



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 9F47 / pdb_00009f47
Title : crystal structure of [FeFe]-hydrogenase CbA5H from Clostridium beijerinckii in Hinact state
Authors : Duan, J.; Rutz, A.; Hofmann, E.; Happe, T.; Kurisu, G.
Deposited on : 2024-04-26
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

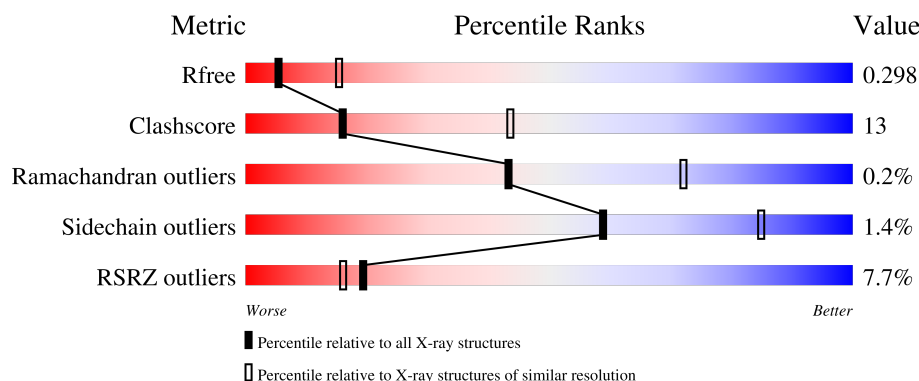
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	674	 6% 67% 24% • 8%
1	B	674	 8% 70% 21% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	402	A	701	-	-	X	-
2	402	B	701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19475 atoms, of which 9665 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 [FeFe]-hydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	621	Total	C	H	N	O	S	0	0	0
			9695	3070	4843	819	927	36			
1	B	618	Total	C	H	N	O	S	0	0	0
			9654	3057	4822	816	923	36			

There are 60 discrepancies between the modelled and reference sequences:

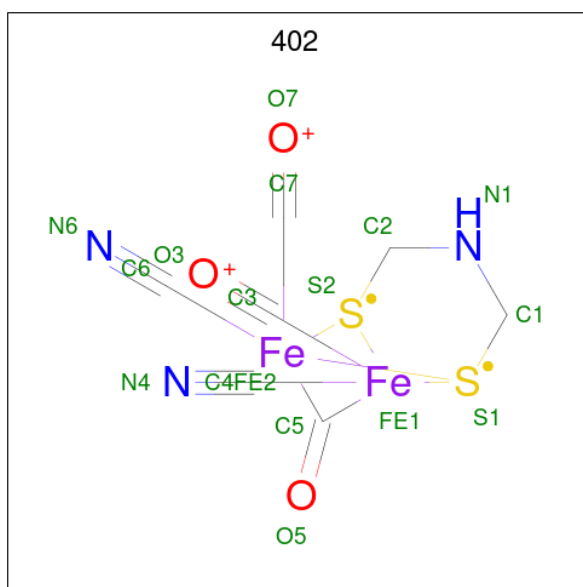
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ASP	-	expression tag	UNP A0A1I9RYV3
A	646	ILE	-	expression tag	UNP A0A1I9RYV3
A	647	TRP	-	expression tag	UNP A0A1I9RYV3
A	648	SER	-	expression tag	UNP A0A1I9RYV3
A	649	VAL	-	expression tag	UNP A0A1I9RYV3
A	650	GLY	-	expression tag	UNP A0A1I9RYV3
A	651	VAL	-	expression tag	UNP A0A1I9RYV3
A	652	LYS	-	expression tag	UNP A0A1I9RYV3
A	653	LEU	-	expression tag	UNP A0A1I9RYV3
A	654	PHE	-	expression tag	UNP A0A1I9RYV3
A	655	GLY	-	expression tag	UNP A0A1I9RYV3
A	656	GLY	-	expression tag	UNP A0A1I9RYV3
A	657	GLY	-	expression tag	UNP A0A1I9RYV3
A	658	SER	-	expression tag	UNP A0A1I9RYV3
A	659	GLY	-	expression tag	UNP A0A1I9RYV3
A	660	GLY	-	expression tag	UNP A0A1I9RYV3
A	661	GLY	-	expression tag	UNP A0A1I9RYV3
A	662	SER	-	expression tag	UNP A0A1I9RYV3
A	663	GLY	-	expression tag	UNP A0A1I9RYV3
A	664	GLY	-	expression tag	UNP A0A1I9RYV3
A	665	GLY	-	expression tag	UNP A0A1I9RYV3
A	666	SER	-	expression tag	UNP A0A1I9RYV3
A	667	TRP	-	expression tag	UNP A0A1I9RYV3
A	668	SER	-	expression tag	UNP A0A1I9RYV3
A	669	HIS	-	expression tag	UNP A0A1I9RYV3

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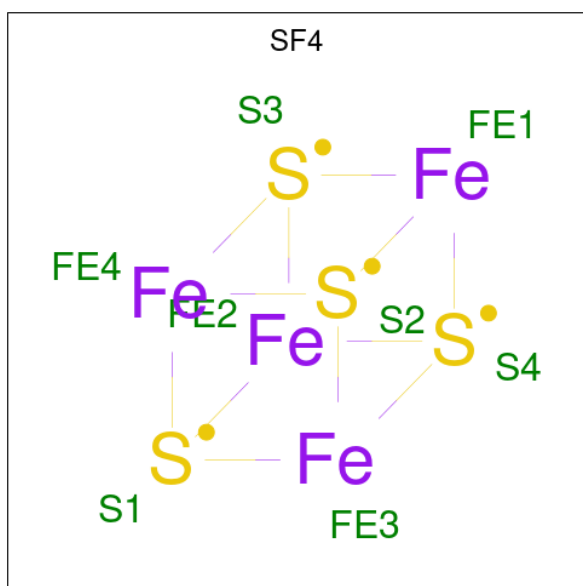
Chain	Residue	Modelled	Actual	Comment	Reference
A	670	PRO	-	expression tag	UNP A0A1I9RYV3
A	671	GLN	-	expression tag	UNP A0A1I9RYV3
A	672	PHE	-	expression tag	UNP A0A1I9RYV3
A	673	GLU	-	expression tag	UNP A0A1I9RYV3
A	674	LYS	-	expression tag	UNP A0A1I9RYV3
B	645	ASP	-	expression tag	UNP A0A1I9RYV3
B	646	ILE	-	expression tag	UNP A0A1I9RYV3
B	647	TRP	-	expression tag	UNP A0A1I9RYV3
B	648	SER	-	expression tag	UNP A0A1I9RYV3
B	649	VAL	-	expression tag	UNP A0A1I9RYV3
B	650	GLY	-	expression tag	UNP A0A1I9RYV3
B	651	VAL	-	expression tag	UNP A0A1I9RYV3
B	652	LYS	-	expression tag	UNP A0A1I9RYV3
B	653	LEU	-	expression tag	UNP A0A1I9RYV3
B	654	PHE	-	expression tag	UNP A0A1I9RYV3
B	655	GLY	-	expression tag	UNP A0A1I9RYV3
B	656	GLY	-	expression tag	UNP A0A1I9RYV3
B	657	GLY	-	expression tag	UNP A0A1I9RYV3
B	658	SER	-	expression tag	UNP A0A1I9RYV3
B	659	GLY	-	expression tag	UNP A0A1I9RYV3
B	660	GLY	-	expression tag	UNP A0A1I9RYV3
B	661	GLY	-	expression tag	UNP A0A1I9RYV3
B	662	SER	-	expression tag	UNP A0A1I9RYV3
B	663	GLY	-	expression tag	UNP A0A1I9RYV3
B	664	GLY	-	expression tag	UNP A0A1I9RYV3
B	665	GLY	-	expression tag	UNP A0A1I9RYV3
B	666	SER	-	expression tag	UNP A0A1I9RYV3
B	667	TRP	-	expression tag	UNP A0A1I9RYV3
B	668	SER	-	expression tag	UNP A0A1I9RYV3
B	669	HIS	-	expression tag	UNP A0A1I9RYV3
B	670	PRO	-	expression tag	UNP A0A1I9RYV3
B	671	GLN	-	expression tag	UNP A0A1I9RYV3
B	672	PHE	-	expression tag	UNP A0A1I9RYV3
B	673	GLU	-	expression tag	UNP A0A1I9RYV3
B	674	LYS	-	expression tag	UNP A0A1I9RYV3

- Molecule 2 is dicarbonyl[bis(cyanide-kappaC)]-mu-(iminodimethanethiolatato-1kappaS:2kappaS)-mu-(oxomethylidene)diiron(2+) (CCD ID: 402) (formula: C₇H₅Fe₂N₃O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	S	0	0
			17	7	2	3	3	2		
2	B	1	Total	C	Fe	N	O	S	0	0
			17	7	2	3	3	2		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe S	0	0
			8	4 4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Cl	0	0
			6	6		
5	B	4	Total	Cl	0	0
			4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total	O	0	0
			15	15		
6	B	17	Total	O	0	0
			17	17		



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	169.00Å 169.00Å 127.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.90 49.26 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.26-2.90) 100.0 (49.26-2.90)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.242 , 0.298 0.242 , 0.298	Depositor DCC
R_{free} test set	2065 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19475	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1968e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 402, CL, ZN

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	0.21	0/4931	0.45	3/6635 (0.0%)
1	B	0.23	0/4910	0.44	2/6604 (0.0%)
All	All	0.22	0/9841	0.45	5/13239 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LYS	CB-CG-CD	-9.03	90.53	111.30
1	A	65	ILE	CB-CG1-CD1	8.22	131.06	113.80
1	A	221	LYS	CA-CB-CG	6.39	126.87	114.10
1	B	377	GLN	CA-C-N	-5.89	112.97	121.98
1	B	377	GLN	C-N-CA	-5.89	112.97	121.98

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	4852	4843	4845	144	0
1	B	4832	4822	4820	114	0
2	A	17	0	5	7	0
2	B	17	0	5	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	0	0	0
3	B	24	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	0	1	0
5	B	4	0	0	1	0
6	A	15	0	0	1	0
6	B	17	0	0	1	0
All	All	9810	9665	9675	256	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 13.

