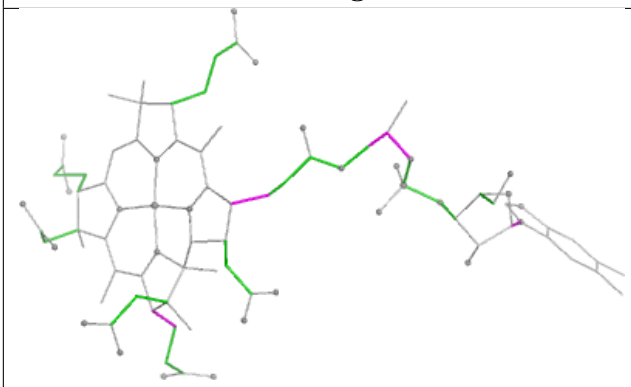
Ligand B12 F 502



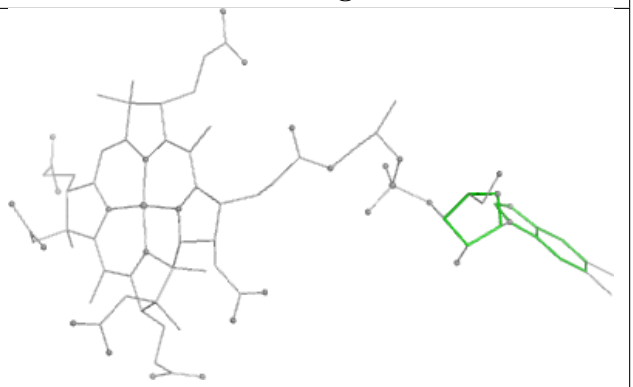
Bond lengths



Bond angles

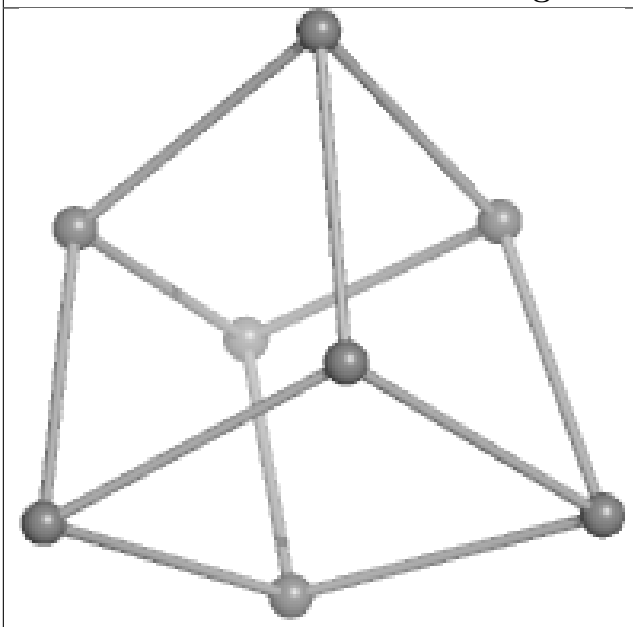


Torsions

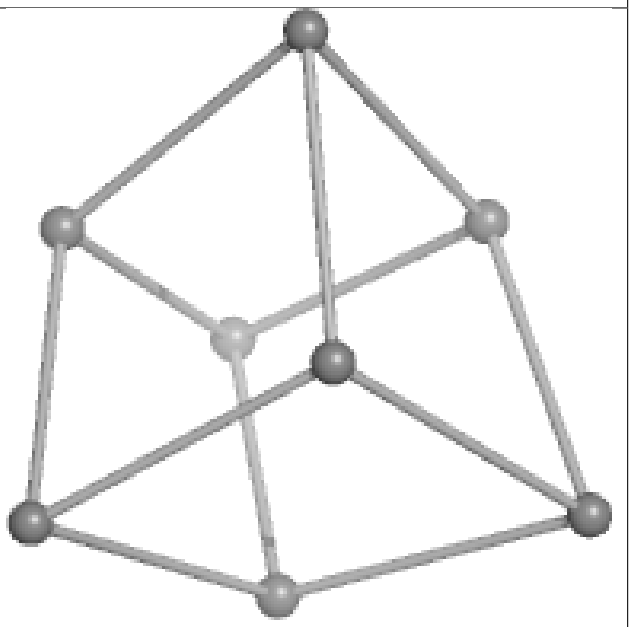


Rings

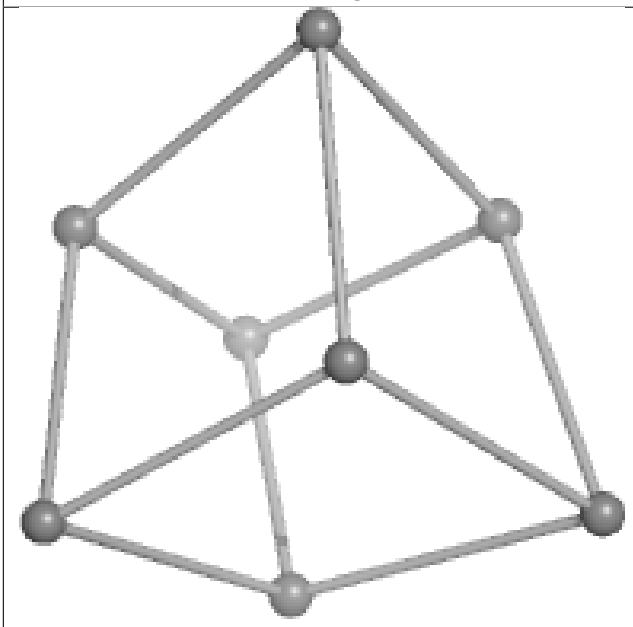
Ligand SF4 F 501



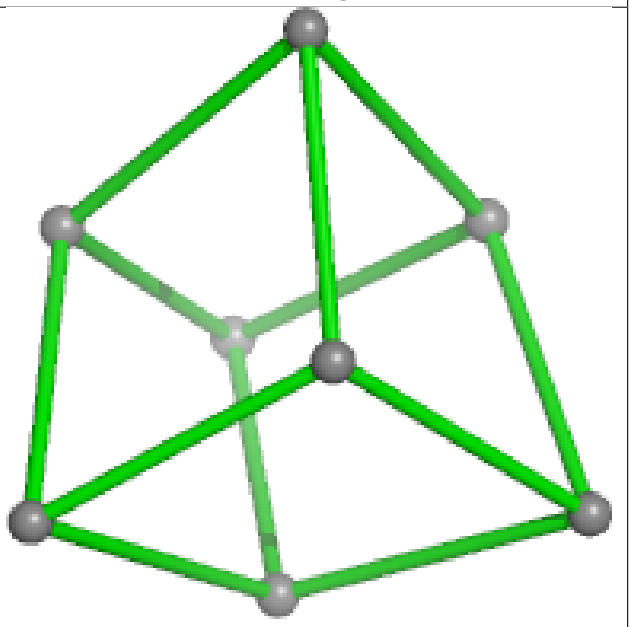
Bond lengths



Bond angles

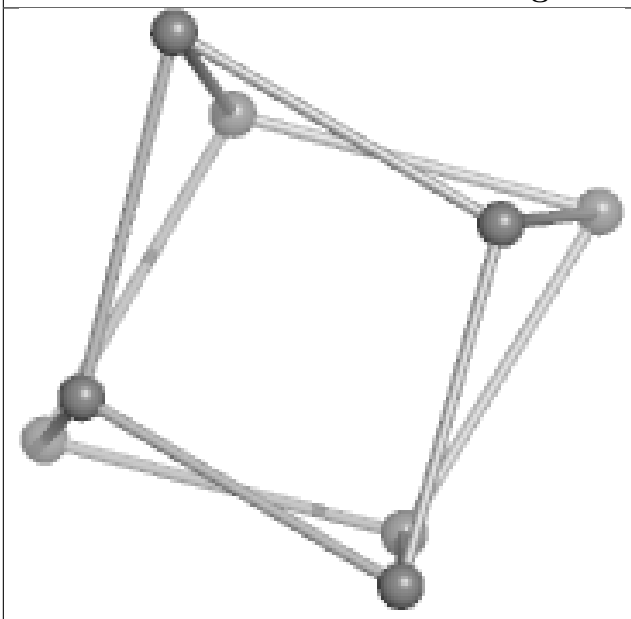


