Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2024 – 07:04 pm GMT

PDB ID	:	8CJC
Title	:	F515A variant of the CODH/ACS complex of C. hydrogenoformans
Authors	:	Ruickoldt, J.; Jeoung, J.; Lennartz, F.; Dobbek, H.
Deposited on	:	2023-02-13
Resolution	:	2.22 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 (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 (i)) were used in the production of this report:

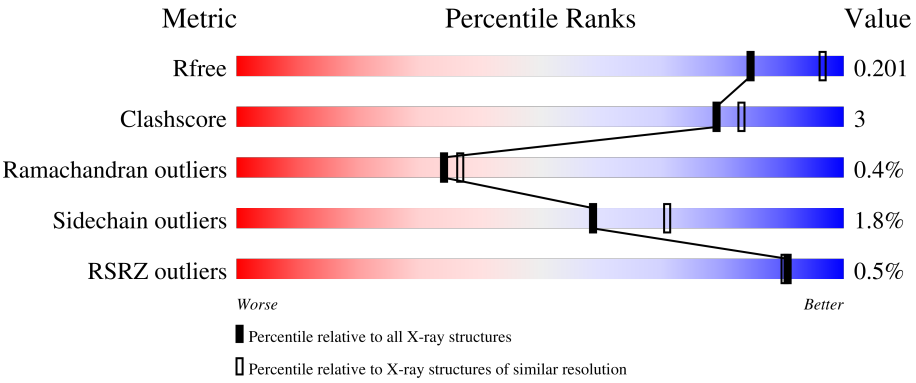
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

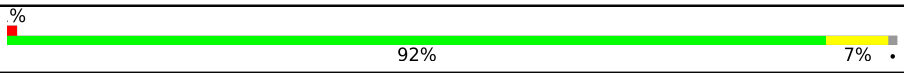
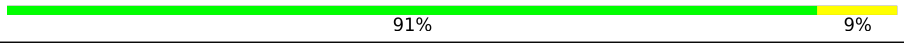
The reported resolution of this entry is 2.22 Å.

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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 <=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	676	
2	B	730	

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
3	RQM	A	701	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11960 atoms, of which 0 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 Carbon monoxide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	669	5147	3264	887	961	35	0	4	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ILE	-	expression tag	UNP A0A1L8D0M5
A	-4	ASN	-	expression tag	UNP A0A1L8D0M5
A	-3	MET	-	expression tag	UNP A0A1L8D0M5
A	-2	PYL	-	expression tag	UNP A0A1L8D0M5
A	-1	ASP	-	expression tag	UNP A0A1L8D0M5
A	0	GLU	-	expression tag	UNP A0A1L8D0M5
A	1	LEU	-	expression tag	UNP A0A1L8D0M5
A	17	ASP	GLU	conflict	UNP A0A1L8D0M5
A	29	ILE	THR	conflict	UNP A0A1L8D0M5
A	73	GLN	MET	conflict	UNP A0A1L8D0M5
A	120	ALA	THR	conflict	UNP A0A1L8D0M5
A	153	THR	ILE	conflict	UNP A0A1L8D0M5
A	159	MET	LEU	conflict	UNP A0A1L8D0M5
A	199	GLU	ASP	conflict	UNP A0A1L8D0M5
A	205	SER	ALA	conflict	UNP A0A1L8D0M5
A	220	ILE	MET	conflict	UNP A0A1L8D0M5
A	389	ILE	VAL	conflict	UNP A0A1L8D0M5
A	393	LEU	PHE	conflict	UNP A0A1L8D0M5
A	494	THR	ALA	conflict	UNP A0A1L8D0M5
A	602	THR	SER	conflict	UNP A0A1L8D0M5