All (256) 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)
1:B:367:CYS:SG	2:B:701:402:N1	2.48	0.86
1:A:19:VAL:HG21	1:A:273:THR:CG2	2.06	0.85
1:A:116:GLN:NE2	1:A:210:CYS:SG	2.53	0.82
1:A:271:ASP:OD1	1:A:273:THR:OG1	1.96	0.82
1:B:40:VAL:HG21	1:B:61:CYS:HB3	1.61	0.81
1:A:131:ASP:OD1	1:A:133:SER:OG	1.99	0.79
1:A:19:VAL:HG11	1:A:455:ILE:HG12	1.66	0.78
1:A:19:VAL:HG13	1:A:277:LEU:HD21	1.66	0.77
1:B:142:GLU:N	1:B:142:GLU:OE1	2.19	0.74
1:B:19:VAL:HG11	1:B:455:ILE:HA	1.68	0.74
1:B:369:PRO:HG2	1:B:425:ALA:HB1	1.70	0.74
1:A:64:LEU:HD12	1:A:68:SER:O	1.88	0.73
1:B:77:LEU:HD13	1:B:106:ILE:HD11	1.70	0.73
1:B:114:ILE:HG23	1:B:115:ILE:HD13	1.70	0.73
1:A:19:VAL:HG21	1:A:273:THR:HG22	1.69	0.73
1:B:507:ARG:NH1	6:B:801:HOH:O	2.23	0.72
1:B:177:LYS:HD2	1:B:177:LYS:N	2.05	0.72
1:B:223:ILE:HD11	1:B:225:CYS:SG	2.31	0.71
1:B:274:MET:HE3	1:B:274:MET:HA	1.71	0.71
1:A:19:VAL:HG21	1:A:273:THR:HG21	1.71	0.71
1:B:271:ASP:OD1	1:B:273:THR:OG1	2.07	0.71
1:A:173:THR:HG22	1:A:177:LYS:HE3	1.74	0.70
1:B:40:VAL:CG2	1:B:61:CYS:HB3	2.23	0.68
1:B:349:LEU:HD21	1:B:534:LEU:HD21	1.75	0.68
1:B:422:PRO:HD2	2:B:701:402:O3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:O	1:B:172:VAL:HG23	1.94	0.68
1:A:16:VAL:HG13	1:A:19:VAL:N	2.08	0.68
1:A:240:GLU:HG3	1:A:241:LEU:HD23	1.76	0.67
1:B:565:MET:HE1	2:B:701:402:N1	2.10	0.67
1:A:250:ASN:O	1:A:373:LYS:NZ	2.25	0.66
1:A:16:VAL:HG13	1:A:19:VAL:H	1.60	0.66
1:A:356:ASP:OD2	1:A:358:SER:OG	2.06	0.64
1:A:367:CYS:SG	2:A:701:402:N1	2.71	0.63
1:A:636:VAL:HG23	1:A:636:VAL:O	1.98	0.62
1:B:19:VAL:HG21	1:B:455:ILE:HG12	1.80	0.61
1:B:430:ALA:HB1	1:B:443:VAL:HB	1.82	0.61
1:A:159:SER:HB2	1:A:163:GLU:HG3	1.81	0.61
1:B:19:VAL:HG21	1:B:455:ILE:CG1	2.31	0.61
1:A:273:THR:HG23	1:A:455:ILE:HD11	1.83	0.60
1:A:251:ARG:HG3	1:A:377:GLN:HG2	1.83	0.60
1:B:57:ILE:HD11	1:B:92:PHE:CG	2.36	0.60
1:A:77:LEU:HD23	1:A:124:TYR:CE1	2.36	0.60
1:A:507:ARG:NH1	6:A:802:HOH:O	2.32	0.60
1:A:368:CYS:N	2:A:701:402:H8	2.16	0.60
1:B:77:LEU:HD13	1:B:106:ILE:CD1	2.31	0.59
1:B:594:GLY:O	1:B:598:ILE:HG13	2.02	0.59
1:B:118:GLU:HG2	1:B:185:MET:HE1	1.83	0.59
1:B:617:TYR:O	1:B:622:ASP:N	2.32	0.59
1:A:496:THR:HG21	1:A:527:LEU:HD13	1.84	0.59
1:B:32:ARG:HD2	1:B:48:VAL:HG13	1.83	0.58
1:B:98:TYR:O	1:B:101:ILE:N	2.37	0.58
1:A:565:MET:HG2	1:A:570:GLY:HA2	1.86	0.58
1:A:77:LEU:HB3	1:A:78:PRO:HD3	1.86	0.57
1:B:565:MET:CE	2:B:701:402:H12	2.34	0.57
1:A:220:LYS:HD3	1:A:220:LYS:N	2.19	0.57
1:B:368:CYS:N	2:B:701:402:H8	2.20	0.57
1:A:75:ILE:HD11	1:A:83:LEU:CD1	2.35	0.56
1:B:13:LEU:O	1:B:22:GLU:HG2	2.04	0.56
1:A:17:PHE:HB3	1:A:65:ILE:HG13	1.87	0.56
1:B:481:ALA:HB1	1:B:494:ALA:HB1	1.87	0.56
1:A:168:ARG:NH2	1:B:631:GLU:OE2	2.39	0.56
1:A:422:PRO:HD2	2:A:701:402:O3	2.05	0.56
1:B:348:ARG:HG2	1:B:359:VAL:HG22	1.86	0.56
1:A:16:VAL:HG12	1:A:20:PHE:N	2.21	0.56
1:B:223:ILE:HD12	1:B:223:ILE:C	2.29	0.56
1:A:514:GLU:HA	1:A:517:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:MET:HE2	1:A:633:LEU:HB3	1.89	0.55
1:B:40:VAL:HG21	1:B:61:CYS:CB	2.33	0.55
1:B:565:MET:HE2	2:B:701:402:H12	1.89	0.55
1:A:346:GLN:NE2	1:A:350:GLU:OE2	2.34	0.55
1:B:264:VAL:HG12	1:B:265:ASP:H	1.72	0.55
1:A:539:ALA:HB2	1:A:548:MET:HE2	1.89	0.54
1:A:545:ALA:HB1	1:A:564:ILE:HD13	1.89	0.54
1:A:310:ASN:HB2	1:A:598:ILE:HD11	1.90	0.54
1:B:477:GLU:OE2	5:B:707:CL:CL	2.63	0.54
1:A:225:CYS:SG	1:A:226:GLY:N	2.81	0.53
1:A:382:MET:HE1	1:A:549:LEU:HB3	1.89	0.53
1:A:40:VAL:HG21	1:A:61:CYS:HB2	1.90	0.53
1:B:348:ARG:HG2	1:B:359:VAL:CG2	2.38	0.53
1:A:617:TYR:O	1:A:622:ASP:N	2.34	0.53
1:B:158:VAL:HG21	1:B:439:MET:SD	2.49	0.53
1:A:222:CYS:O	1:A:244:LYS:HE2	2.08	0.53
1:A:240:GLU:O	1:A:243:LYS:HB3	2.09	0.53
1:B:453:ILE:O	1:B:457:GLU:HG3	2.07	0.53
1:A:259:VAL:HG22	1:A:267:ILE:HG21	1.91	0.52
1:B:622:ASP:O	1:B:623:HIS:HB3	2.08	0.52
1:A:421:MET:HE1	2:A:701:402:O5	2.09	0.52
1:A:223:ILE:HD11	1:A:225:CYS:CB	2.40	0.52
1:A:137:TYR:O	1:A:140:VAL:HG22	2.09	0.52
1:A:362:PRO:O	1:A:385:VAL:HG13	2.09	0.52
1:A:548:MET:O	1:A:552:ILE:HG13	2.10	0.52
1:B:565:MET:CE	2:B:701:402:C1	2.88	0.52
1:A:400:ALA:HB2	1:A:475:MET:HE1	1.92	0.52
1:A:101:ILE:HG23	1:A:103:ARG:H	1.75	0.52
1:B:215:LYS:HB3	1:B:249:TYR:CE2	2.44	0.52
1:A:65:ILE:HG22	1:A:66:ASN:N	2.23	0.52
1:A:496:THR:HG22	1:A:500:LEU:HD22	1.92	0.51
1:B:97:PHE:HB3	1:B:101:ILE:HD12	1.92	0.51
1:A:604:LEU:HD22	1:A:609:GLU:HB3	1.91	0.51
1:A:77:LEU:HD23	1:A:124:TYR:HE1	1.74	0.51
1:A:211:ASN:HB3	1:A:272:ASN:OD1	2.11	0.51
1:A:369:PRO:O	1:A:372:ILE:HD12	2.10	0.51
1:A:77:LEU:HD13	1:A:106:ILE:HD11	1.93	0.51
1:A:131:ASP:OD1	1:A:131:ASP:C	2.53	0.51
1:A:183:ASN:OD1	1:A:185:MET:N	2.43	0.51
1:B:223:ILE:HD12	1:B:224:GLY:N	2.26	0.50
1:B:306:GLU:HG3	1:B:307:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:THR:HG22	1:B:449:THR:N	2.27	0.50
1:B:34:ILE:HB	1:B:46:ILE:CD1	2.41	0.50
1:A:75:ILE:O	1:A:80:GLY:HA3	2.11	0.49
1:B:13:LEU:C	1:B:13:LEU:HD23	2.38	0.49
1:B:128:LYS:HB3	1:B:134:TYR:CE2	2.48	0.49
1:A:222:CYS:O	1:A:244:LYS:CE	2.61	0.49
1:A:234:VAL:O	1:A:251:ARG:NH1	2.46	0.49
1:B:122:ILE:HG21	1:B:148:PHE:HB2	1.95	0.49
1:B:38:GLY:HA3	1:B:107:VAL:H	1.78	0.49
1:B:221:LYS:NZ	1:B:264:VAL:HG12	2.27	0.49
1:A:66:ASN:O	1:A:67:LYS:HD2	2.13	0.49
1:A:511:ILE:HD13	1:A:606:ARG:CZ	2.43	0.49
1:B:336:LEU:HD13	1:B:613:VAL:HG13	1.95	0.49
1:A:594:GLY:O	1:A:598:ILE:HG13	2.14	0.48
1:A:216:LEU:HB3	1:A:249:TYR:HE2	1.77	0.48
1:A:236:CYS:SG	1:A:251:ARG:HB3	2.54	0.48
1:A:140:VAL:HG13	1:A:178:MET:HE3	1.95	0.48
1:B:424:ILE:HA	1:B:427:LYS:HD2	1.95	0.48
1:A:192:PHE:O	1:A:196:ILE:HG13	2.14	0.48
1:A:622:ASP:O	1:A:623:HIS:HB3	2.14	0.48
1:B:139:VAL:HG13	1:B:140:VAL:HG13	1.96	0.48
1:B:401:LYS:NZ	1:B:441:TYR:O	2.47	0.47
1:A:211:ASN:O	1:A:214:VAL:HG12	2.13	0.47
1:A:367:CYS:HB2	2:A:701:402:C6	2.44	0.47
1:B:220:LYS:HD3	1:B:220:LYS:N	2.30	0.47
1:B:448:THR:HG22	1:B:450:ARG:H	1.79	0.47
1:B:548:MET:O	1:B:552:ILE:HD12	2.14	0.47
1:B:565:MET:HE1	2:B:701:402:C1	2.44	0.47
1:A:223:ILE:HD12	1:A:223:ILE:O	2.15	0.47
1:A:311:VAL:O	1:A:315:ILE:HG13	2.14	0.47
1:A:631:GLU:OE2	1:B:168:ARG:NH2	2.48	0.47
1:A:221:LYS:NZ	1:A:265:ASP:HB3	2.29	0.47
1:B:16:VAL:HG12	1:B:20:PHE:HB2	1.97	0.47
1:B:617:TYR:O	1:B:622:ASP:HA	2.15	0.47
1:A:477:GLU:OE2	5:A:706:CL:CL	2.70	0.46
1:A:636:VAL:O	1:A:636:VAL:CG2	2.63	0.46
1:B:420:ILE:HD13	1:B:452:LEU:HD22	1.97	0.46
1:A:240:GLU:O	1:A:241:LEU:O	2.34	0.46
1:B:216:LEU:HD13	1:B:269:ALA:HB2	1.96	0.46
1:B:496:THR:HG21	1:B:527:LEU:HD13	1.96	0.46
1:A:32:ARG:HE	1:A:48:VAL:HG13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:TYR:O	1:B:140:VAL:HG22	2.16	0.46
1:A:41:ASN:O	1:A:61:CYS:O	2.33	0.46
1:B:35:ALA:HB2	1:B:45:ILE:HD12	1.98	0.46
1:B:273:THR:HG23	1:B:455:ILE:HD11	1.98	0.46
1:A:31:GLY:C	1:A:103:ARG:HH22	2.24	0.46
1:A:180:GLN:OE1	1:A:181:LYS:N	2.49	0.46
1:B:86:ASP:OD1	1:B:86:ASP:N	2.48	0.46
1:B:170:LEU:O	1:B:174:VAL:HG23	2.16	0.46
1:A:82:PHE:HB2	1:A:184:ILE:HD12	1.97	0.46
1:B:478:TYR:CE1	1:B:483:ILE:HD13	2.51	0.46
1:A:223:ILE:HD11	1:A:225:CYS:HB3	1.98	0.46
1:A:446:VAL:O	1:A:447:ILE:HD12	2.16	0.46
1:A:265:ASP:OD1	1:A:265:ASP:O	2.34	0.45
1:A:401:LYS:NZ	1:A:441:TYR:O	2.48	0.45
1:A:19:VAL:O	1:A:458:ASN:HB2	2.16	0.45
1:B:274:MET:HA	1:B:274:MET:CE	2.45	0.45
1:A:379:TYR:HB3	1:A:382:MET:HE3	1.98	0.45
1:A:385:VAL:HB	1:A:386:PRO:CD	2.47	0.45
1:A:571:CYS:CB	2:A:701:402:C4	2.94	0.45
1:B:17:PHE:C	1:B:19:VAL:H	2.24	0.45
1:B:348:ARG:HD3	1:B:360:LYS:O	2.17	0.45
1:B:481:ALA:HB1	1:B:494:ALA:CB	2.47	0.45
1:A:220:LYS:HD3	1:A:220:LYS:H	1.82	0.45
1:B:18:SER:O	1:B:19:VAL:HB	2.16	0.45
1:B:19:VAL:HG22	1:B:277:LEU:HD11	1.99	0.45
1:A:19:VAL:O	1:A:458:ASN:CB	2.65	0.45
1:B:448:THR:CG2	1:B:449:THR:N	2.80	0.45
1:A:367:CYS:HB3	1:A:392:PRO:HD2	1.99	0.45
1:A:220:LYS:H	1:A:220:LYS:CD	2.30	0.45
1:A:508:PHE:N	1:A:508:PHE:CD2	2.83	0.45
1:A:220:LYS:N	1:A:220:LYS:CD	2.80	0.45
1:A:150:ILE:HG23	1:A:163:GLU:HB3	1.98	0.44
1:A:496:THR:CG2	1:A:500:LEU:HD22	2.47	0.44
1:A:240:GLU:CG	1:A:241:LEU:HD23	2.45	0.44
1:A:85:GLU:OE1	1:A:85:GLU:C	2.60	0.44
1:A:508:PHE:N	1:A:508:PHE:HD2	2.16	0.44
1:A:64:LEU:O	1:A:65:ILE:C	2.59	0.44
1:A:67:LYS:HD2	1:A:67:LYS:HA	1.78	0.44
1:B:362:PRO:O	1:B:385:VAL:HG13	2.17	0.44
1:A:240:GLU:O	1:A:241:LEU:C	2.61	0.44
1:A:274:MET:HE1	1:A:277:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:MET:SD	1:A:608:ASN:HA	2.58	0.44
1:A:373:LYS:NZ	1:A:377:GLN:OE1	2.51	0.44
1:A:480:GLY:O	1:A:484:ILE:HG12	2.18	0.44
1:B:623:HIS:ND1	1:B:624:PRO:O	2.51	0.43
1:A:34:ILE:HG22	1:A:35:ALA:N	2.33	0.43
1:B:275:LEU:HD12	1:B:275:LEU:O	2.18	0.43
1:B:422:PRO:CD	2:B:701:402:O3	2.64	0.43
1:B:535:ARG:HH21	1:B:557:GLU:HB3	1.83	0.43
1:B:311:VAL:O	1:B:315:ILE:HG13	2.18	0.43
1:A:17:PHE:HD2	1:A:65:ILE:HG21	1.83	0.43
1:B:604:LEU:HD22	1:B:609:GLU:HB3	1.99	0.43
1:B:274:MET:HE3	1:B:274:MET:CA	2.45	0.43
1:B:514:GLU:HA	1:B:517:ARG:HG3	2.00	0.43
1:A:68:SER:CB	1:A:111:GLU:HG3	2.49	0.43
1:A:346:GLN:OE1	1:A:502:LYS:HG3	2.19	0.43
1:B:371:TRP:HA	1:B:374:PHE:HB3	2.01	0.43
1:A:400:ALA:CB	1:A:475:MET:HE1	2.48	0.42
1:B:140:VAL:HG23	1:B:144:ILE:HG13	2.01	0.42
1:B:219:THR:OG1	1:B:266:ALA:O	2.24	0.42
1:B:515:GLY:HA3	1:B:525:CYS:SG	2.59	0.42
1:A:226:GLY:HA2	1:A:229:LYS:HD2	2.01	0.42
1:B:75:ILE:CG1	1:B:83:LEU:HD13	2.49	0.42
1:B:480:GLY:HA2	1:B:483:ILE:HG22	1.99	0.42
1:A:40:VAL:HA	1:A:64:LEU:HA	2.00	0.42
1:A:48:VAL:HG11	1:A:94:PHE:HZ	1.83	0.42
1:A:219:THR:OG1	1:A:266:ALA:O	2.31	0.42
1:B:37:CYS:O	1:B:37:CYS:SG	2.76	0.42
1:A:492:ILE:HG12	1:A:536:ILE:HG21	2.02	0.42
1:B:483:ILE:HG13	1:B:595:LEU:HD22	2.02	0.42
1:A:83:LEU:HD23	1:A:87:SER:CB	2.50	0.42
1:A:427:LYS:HG2	1:A:446:VAL:HB	2.01	0.42
1:B:125:LEU:HD23	1:B:125:LEU:O	2.19	0.42
1:B:617:TYR:O	1:B:622:ASP:CA	2.68	0.42
1:A:122:ILE:HG23	1:A:144:ILE:CG2	2.50	0.42
1:A:571:CYS:SG	2:A:701:402:H12	2.59	0.42
1:B:289:THR:HG23	1:B:324:VAL:HG11	2.02	0.41
1:A:79:PHE:HE1	1:A:134:TYR:CZ	2.38	0.41
1:B:83:LEU:N	1:B:83:LEU:HD12	2.35	0.41
1:A:352:HIS:CG	1:A:361:LEU:HD11	2.54	0.41
1:B:32:ARG:CD	1:B:48:VAL:HG13	2.49	0.41
1:A:314:LYS:NZ	1:A:468:ASP:OD1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:O	1:A:15:SER:OG	2.28	0.41
1:A:32:ARG:NE	1:A:48:VAL:HG13	2.35	0.41
1:A:38:GLY:HA3	1:A:107:VAL:H	1.85	0.41
1:A:124:TYR:C	1:A:124:TYR:CD2	2.99	0.41
1:A:229:LYS:HG2	1:A:230:ARG:N	2.35	0.41
1:A:157:GLY:O	1:A:203:LYS:HE3	2.21	0.41
1:B:13:LEU:O	1:B:22:GLU:O	2.38	0.41
1:B:36:ILE:HG12	1:B:46:ILE:HD11	2.02	0.41
1:A:77:LEU:CD2	1:A:124:TYR:CE1	3.03	0.41
1:A:259:VAL:HG22	1:A:267:ILE:CG2	2.51	0.41
1:A:545:ALA:O	1:A:549:LEU:HG	2.20	0.41
1:B:33:LYS:HE2	1:B:103:ARG:NH1	2.36	0.41
1:B:57:ILE:HD11	1:B:92:PHE:CD2	2.56	0.41
1:B:76:GLY:HA2	1:B:102:ALA:HB3	2.01	0.41
1:A:48:VAL:HG11	1:A:94:PHE:CZ	2.55	0.41
1:A:75:ILE:HB	1:A:81:GLY:H	1.86	0.41
1:B:101:ILE:HG23	1:B:103:ARG:H	1.86	0.41
1:A:521:GLY:O	1:A:539:ALA:HA	2.21	0.40
1:A:77:LEU:HD12	1:A:77:LEU:HA	1.94	0.40
1:A:84:THR:OG1	1:A:85:GLU:N	2.49	0.40
1:B:75:ILE:O	1:B:80:GLY:HA3	2.21	0.40
1:B:288:ILE:HG22	1:B:326:TYR:HB2	2.03	0.40
1:A:220:LYS:H	1:A:220:LYS:HE2	1.87	0.40
1:B:74:GLN:HB2	1:B:117:PHE:HZ	1.86	0.40
1:B:177:LYS:C	1:B:178:MET:HE2	2.46	0.40
1:B:135:LYS:O	1:B:138:GLU:HB2	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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	617/674 (92%)	583 (94%)	32 (5%)	2 (0%)	36	65
1	B	612/674 (91%)	580 (95%)	31 (5%)	1 (0%)	43	72
All	All	1229/1348 (91%)	1163 (95%)	63 (5%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	B	19	VAL
1	A	19	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	523/565 (93%)	515 (98%)	8 (2%)	57	84
1	B	521/565 (92%)	514 (99%)	7 (1%)	61	86
All	All	1044/1130 (92%)	1029 (99%)	15 (1%)	59	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	225	CYS
1	A	229	LYS
1	A	264	VAL
1	A	367	CYS
1	A	377	GLN
1	A	479	THR
1	A	632	LEU
1	B	18	SER
1	B	46	ILE
1	B	61	CYS
1	B	160	ASN
1	B	264	VAL