Torsions

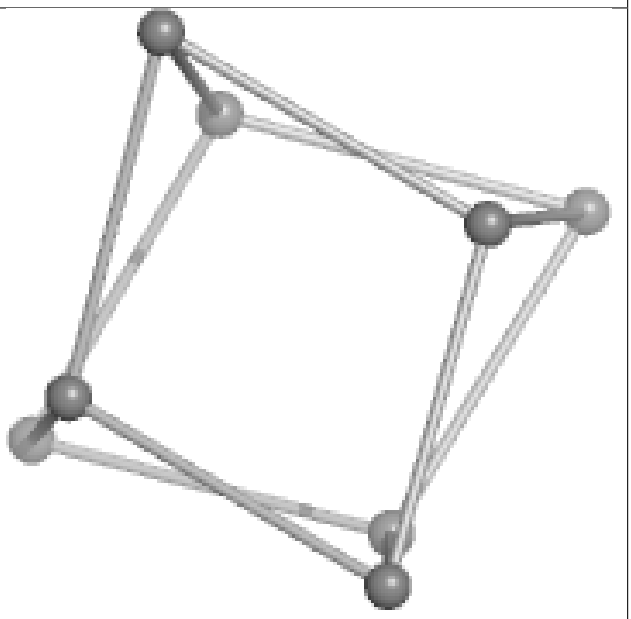


Rings

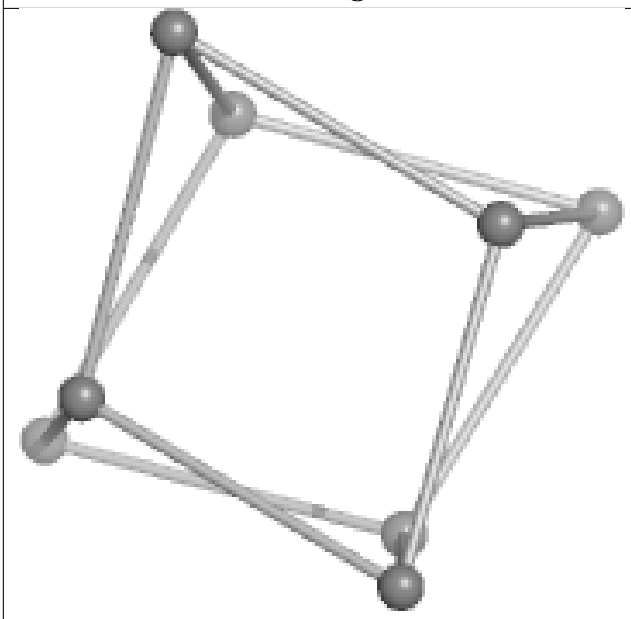
Ligand SF4 C 701



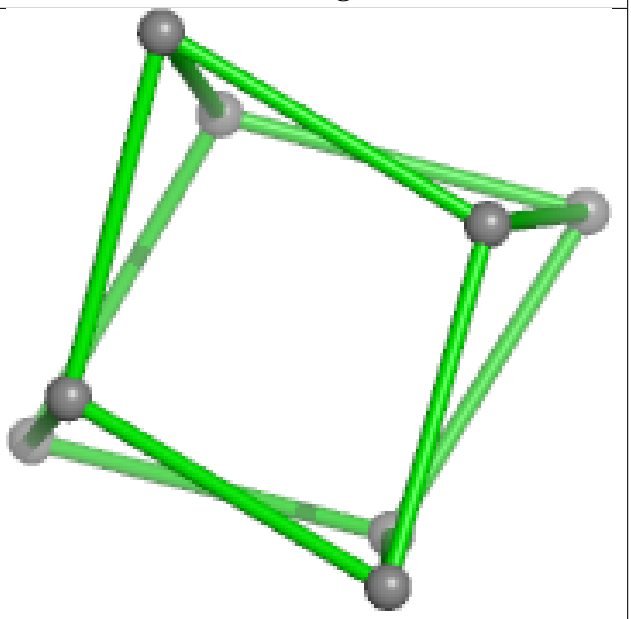
Bond lengths



Bond angles

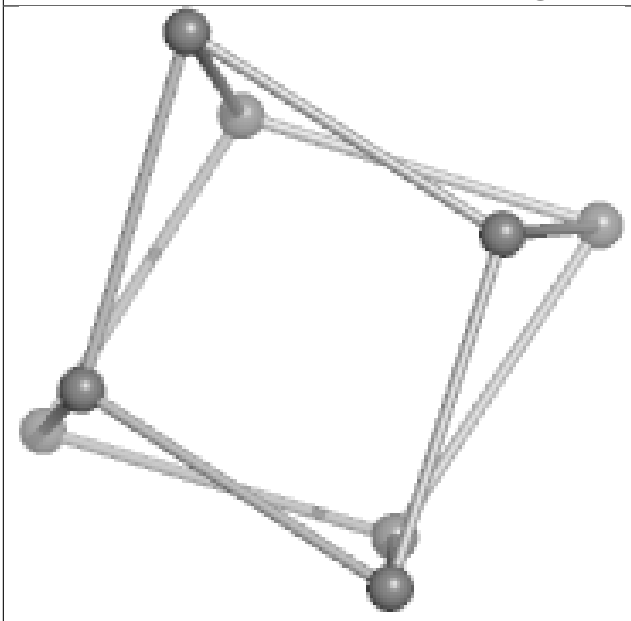


Torsions

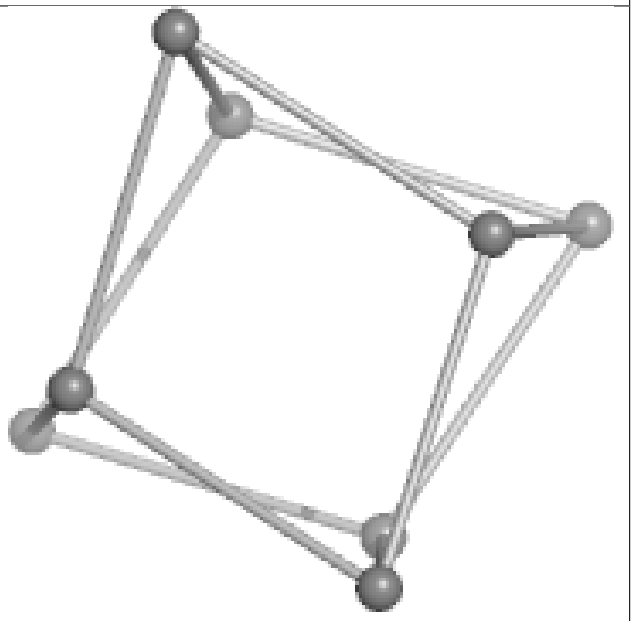


Rings

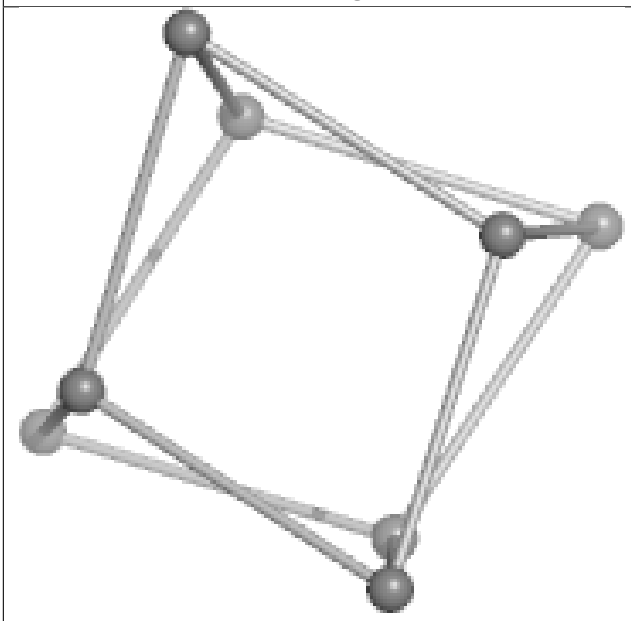
Ligand SF4 B 702



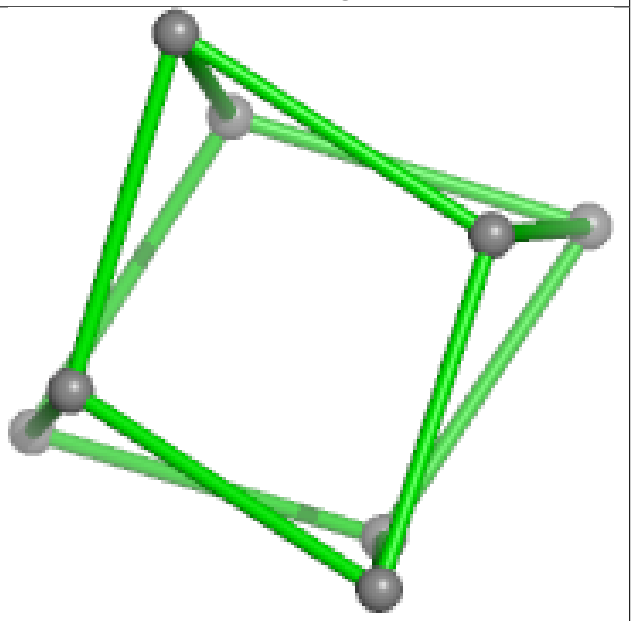