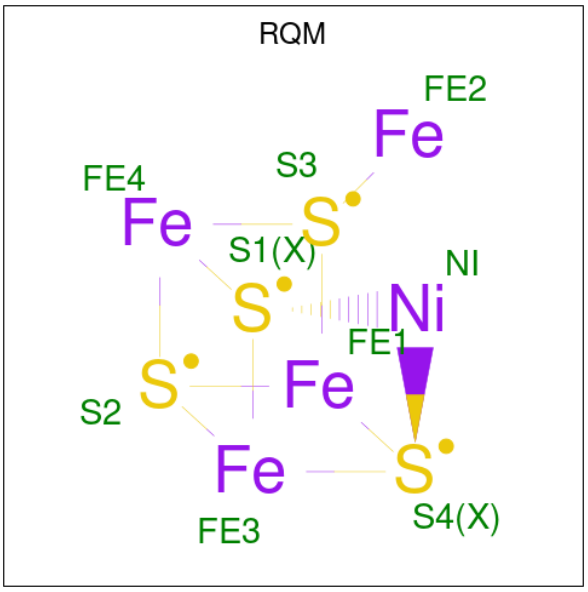
- Molecule 2 is a protein called CO-methylating acetyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	730	5812	3726	976	1081	29	0	7	0

There are 3 discrepancies between the modelled and reference sequences:

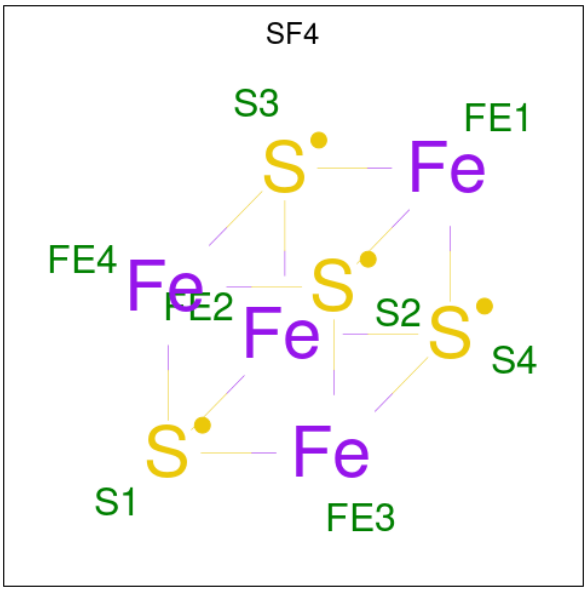
Chain	Residue	Modelled	Actual	Comment	Reference
B	515	ALA	PHE	engineered mutation	UNP Q3ACS4
B	733	ARG	-	expression tag	UNP Q3ACS4
B	734	SER	-	expression tag	UNP Q3ACS4

- Molecule 3 is Fe(3)-Ni(1)-S(4) cluster (three-letter code: RQM) (formula: Fe_4NiS_4) (labeled as "Ligand of Interest" by depositor).



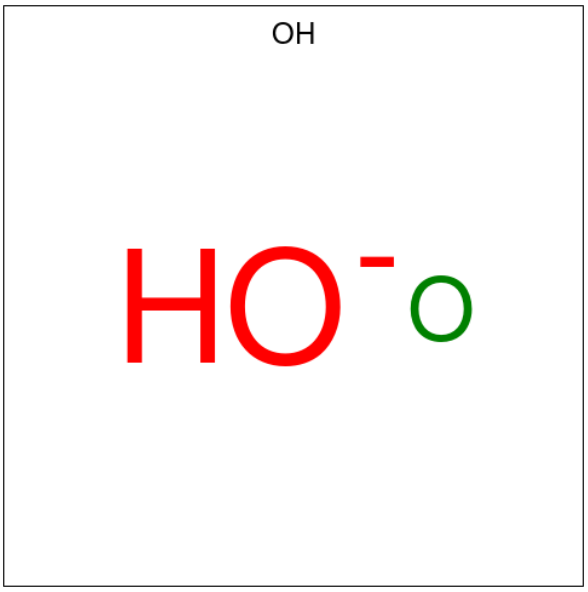
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	Ni	S		
3	A	1	9	4	1	4	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