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Mol	Chain	Res	Type
1	B	359	VAL
1	B	636	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	ASN
1	A	462	ASN
1	B	378	ASN

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 20 ligands modelled in this entry, 12 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	$\# Z > 2$
3	SF4	A	703	1	0,12,12	-	-	-		
3	SF4	B	704	1	0,12,12	-	-	-		
2	402	A	701	1	15,19,19	2.27	6 (40%)	1,36,36	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	B	703	1	0,12,12	-	-	-		
3	SF4	A	704	1	0,12,12	-	-	-		
3	SF4	A	702	1	0,12,12	-	-	-		
2	402	B	701	1	15,19,19	2.28	6 (40%)	1,36,36	0.93	0
3	SF4	B	702	1	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
3	SF4	A	703	1	-	-	0/6/5/5
3	SF4	B	704	1	-	-	0/6/5/5
2	402	A	701	1	-	-	0/5/3/3
3	SF4	B	703	1	-	-	0/6/5/5
3	SF4	A	704	1	-	-	0/6/5/5
3	SF4	A	702	1	-	-	0/6/5/5
2	402	B	701	1	-	-	0/5/3/3
3	SF4	B	702	1	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	402	S2-FE2	5.04	2.33	2.26
2	A	701	402	S2-FE2	5.02	2.33	2.26
2	B	701	402	S2-FE1	5.01	2.33	2.26
2	A	701	402	S2-FE1	5.00	2.33	2.26
2	B	701	402	C1-S1	2.66	1.89	1.85
2	A	701	402	C1-S1	2.61	1.89	1.85
2	B	701	402	C6-N6	2.34	1.18	1.15
2	A	701	402	C2-S2	2.30	1.89	1.85
2	B	701	402	C2-S2	2.29	1.89	1.85
2	A	701	402	C4-N4	2.29	1.18	1.15
2	A	701	402	C6-N6	2.28	1.18	1.15
2	B	701	402	C4-N4	2.27	1.18	1.15

There are no bond angle outliers.

There are no chirality outliers.

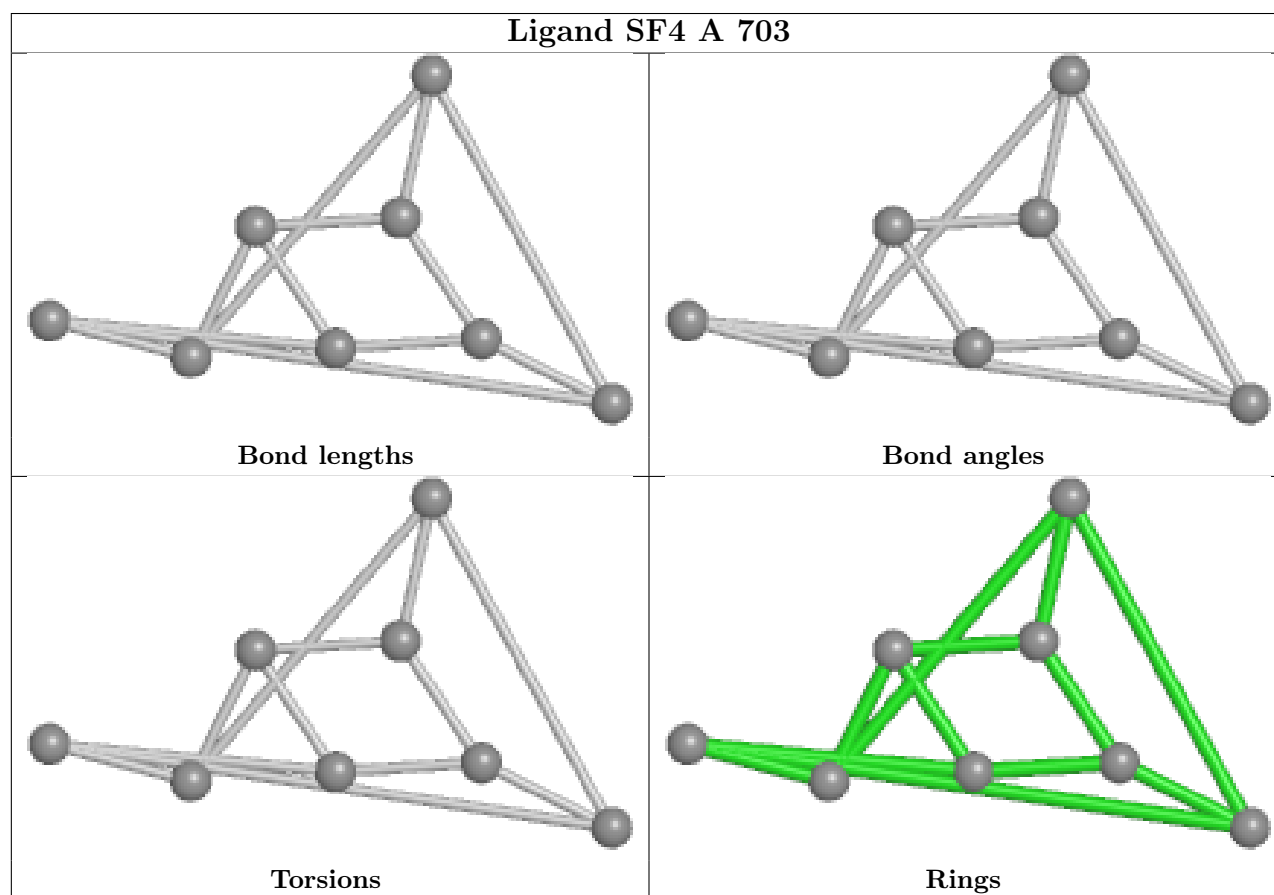
There are no torsion outliers.