Bond lengths



Bond angles

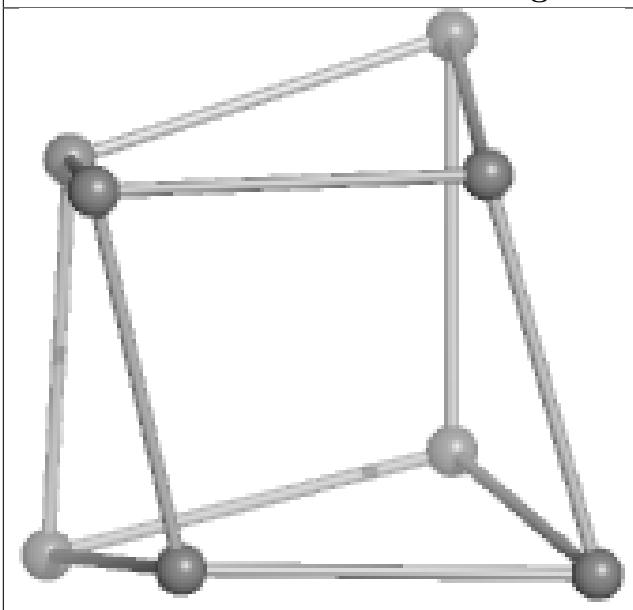


Torsions

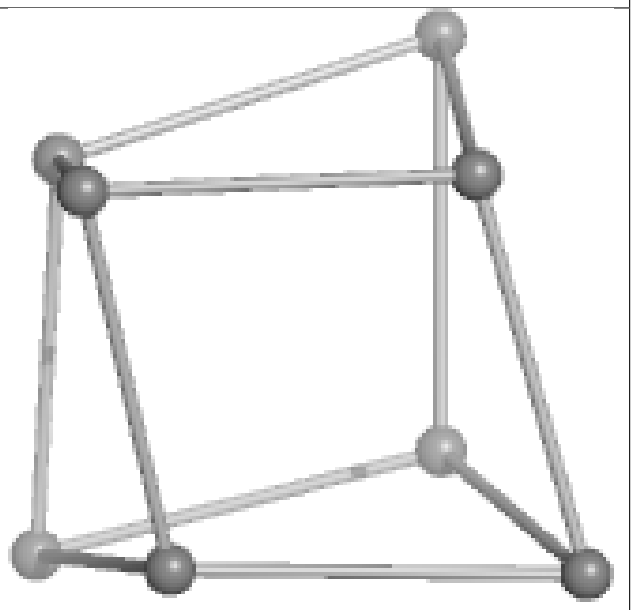


Rings

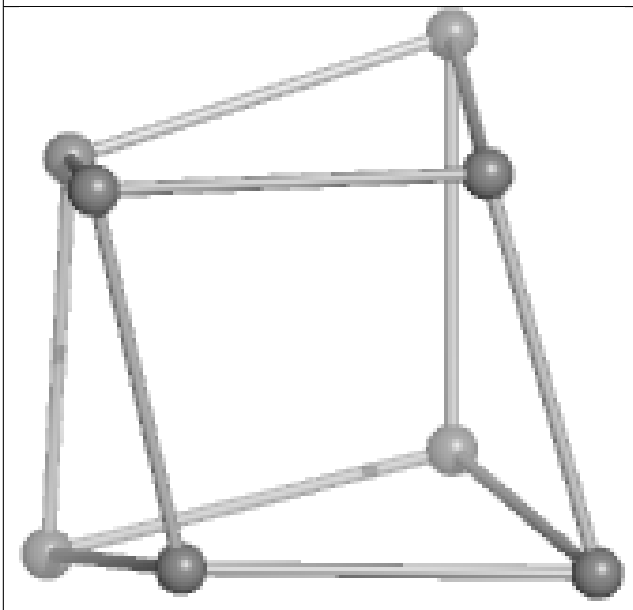
Ligand SF4 D 801



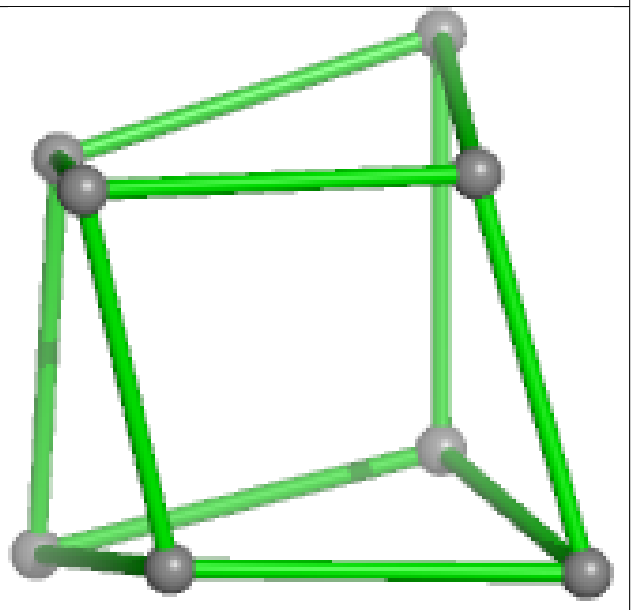
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

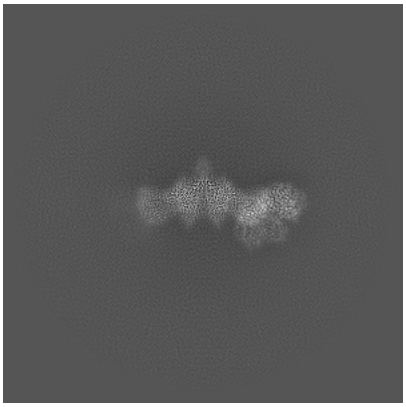
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50900. These allow visual