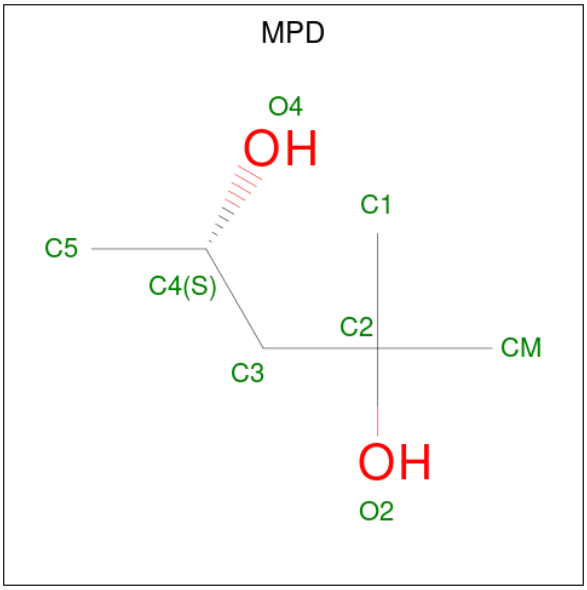
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	A	1	Total O 1 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

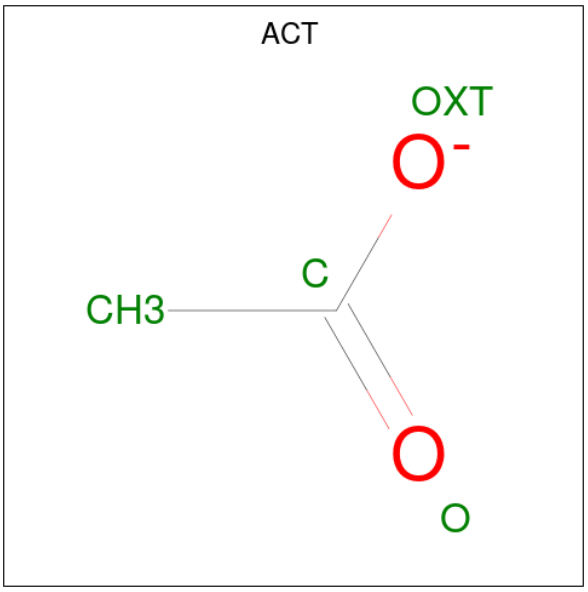


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Ni 2 2	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Na 1 1	0	0

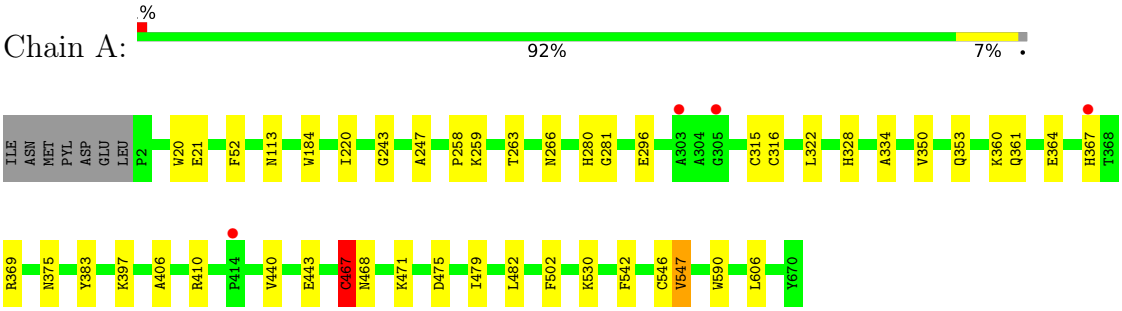
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	399	Total O 399 399	0	0
10	B	540	Total O 540 540	0	0

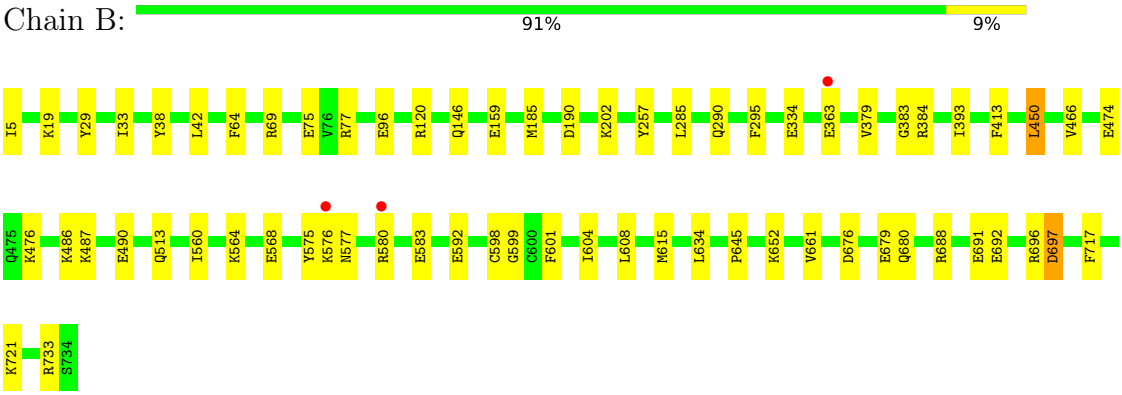
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Carbon monoxide dehydrogenase