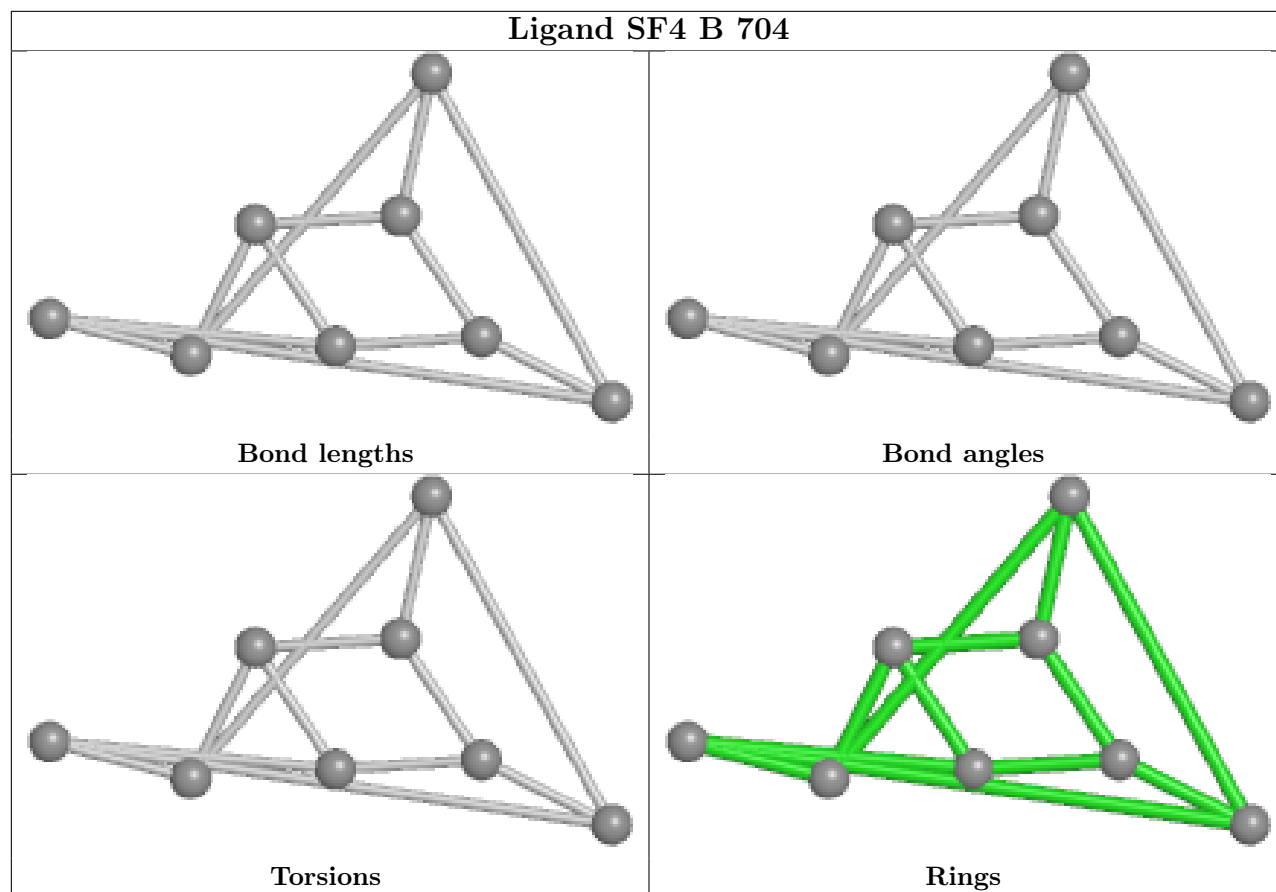
There are no ring outliers.

2 monomers are involved in 16 short contacts:

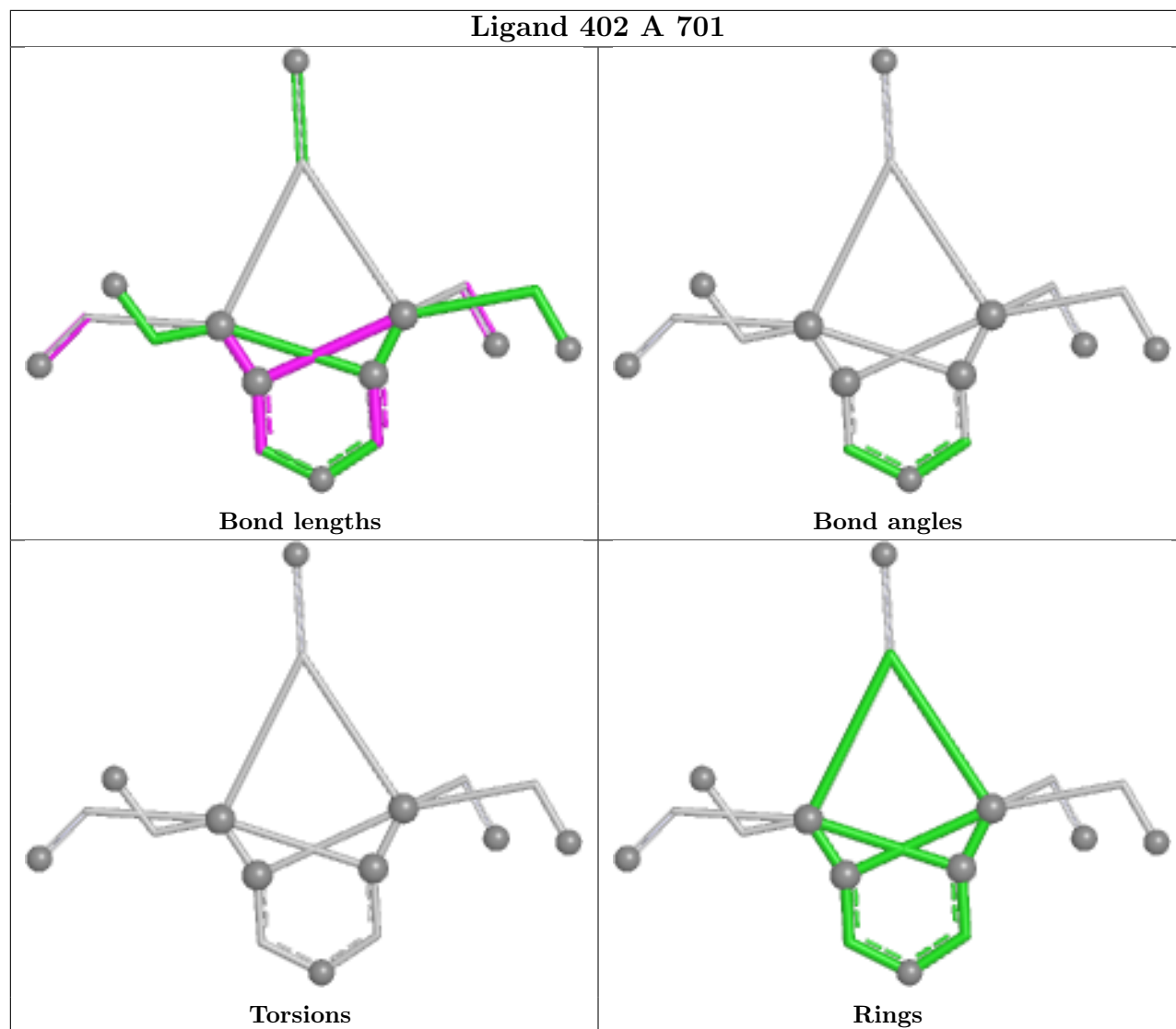
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	402	7	0
2	B	701	402	9	0

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 than 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.