inspection of the internal detail of the map and identification of artifacts.

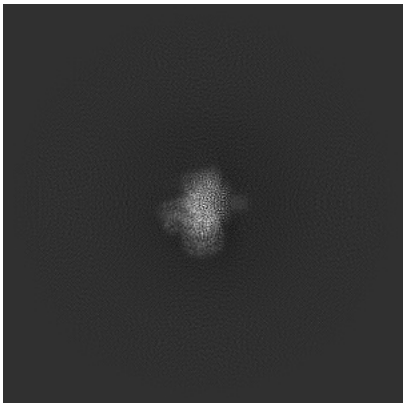
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

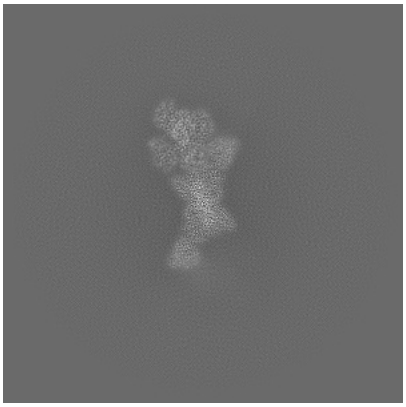
6.1.1 Primary map



X



Y

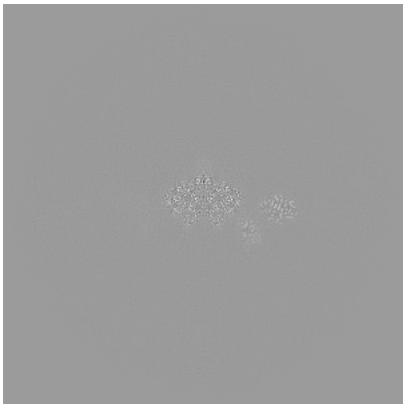


Z

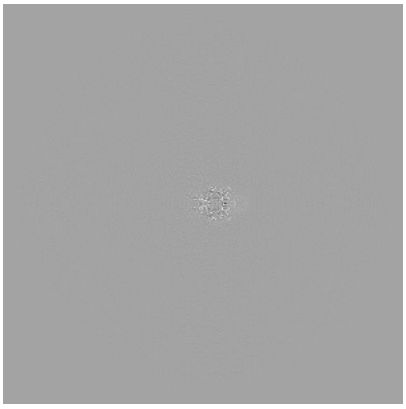
The images above show the map projected in three orthogonal directions.