• Molecule 2: CO-methylating acetyl-CoA synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.13Å 142.13Å 290.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 2.22 48.45 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-2.22) 99.9 (48.45-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.158 , 0.202 0.156 , 0.201	Depositor DCC
R_{free} test set	2101 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11960	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, OH, MPD, SF4, NI, ACT, RQM

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	0.46	1/5259 (0.0%)	0.62	1/7118 (0.0%)
2	B	0.46	0/5963	0.65	1/8071 (0.0%)
All	All	0.46	1/11222 (0.0%)	0.64	2/15189 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	CYS	CB-SG	5.92	1.92	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	590	TRP	CA-CB-CG	5.86	124.82	113.70
2	B	450	LEU	CA-CB-CG	5.20	127.26	115.30

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	5147	0	5168	23	0
2	B	5812	0	5798	36	0
3	A	9	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	12	0	0	0	0
4	B	8	0	0	0	0
5	A	2	0	0	1	0
6	A	16	0	28	1	0
6	B	8	0	14	3	0
7	B	2	0	0	0	0
8	B	4	0	3	0	0
9	B	1	0	0	0	0
10	A	399	0	0	2	1
10	B	540	0	0	7	0
All	All	11960	0	11011	62	1

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 3.

All (62) 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:A:467:CYS:HB3	3:A:701:RQM:S2	2.07	0.92
1:A:546[B]:CYS:SG	10:A:802:HOH:O	2.28	0.90
2:B:688:ARG:NH1	2:B:691:GLU:OE2	2.11	0.84
2:B:486:LYS:HE2	2:B:490:GLU:OE2	1.79	0.82
2:B:120[A]:ARG:NH1	10:B:901:HOH:O	2.13	0.67
1:A:316:CYS:SG	1:A:546[B]:CYS:HB3	2.42	0.60
1:A:280:HIS:HB3	1:A:350:VAL:HG12	1.82	0.59
2:B:19:LYS:NZ	10:B:911:HOH:O	2.36	0.59
1:A:369:ARG:HD3	1:A:383:TYR:CE1	2.38	0.59
2:B:5:ILE:N	10:B:910:HOH:O	2.36	0.59
2:B:513:GLN:NE2	2:B:577:ASN:O	2.35	0.58
2:B:575:TYR:CZ	2:B:580:ARG:HG2	2.39	0.57
2:B:564:LYS:HE3	2:B:592:GLU:OE2	2.05	0.56
6:A:706:MPD:O4	6:A:706:MPD:O2	2.18	0.56
1:A:367:HIS:CE1	1:A:410:ARG:HD3	2.42	0.55
2:B:75:GLU:OE1	2:B:77:ARG:NH1	2.31	0.55
2:B:568:GLU:OE1	10:B:902:HOH:O	2.18	0.55
1:A:369:ARG:HG3	1:A:406:ALA:HB2	1.90	0.54
1:A:369:ARG:HD3	1:A:383:TYR:CZ	2.44	0.53
2:B:688:ARG:O	2:B:692:GLU:HG3	2.09	0.52
2:B:290[A]:GLN:HB2	2:B:295:PHE:O	2.10	0.52
2:B:560:ILE:HD11	2:B:568:GLU:HG2	1.92	0.52
2:B:717:PHE:O	2:B:721:LYS:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:TYR:CZ	2:B:42:LEU:HD11	2.46	0.51
1:A:296:GLU:OE1	1:A:397:LYS:NZ	2.32	0.49