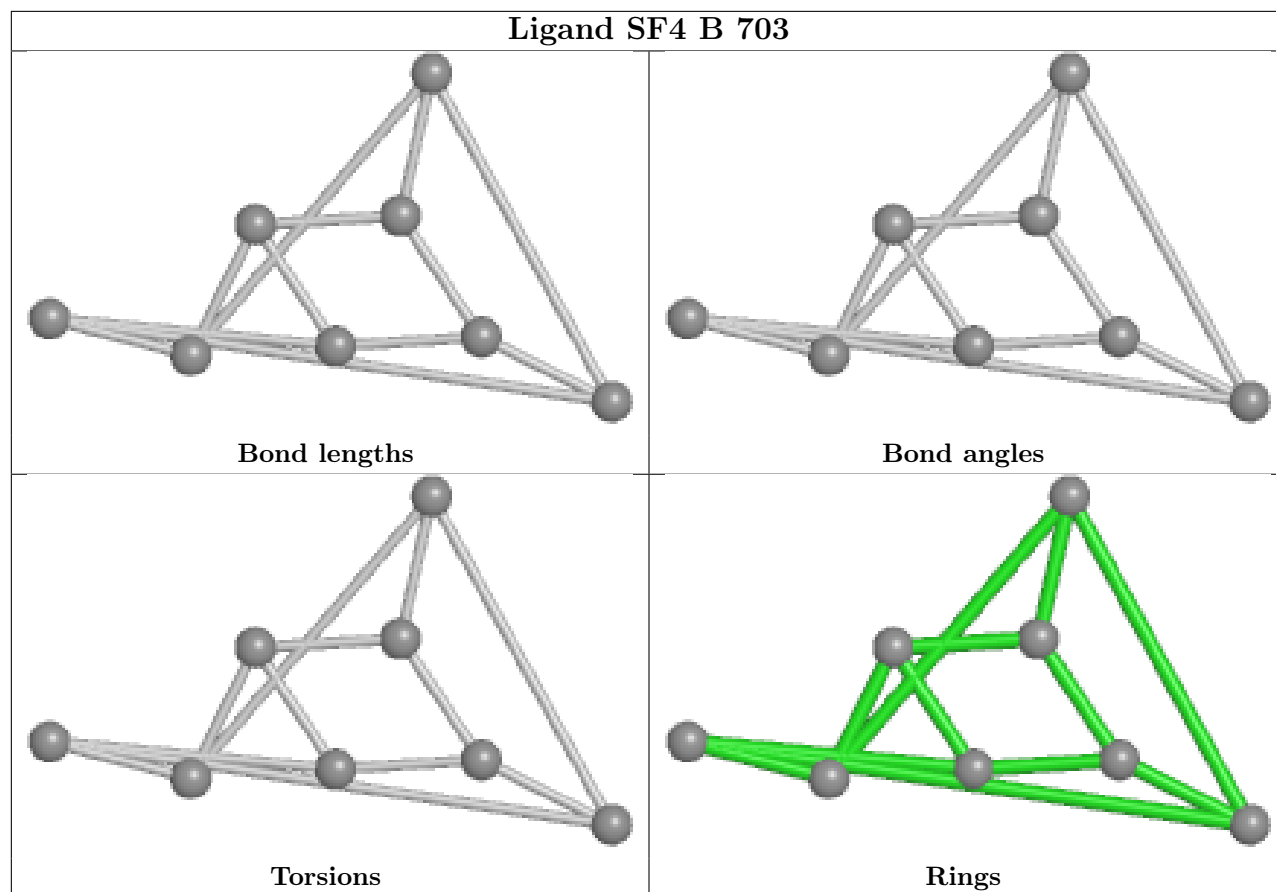




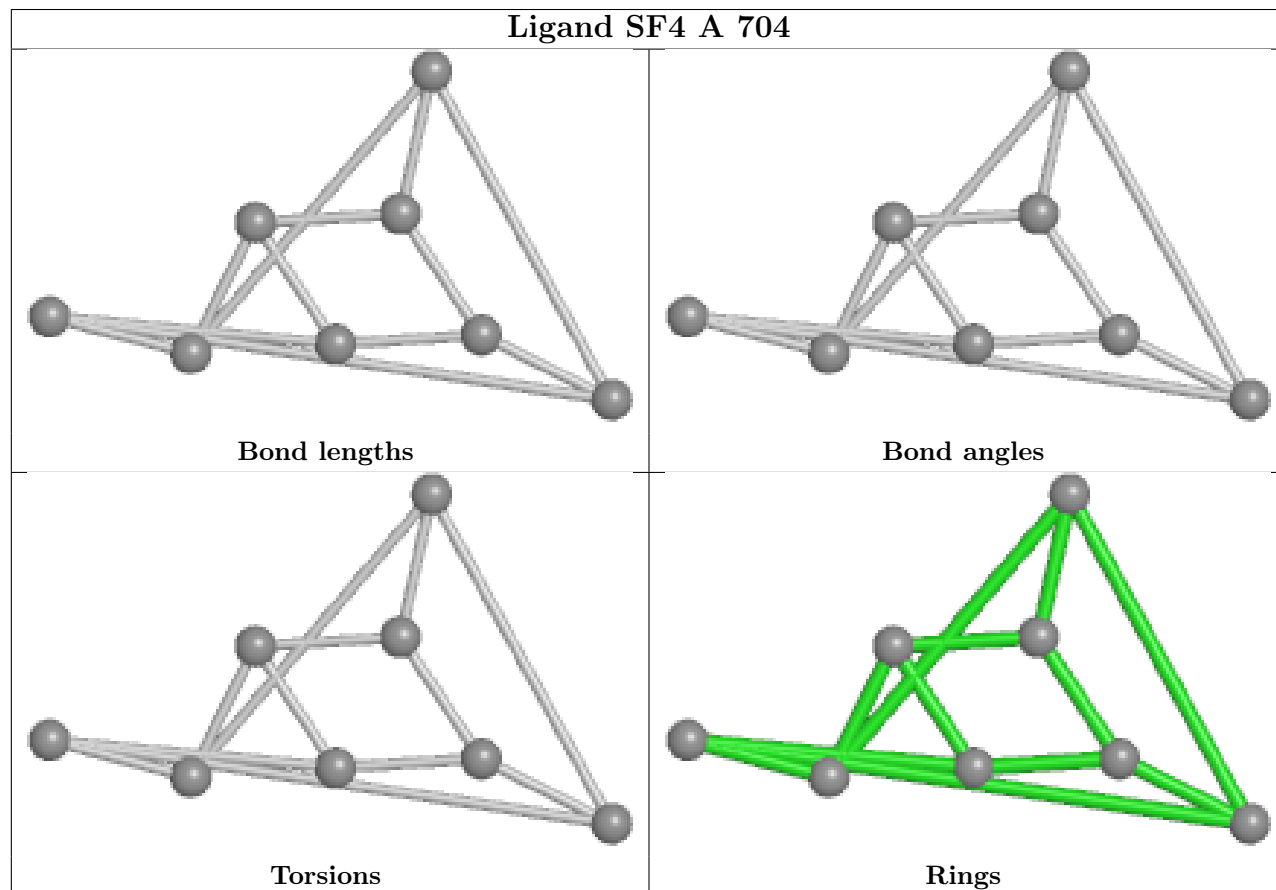
Ligand 402 A 701

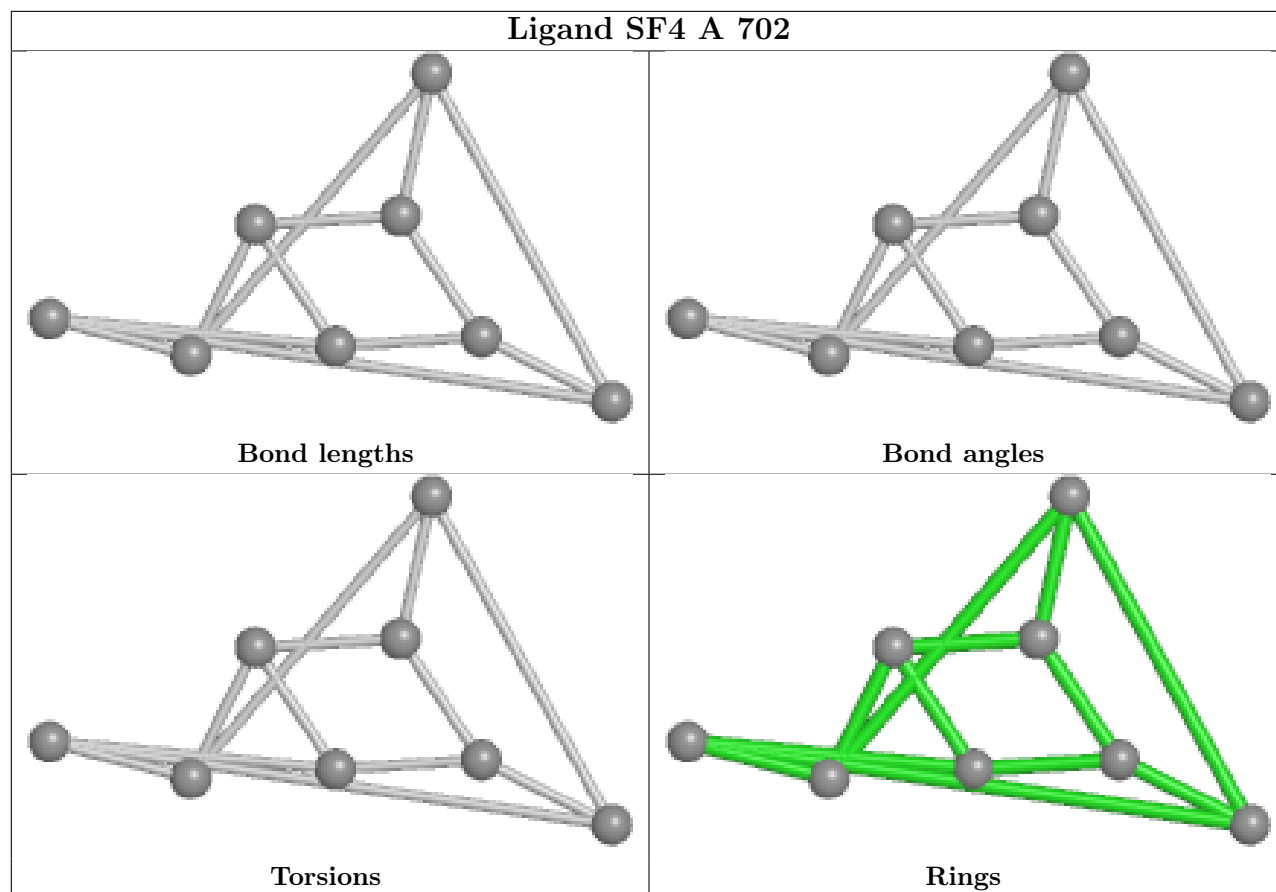


Ligand SF4 B 703

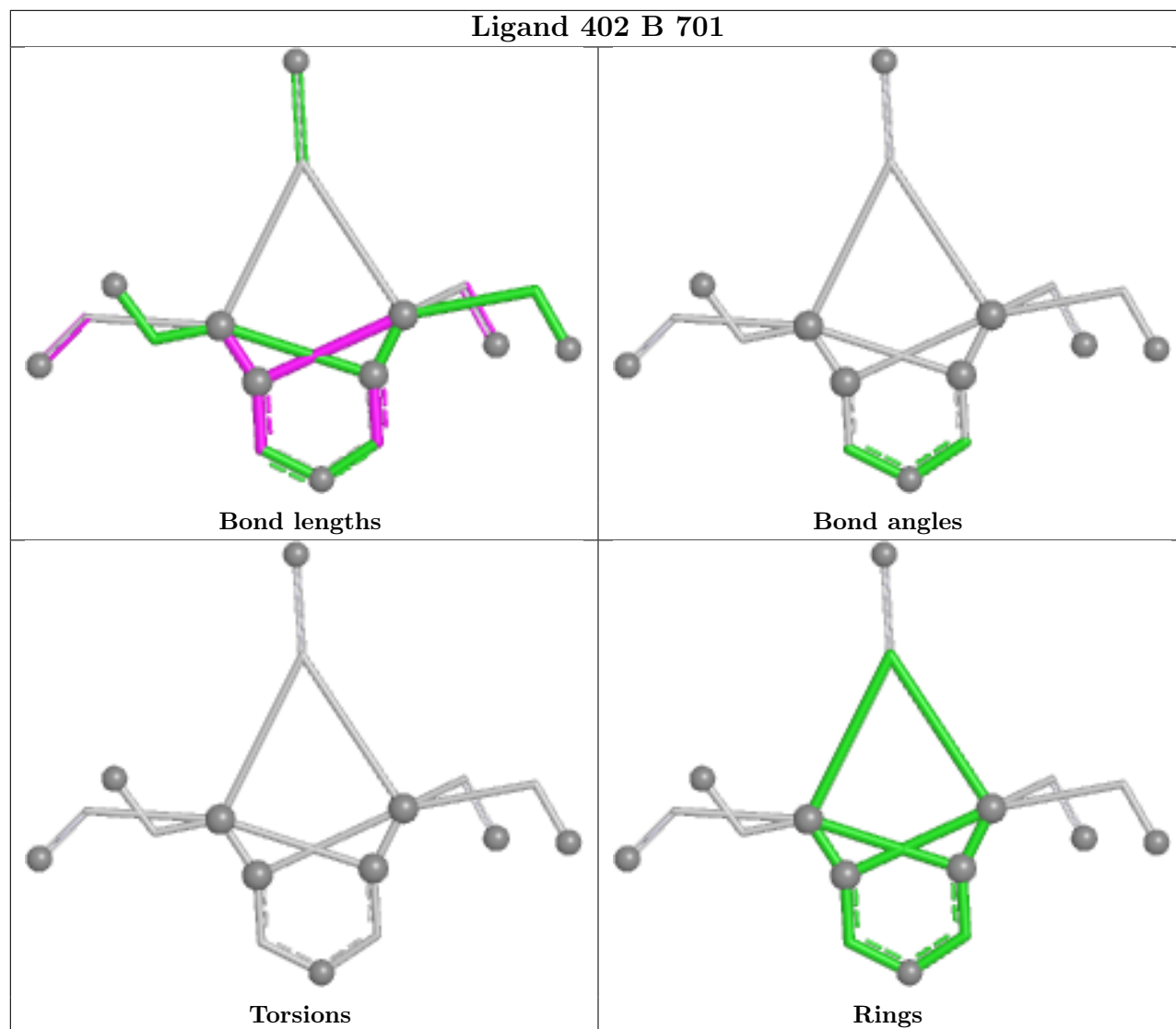


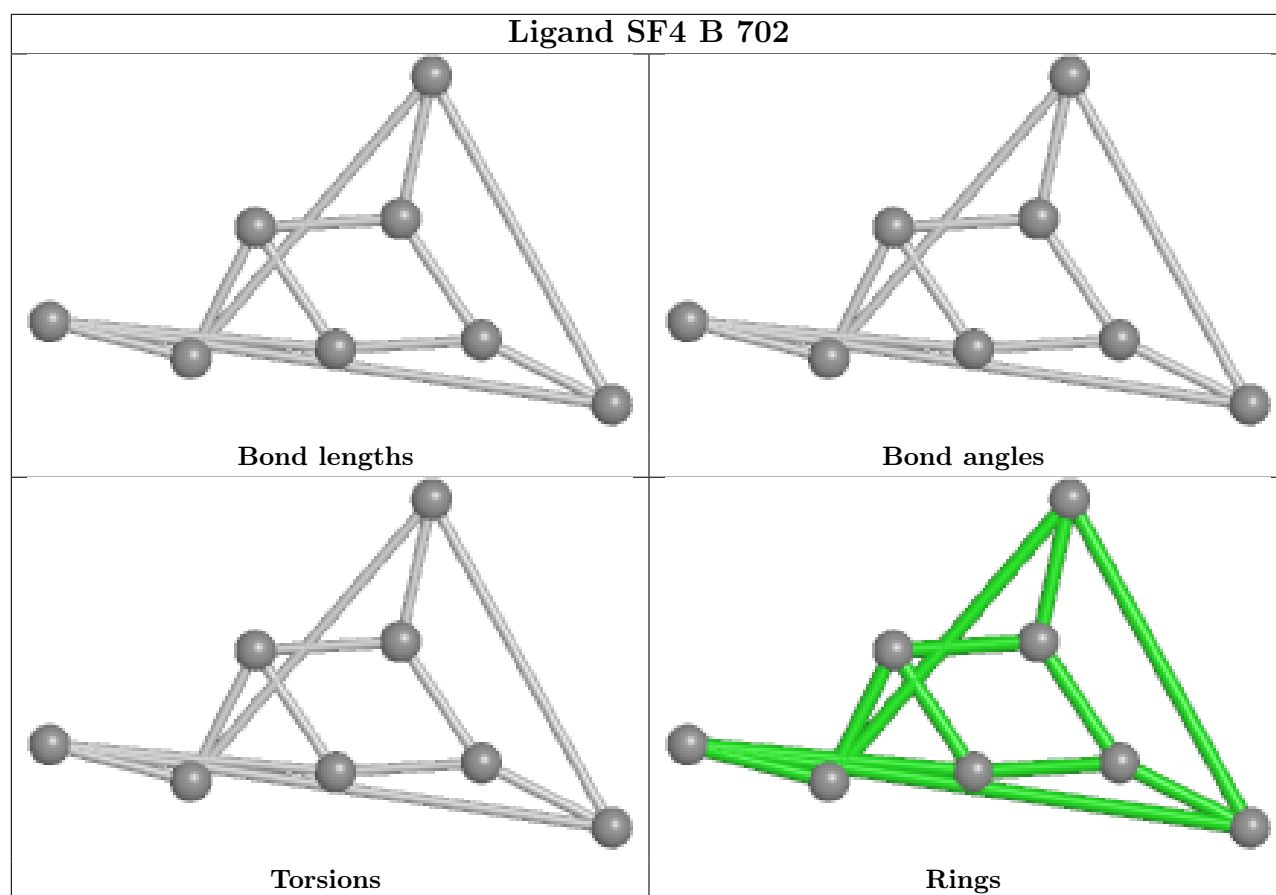
Ligand SF4 A 704





Ligand 402 B 701





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	621/674 (92%)	0.67	41 (6%)	24 19	59, 87, 135, 192	0
1	B	618/674 (91%)	0.75	55 (8%)	15 13	58, 88, 153, 203	0
All	All	1239/1348 (91%)	0.71	96 (7%)	19 16	58, 87, 144, 203	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	VAL	5.6
1	A	19	VAL	5.0
1	A	17	PHE	4.8
1	B	101	ILE	4.5
1	A	20	PHE	4.3
1	B	17	PHE	4.3
1	A	96	ILE	4.1
1	B	20	PHE	3.9
1	B	21	SER	3.9
1	B	45	ILE	3.8
1	B	239	GLY	3.8
1	B	52	ALA	3.8
1	B	241	LEU	3.8
1	A	77	LEU	3.7
1	A	54	LEU	3.6
1	B	92	PHE	3.5
1	B	57	ILE	3.5
1	B	225	CYS	3.4
1	B	60	LEU	3.3
1	B	48	VAL	3.3
1	A	264	VAL	3.3
1	B	49	PRO	3.3
1	B	105	ILE	3.3
1	A	639	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	88	LEU	3.3
1	B	22	GLU	3.2
1	B	96	ILE	3.2
1	B	94	PHE	3.1
1	A	516	LEU	3.1
1	A	383	LEU	3.1
1	A	15	SER	3.1
1	B	87	SER	3.1
1	A	229	LYS	3.1
1	B	37	CYS	3.0
1	A	263	PRO	3.0
1	B	13	LEU	3.0
1	B	79	PHE	2.9
1	B	104	THR	2.9
1	B	97	PHE	2.9
1	B	31	GLY	2.9
1	B	102	ALA	2.9
1	B	44	GLY	2.8
1	B	18	SER	2.8
1	B	46	ILE	2.8
1	B	98	TYR	2.8
1	B	447	ILE	2.7
1	A	102	ALA	2.7
1	B	266	ALA	2.7
1	B	14	GLY	2.7
1	B	19	VAL	2.7
1	B	616	ILE	2.6
1	B	227	ALA	2.6
1	A	18	SER	2.6
1	B	264	VAL	2.6
1	B	15	SER	2.5
1	B	263	PRO	2.5
1	B	70	PHE	2.5
1	A	45	ILE	2.5
1	A	566	ALA	2.5
1	A	65	ILE	2.4
1	A	466	ILE	2.4
1	A	38	GLY	2.4
1	A	244	LYS	2.4
1	B	47	GLU	2.4
1	B	262	CYS	2.4
1	A	451	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	2.4
1	A	36	ILE	2.4
1	A	103	ARG	2.3
1	B	132	GLY	2.3
1	B	249	TYR	2.3
1	A	613	VAL	2.3
1	A	78	PRO	2.3
1	A	80	GLY	2.3
1	B	55	ASN	2.2
1	A	16	VAL	2.2