6.2 Central slices

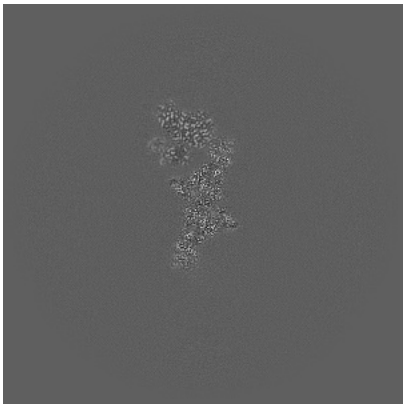
6.2.1 Primary map



X Index: 280



Y Index: 280

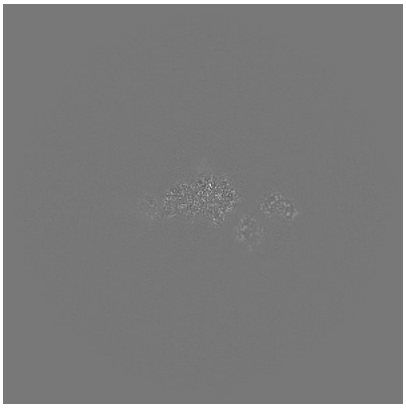


Z Index: 280

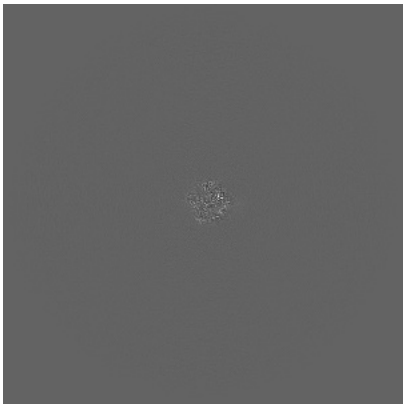
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

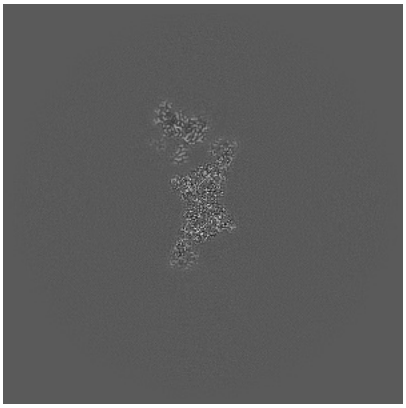
6.3.1 Primary map



X Index: 272



Y Index: 270

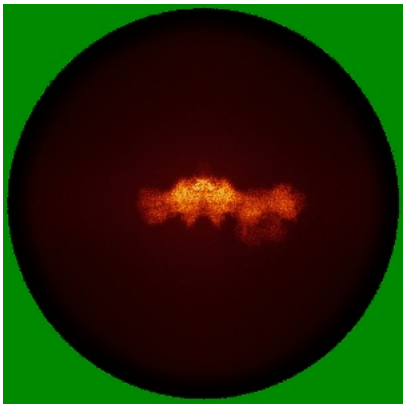


Z Index: 287

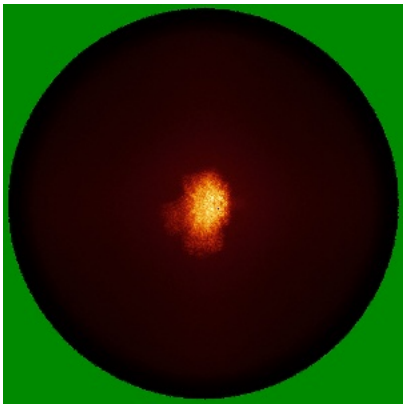
The images above show the largest variance slices of the map in three orthogonal directions.

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

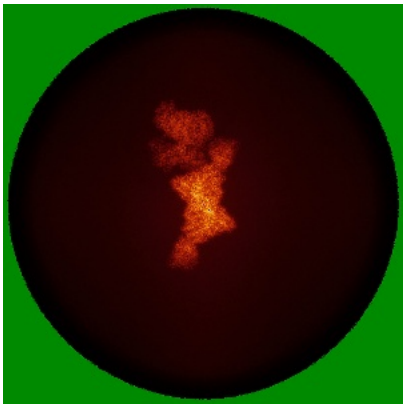
6.4.1 Primary map



X



Y

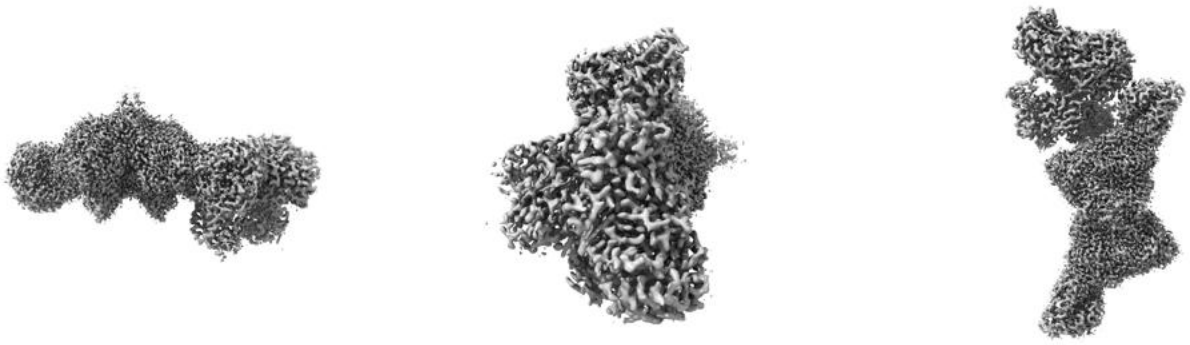


Z

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.