1	B	245	HIS	2.2
1	A	12	ALA	2.2
1	A	471	ILE	2.2
1	A	492	ILE	2.2
1	A	241	LEU	2.2
1	A	49	PRO	2.1
1	B	41	ASN	2.1
1	A	259	VAL	2.1
1	A	106	ILE	2.1
1	A	184	ILE	2.1
1	B	182	HIS	2.1
1	B	321	LYS	2.1
1	B	240	GLU	2.1
1	A	428	TYR	2.1
1	A	13	LEU	2.0
1	A	218	ILE	2.0
1	A	23	GLU	2.0
1	B	42	ASN	2.0
1	B	587	ALA	2.0
1	B	274	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

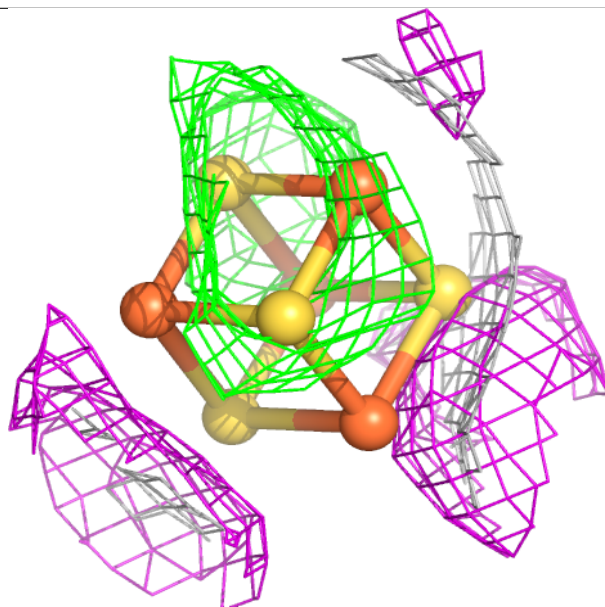
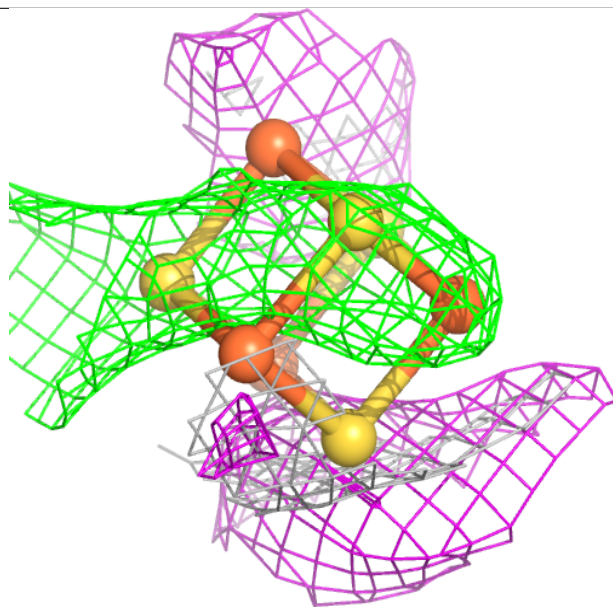
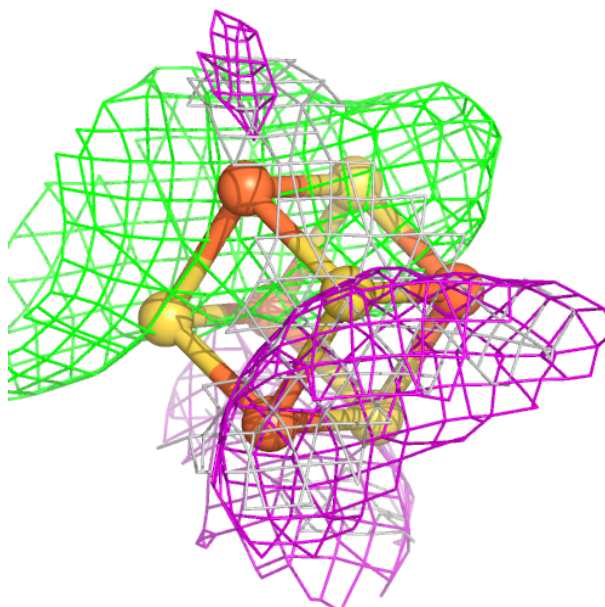
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	A	707	1/1	0.81	0.30	101,101,101,101	0
5	CL	B	706	1/1	0.83	0.13	103,103,103,103	0
5	CL	A	710	1/1	0.85	0.41	94,94,94,94	0
5	CL	A	708	1/1	0.85	0.32	91,91,91,91	0
5	CL	A	706	1/1	0.86	0.22	73,73,73,73	0
5	CL	B	707	1/1	0.86	0.21	73,73,73,73	0
3	SF4	B	703	8/8	0.87	0.13	112,133,153,164	0
5	CL	A	711	1/1	0.90	0.41	100,100,100,100	0
5	CL	A	709	1/1	0.95	0.22	93,93,93,93	0
5	CL	B	709	1/1	0.95	0.15	84,84,84,84	0
3	SF4	A	703	8/8	0.96	0.08	94,107,149,157	0
2	402	B	701	17/17	0.97	0.12	52,69,89,104	0
5	CL	B	708	1/1	0.97	0.24	86,86,86,86	0
3	SF4	A	704	8/8	0.97	0.06	76,94,103,113	0
3	SF4	B	704	8/8	0.98	0.04	74,81,91,101	0
4	ZN	B	705	1/1	0.98	0.10	95,95,95,95	0
3	SF4	B	702	8/8	0.98	0.06	68,78,91,92	0
2	402	A	701	17/17	0.98	0.11	68,77,94,104	0
4	ZN	A	705	1/1	0.99	0.08	76,76,76,76	0
3	SF4	A	702	8/8	0.99	0.04	60,71,83,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

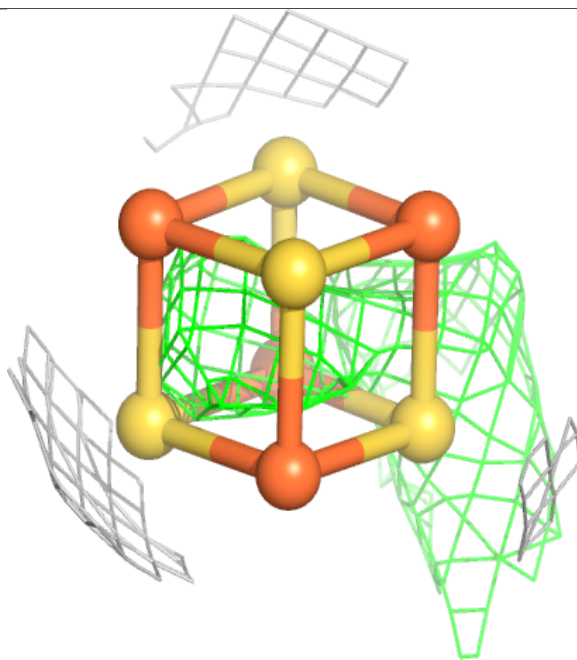
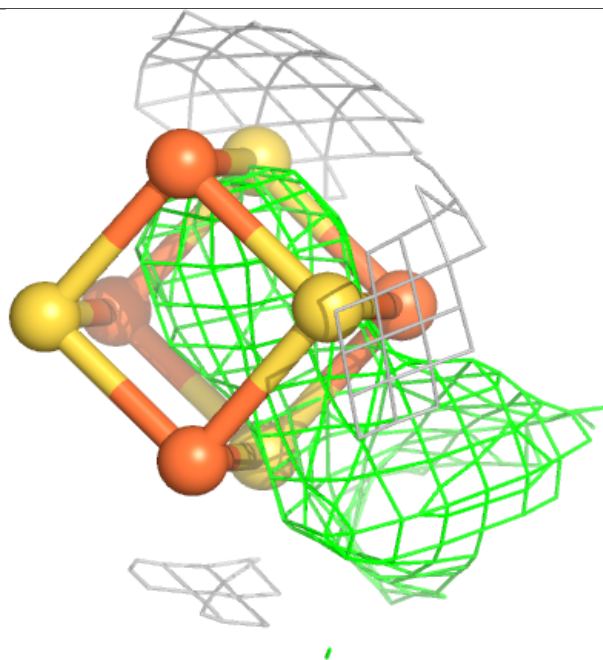
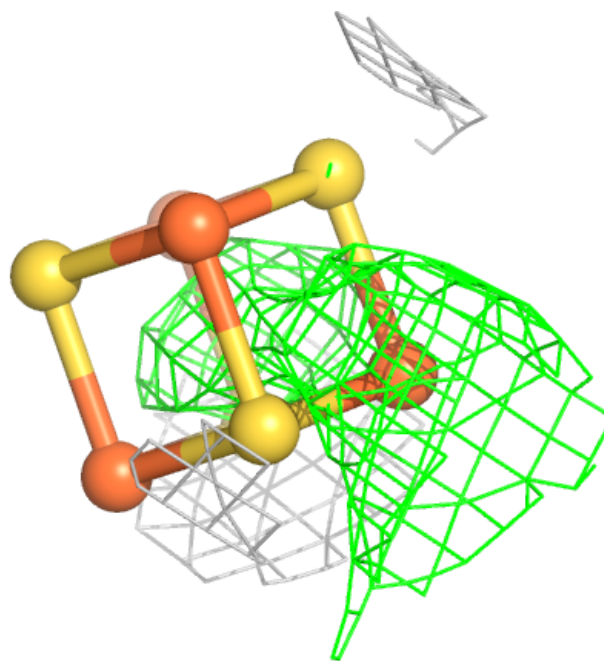
Electron density around SF4 B 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



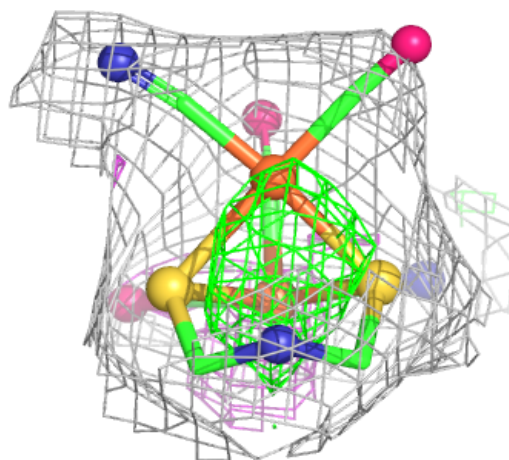
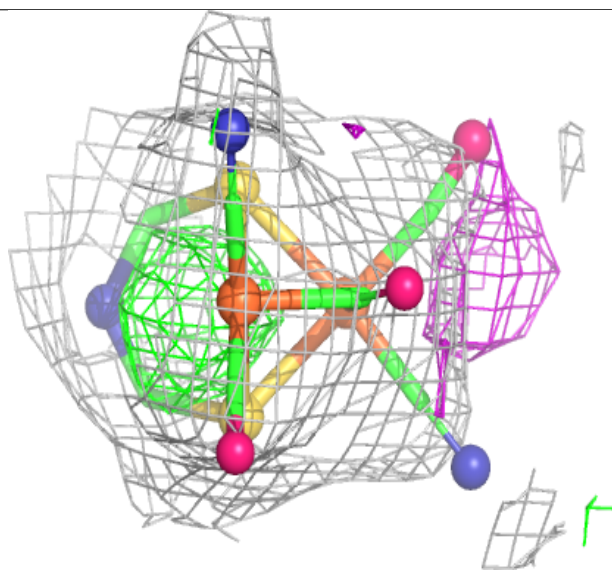
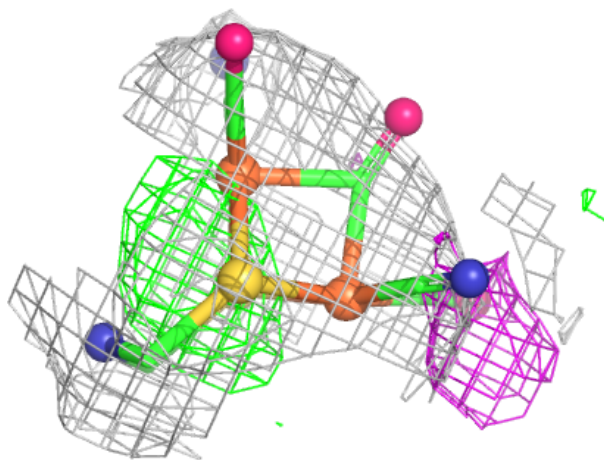
Electron density around SF4 A 703:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



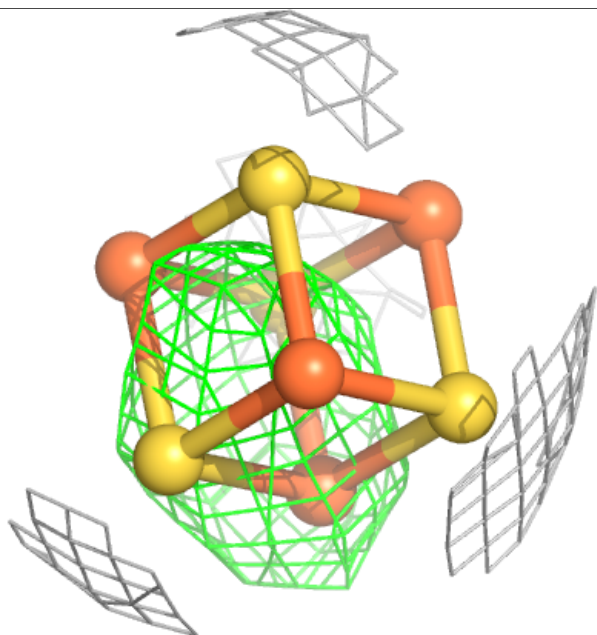
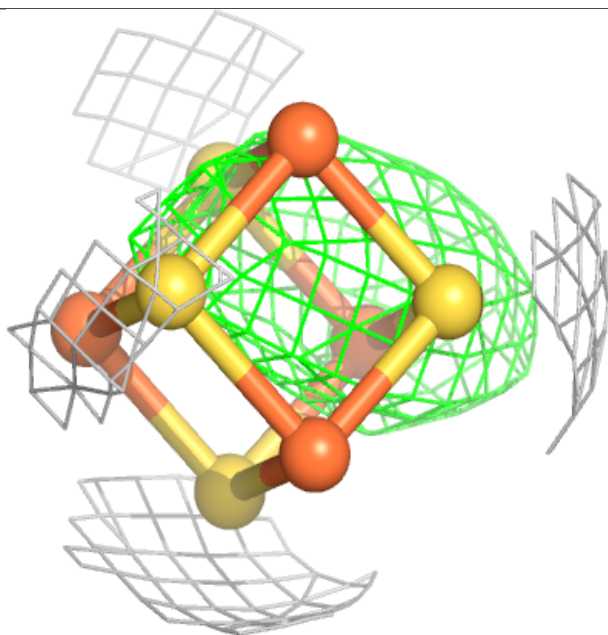
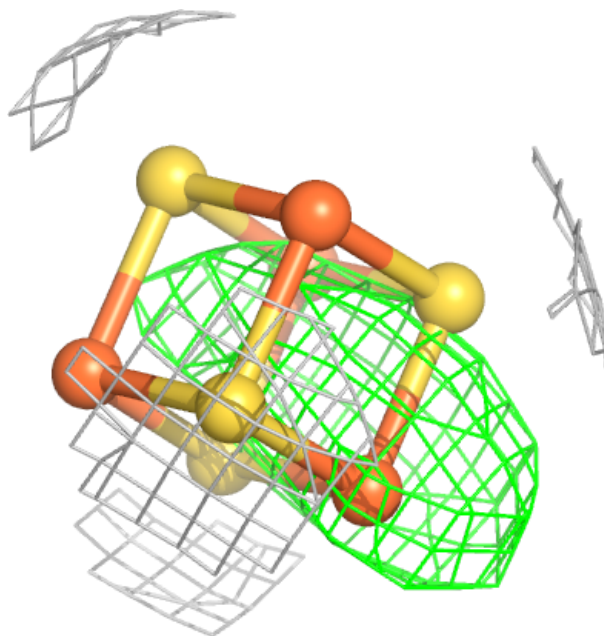
Electron density around 402 B 701:

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and green (positive)



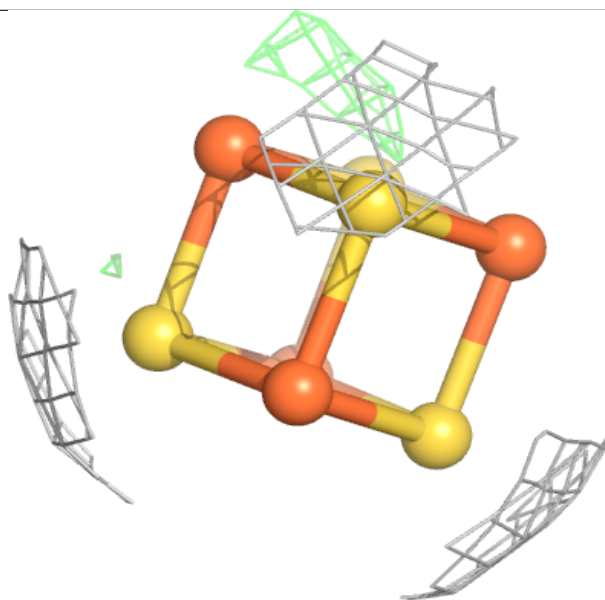
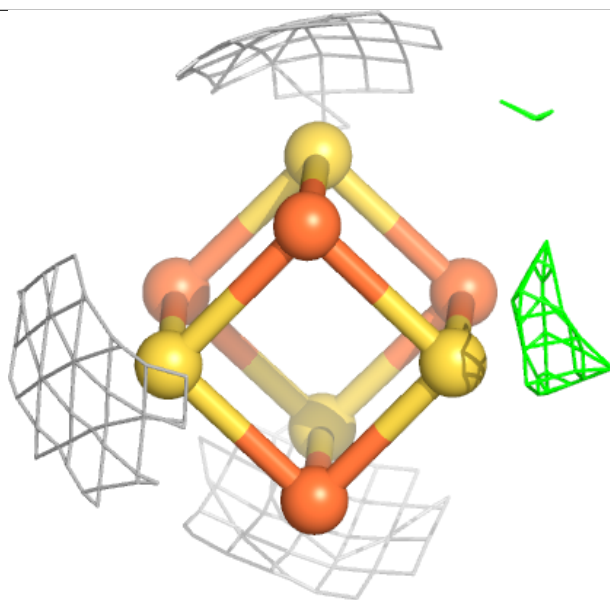
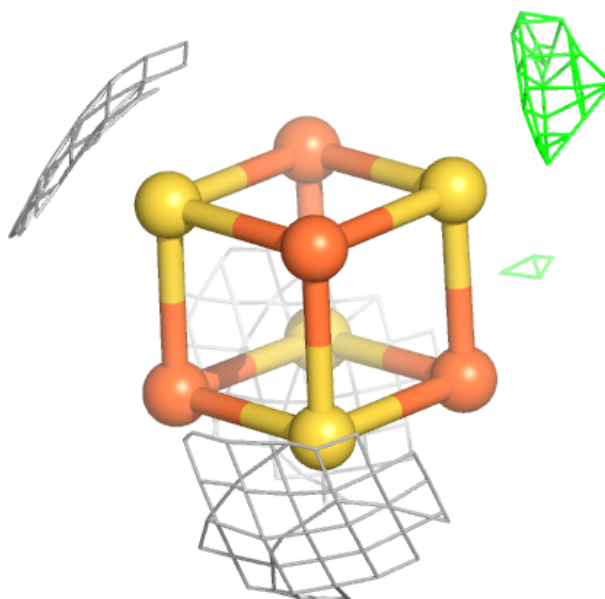
Electron density around SF4 A 704:

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and green (positive)



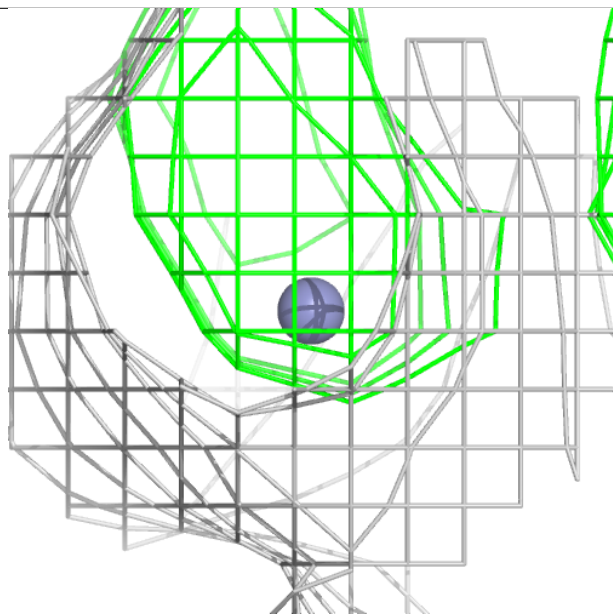
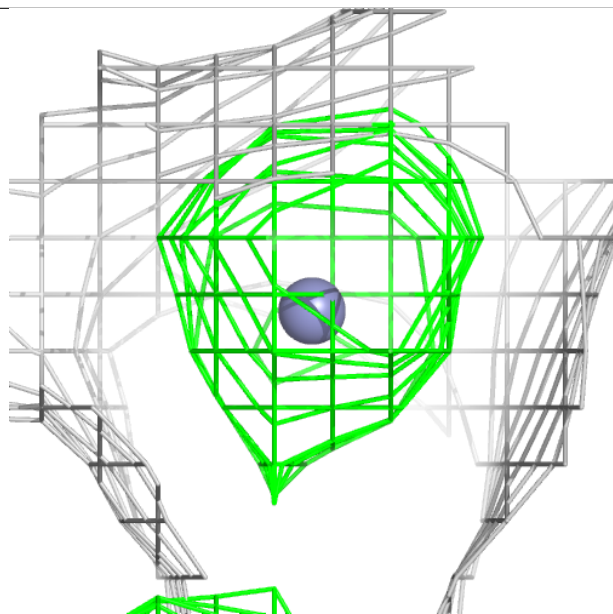
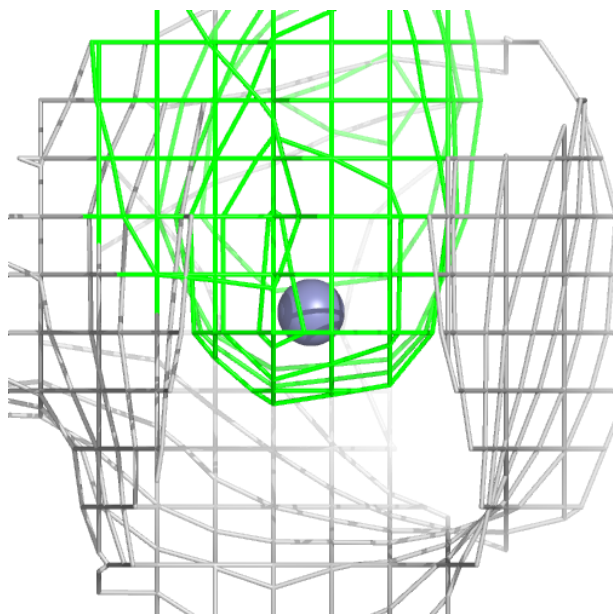
Electron density around SF4 B 704:

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and green (positive)