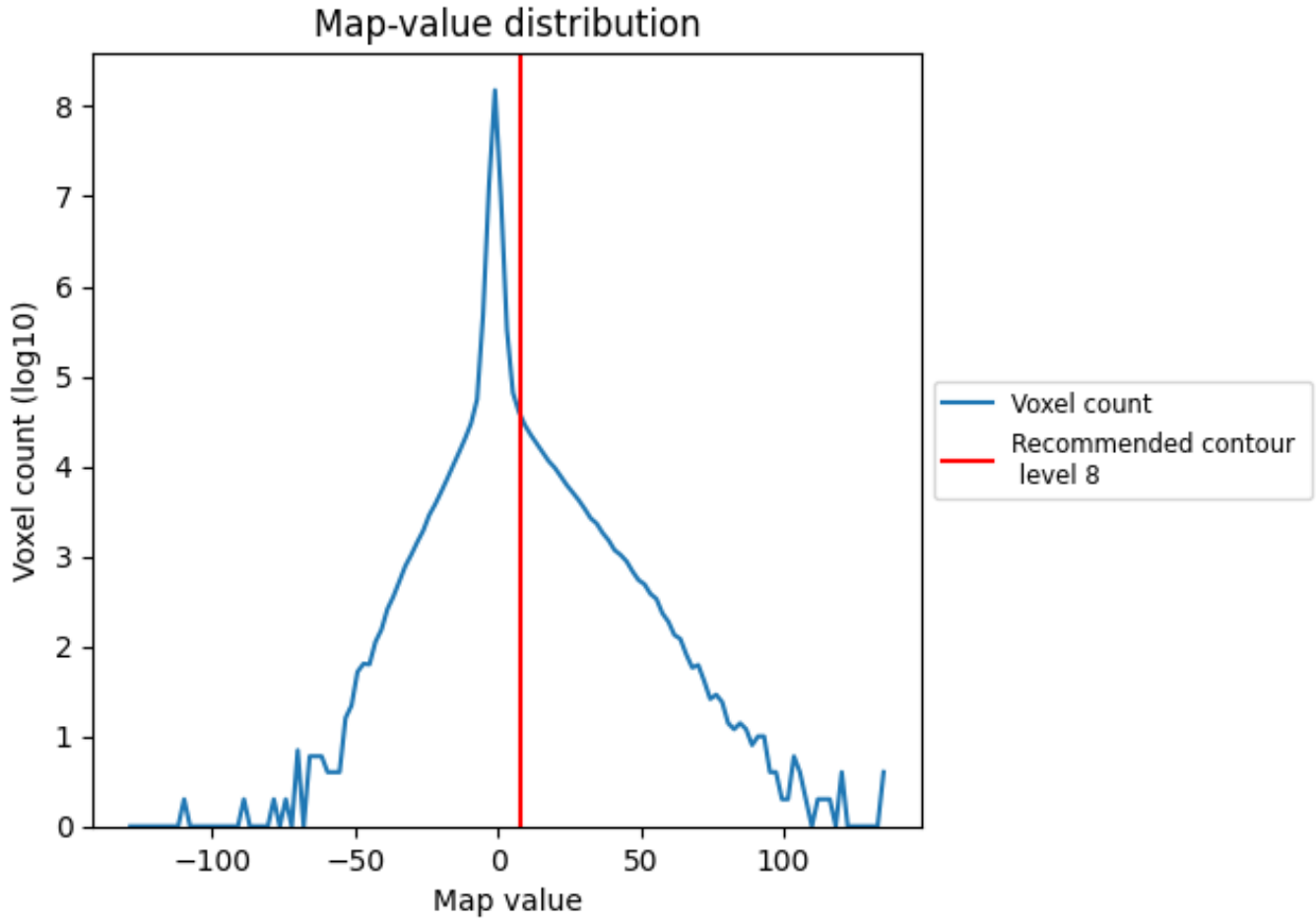
6.6 Mask visualisation (i)

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

7 Map analysis

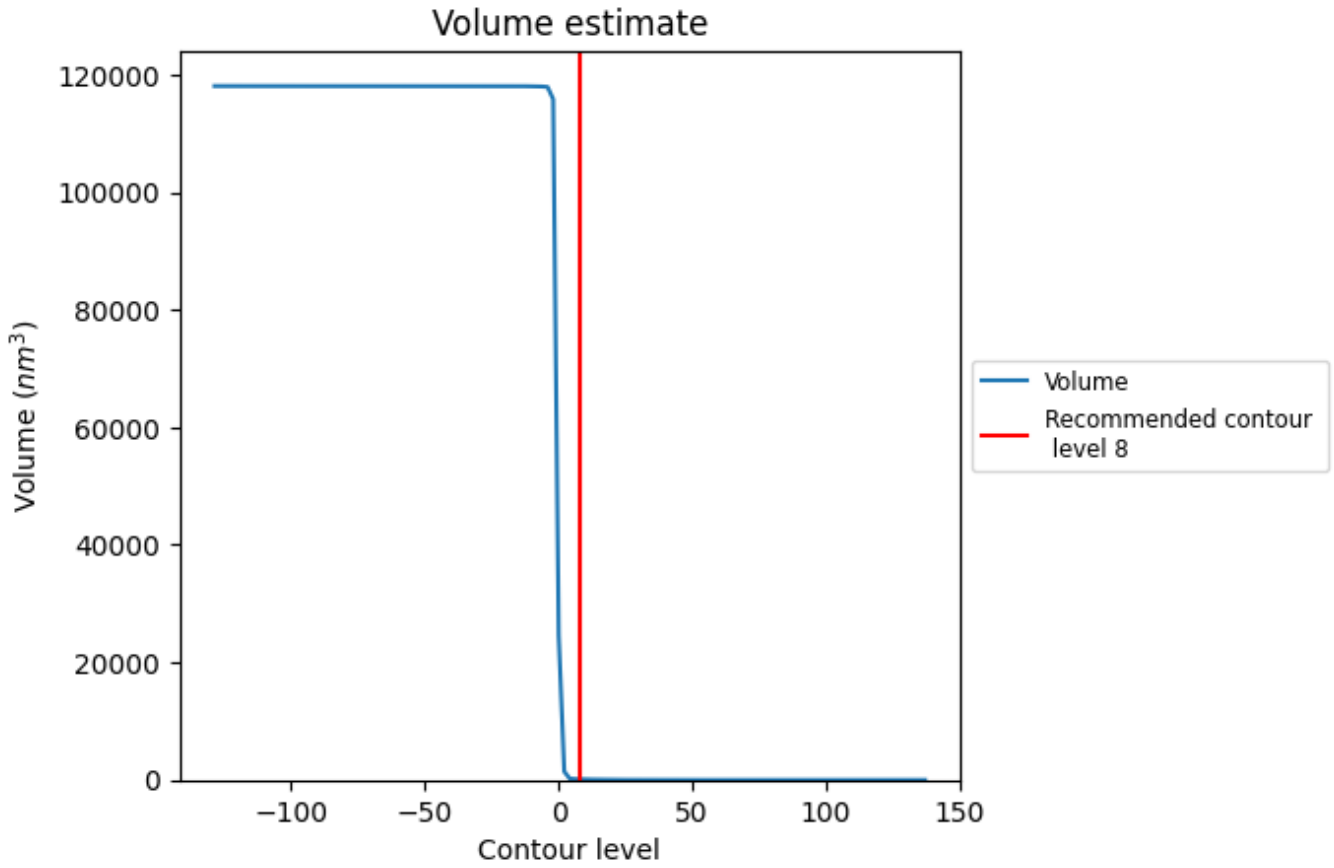
This section contains the results of statistical analysis of the map.

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.

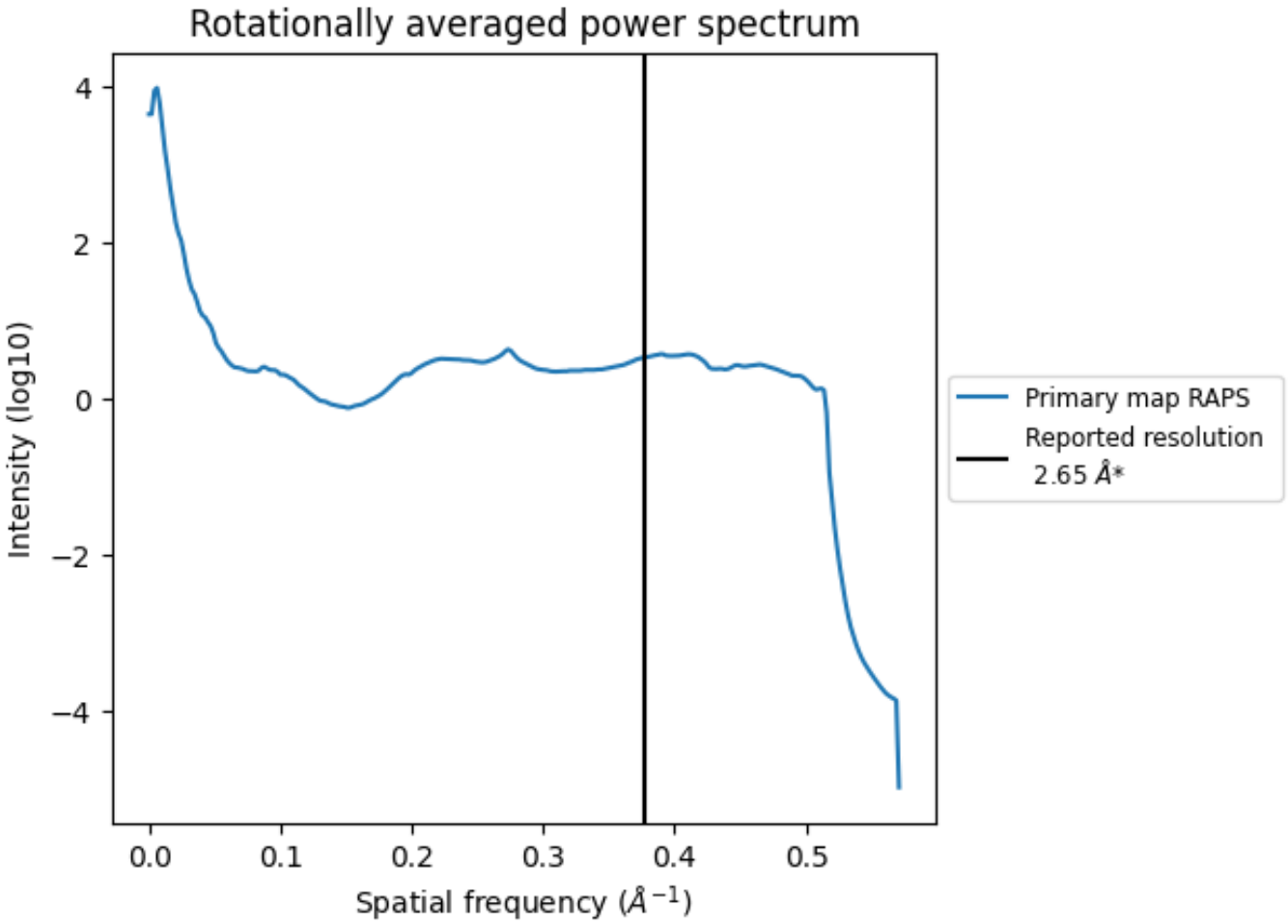
7.2 Volume estimate



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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 0.377 Å^{-1}

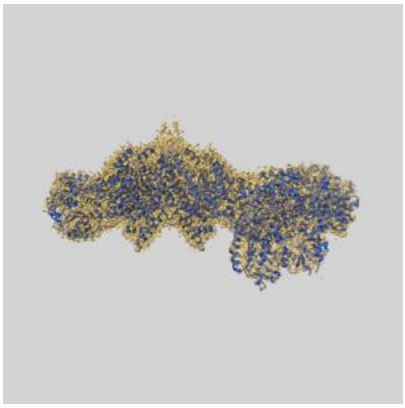
8 Fourier-Shell correlation

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

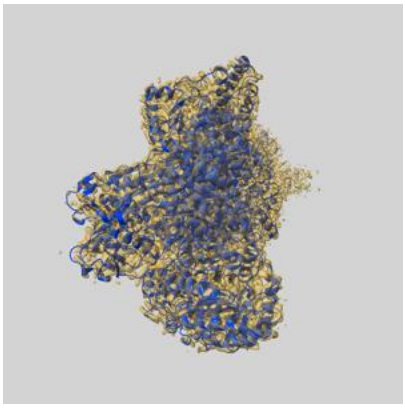
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50900 and PDB model 9FZZ. Per-residue inclusion information can be found in section 3 on page 7.

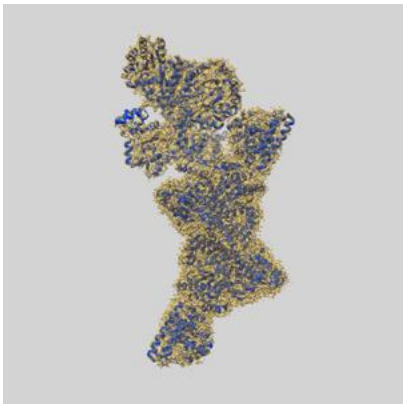
9.1 Map-model overlay



X



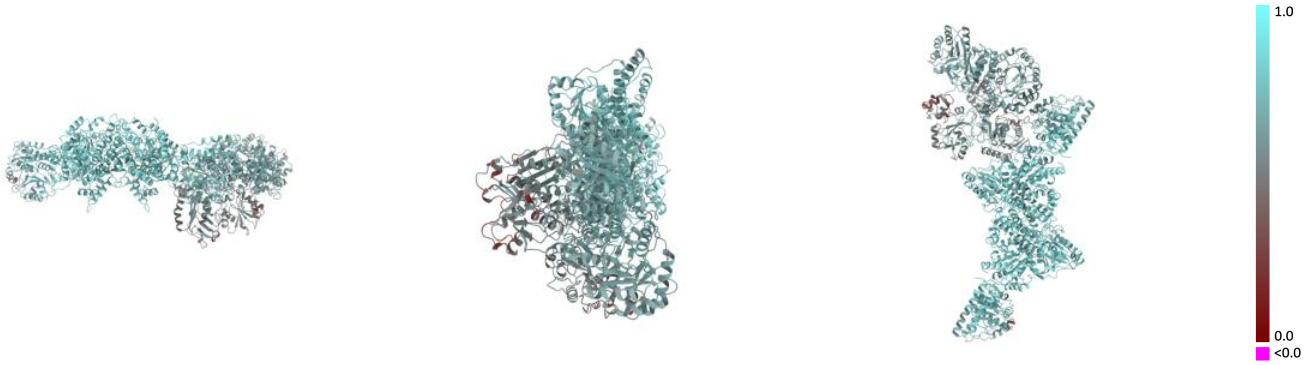
Y



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.