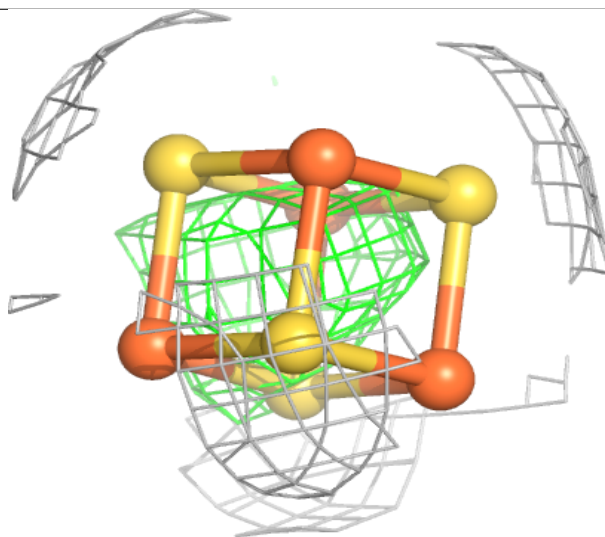
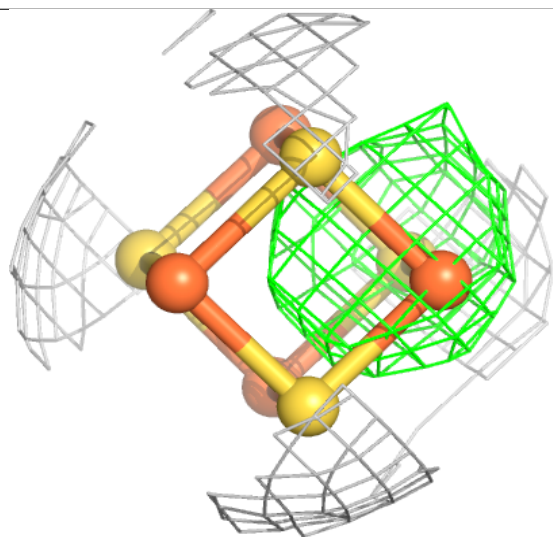
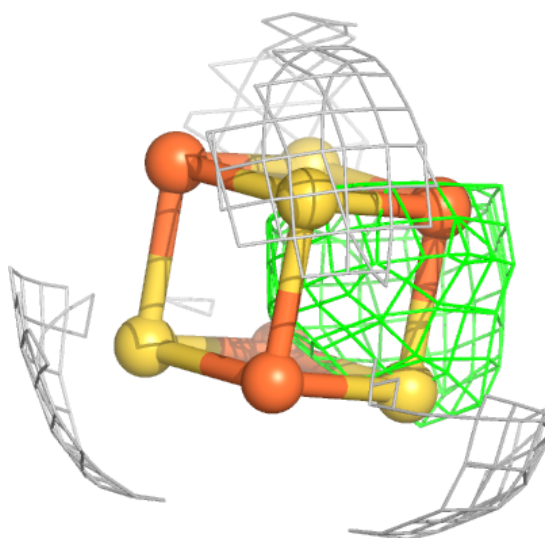
Electron density around ZN B 705:

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and green (positive)



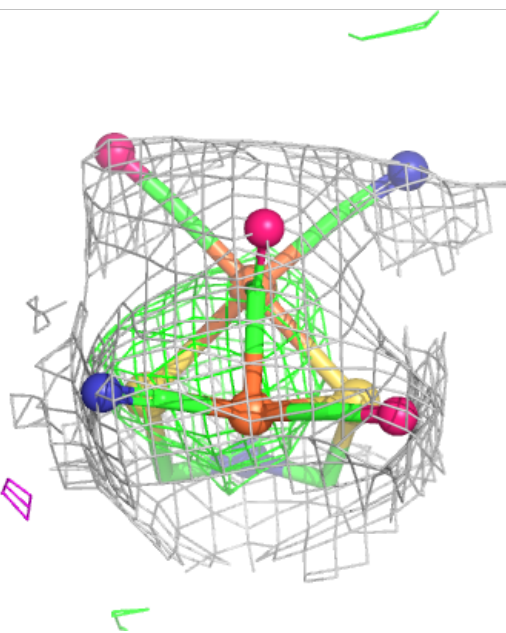
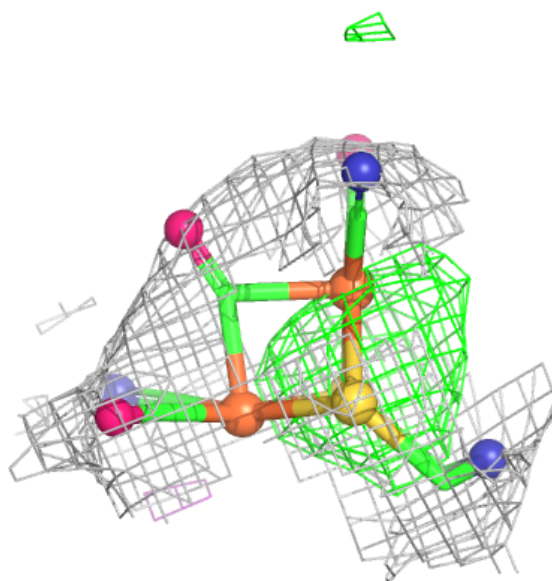
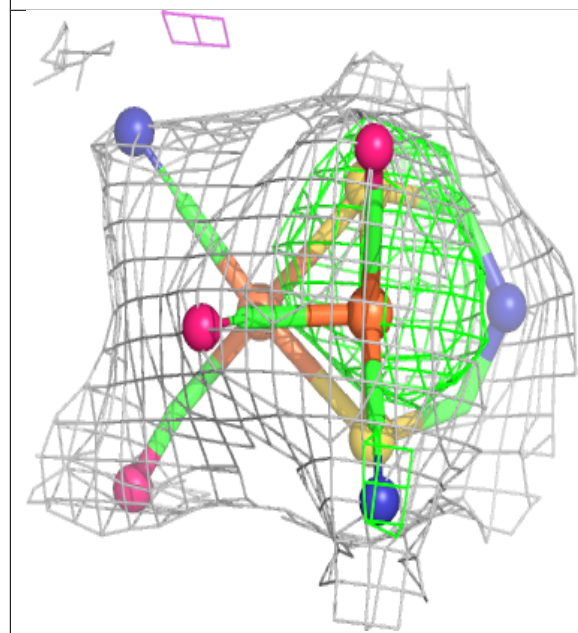
Electron density around SF4 B 702:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



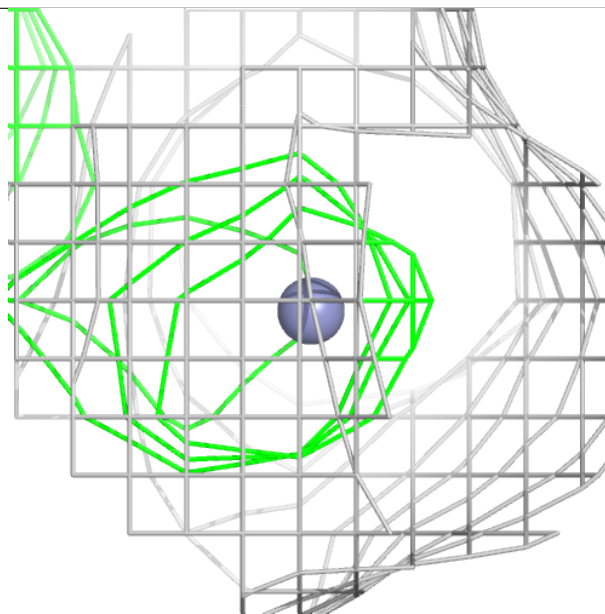
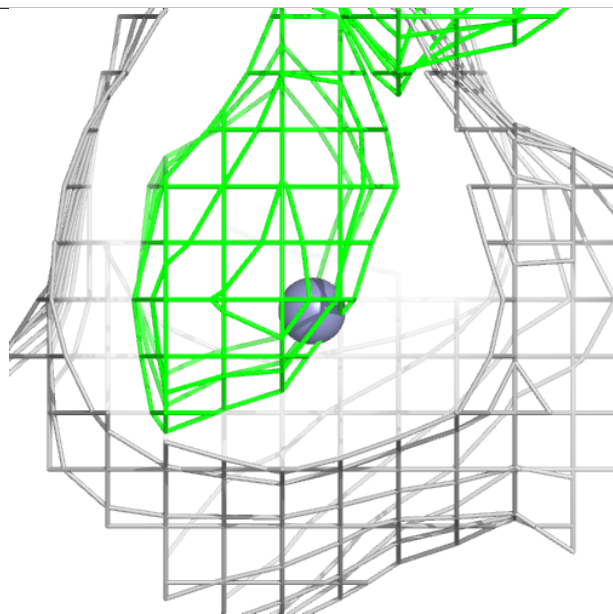
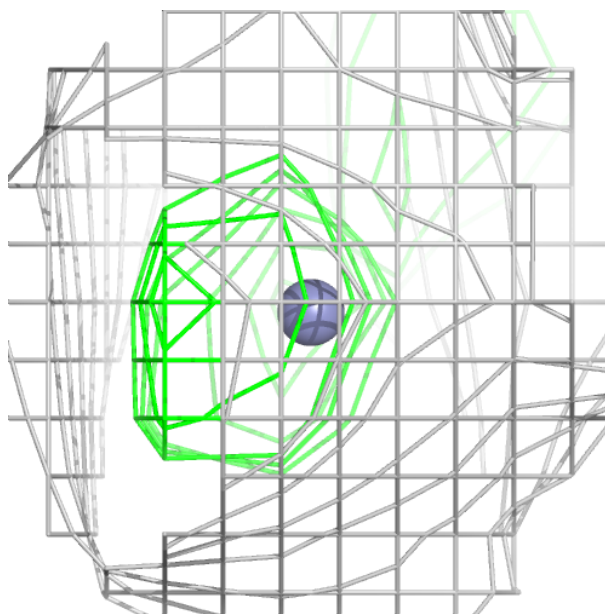
Electron density around 402 A 701:

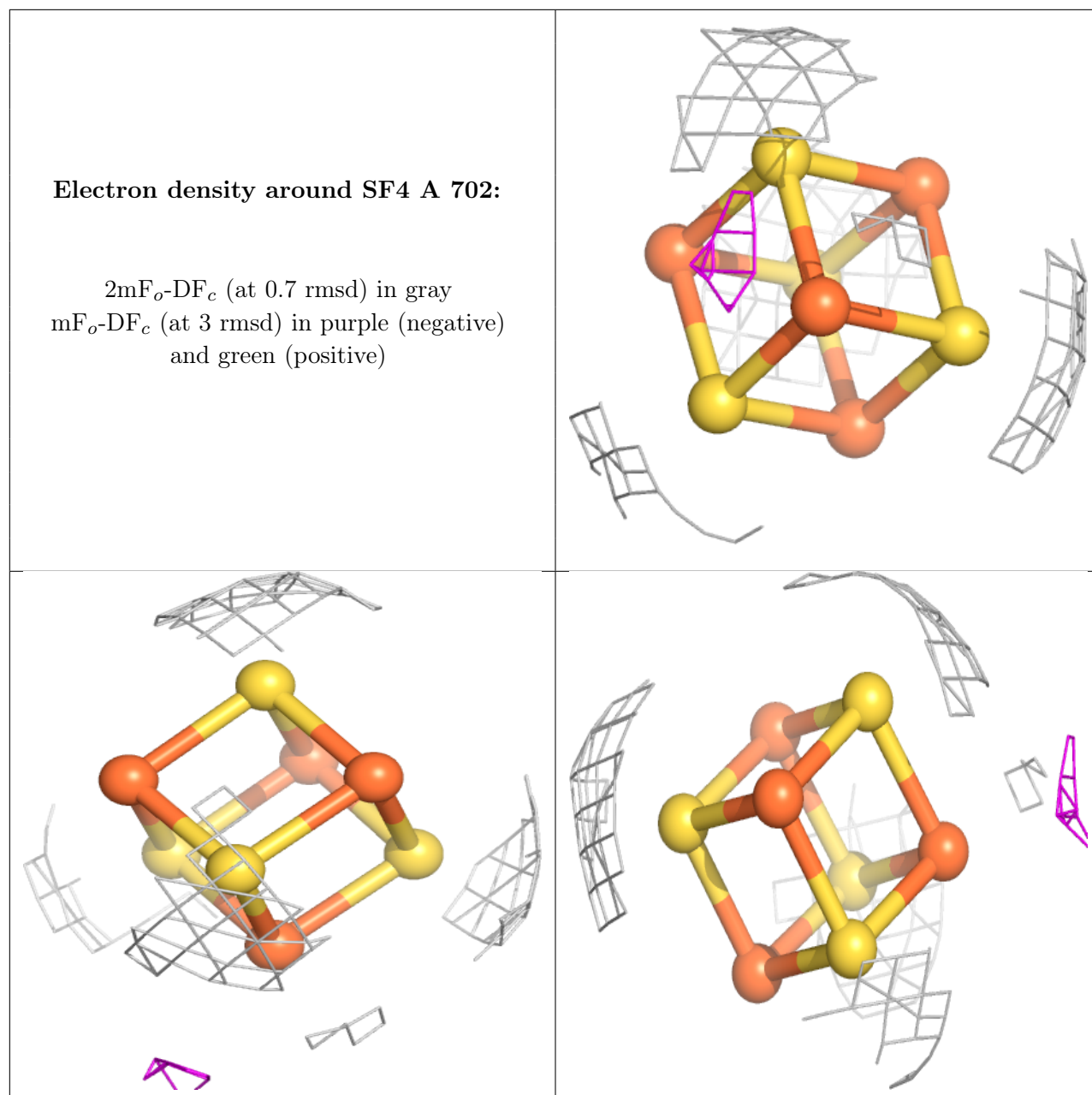
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.