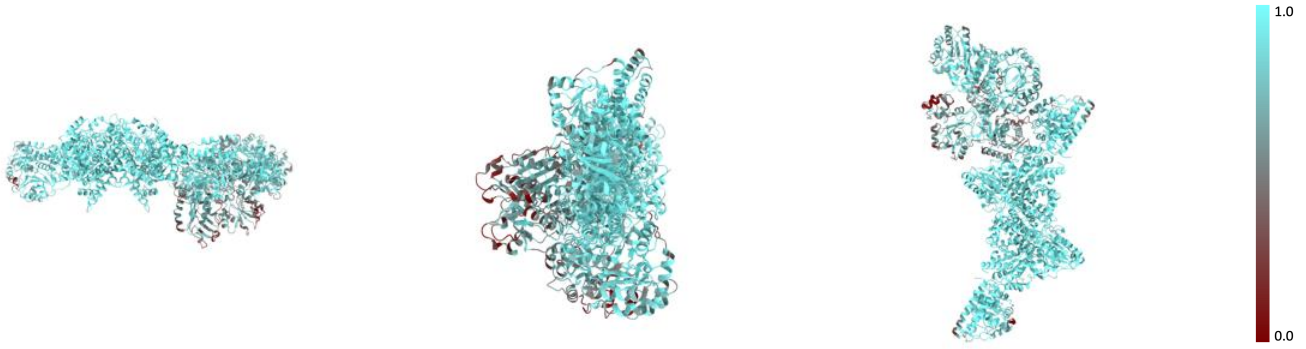
9.2 Q-score mapped to coordinate model (i)



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.

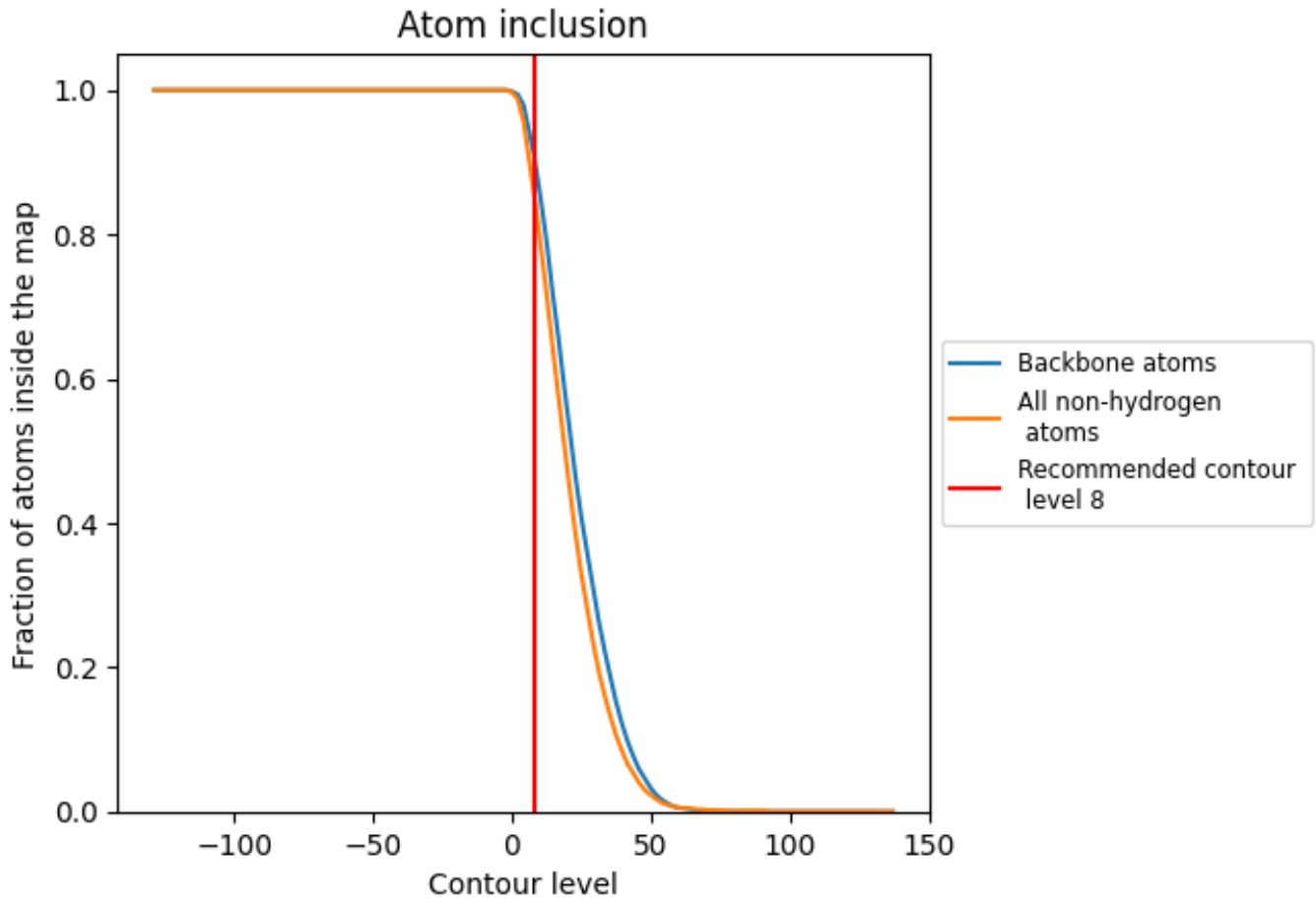
9.3 Atom inclusion mapped to coordinate model (i)



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, 91% of all backbone atoms, 86% 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	0.8580	0.6750
A	0.8840	0.6960
B	0.9680	0.7610
C	0.9670	0.7610
D	0.7610	0.6150
E	0.8460	0.6190
F	0.7040	0.5570