2:B:393:ILE:HD13	2:B:466:VAL:HG22	1.94	0.48
2:B:285:LEU:HB2	2:B:290[A]:GLN:OE1	2.14	0.47
2:B:379:VAL:CG2	2:B:383:GLY:HA3	2.45	0.47
2:B:486:LYS:NZ	10:B:903:HOH:O	2.19	0.47
2:B:29:TYR:CZ	2:B:33:ILE:HD11	2.50	0.47
2:B:575:TYR:CE2	2:B:580:ARG:HG2	2.49	0.47
1:A:360:LYS:HE3	1:A:364:GLU:OE1	2.15	0.46
2:B:583:GLU:HG2	6:B:806:MPD:H52	1.97	0.46
2:B:487:LYS:NZ	10:B:916:HOH:O	2.47	0.46
1:A:52:PHE:CZ	1:A:471:LYS:HA	2.51	0.45
1:A:440:VAL:HG22	1:A:530:LYS:HG3	1.98	0.45
2:B:575:TYR:CG	6:B:806:MPD:H11	2.51	0.45
1:A:334:ALA:HB2	1:A:468:ASN:HB2	1.98	0.45
1:A:247:ALA:HB3	1:A:547:VAL:HG21	1.99	0.45
1:A:360:LYS:HG2	10:A:986:HOH:O	2.17	0.45
2:B:69:ARG:NH1	2:B:75:GLU:HG3	2.32	0.44
2:B:645:PRO:HB2	2:B:733:ARG:HG2	1.99	0.44
2:B:64:PHE:CE2	2:B:75:GLU:HG2	2.52	0.44
1:A:263:THR:HG21	1:A:322:LEU:HG	2.00	0.44
3:A:701:RQM:S4	5:A:704:OH:O	2.76	0.44
6:B:806:MPD:H52	6:B:806:MPD:H12	2.00	0.43
1:A:258:PRO:O	1:A:259:LYS:HE3	2.19	0.43
2:B:33:ILE:HD13	2:B:33:ILE:HG21	1.81	0.43
1:A:20:TRP:CE2	1:A:21:GLU:HG3	2.53	0.43
2:B:652:LYS:HE3	2:B:680:GLN:HE22	1.82	0.43
2:B:608:LEU:HD11	2:B:615:MET:HB3	2.00	0.43
1:A:113:ASN:OD1	1:A:243:GLY:HA3	2.20	0.42
1:A:281:GLY:H	1:A:315[B]:CYS:HG	1.67	0.42
2:B:676:ASP:HA	2:B:679:GLU:HB2	2.01	0.42
2:B:476:LYS:HD2	2:B:476:LYS:HA	1.82	0.42
2:B:604:ILE:HG21	2:B:634:LEU:HG	2.02	0.42
1:A:482:LEU:HD22	1:A:502:PHE:CD1	2.55	0.41
1:A:475:ASP:O	1:A:479:ILE:HG12	2.21	0.41
2:B:159:GLU:HG3	2:B:185:MET:HB3	2.01	0.41
1:A:443:GLU:H	1:A:443:GLU:CD	2.25	0.41
2:B:413:PHE:O	2:B:450:LEU:HD21	2.21	0.40
2:B:202:LYS:HE2	10:B:907:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1039:HOH:O	10:A:1039:HOH:O[10_444]	2.14	0.06

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	671/676 (99%)	640 (95%)	29 (4%)	2 (0%)	41	45
2	B	735/730 (101%)	720 (98%)	11 (2%)	4 (0%)	29	30
All	All	1406/1406 (100%)	1360 (97%)	40 (3%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	697	ASP
1	A	266	ASN
2	B	190	ASP
2	B	599	GLY
1	A	353	GLN
2	B	661	VAL

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 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	552/554 (100%)	542 (98%)	10 (2%)	59	71
2	B	618/611 (101%)	606 (98%)	12 (2%)	57	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1170/1165 (100%)	1148 (98%)	22 (2%)	59 69

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	TRP
1	A	220	ILE
1	A	328	HIS
1	A	361	GLN
1	A	375[A]	ASN
1	A	375[B]	ASN
1	A	467	CYS
1	A	542	PHE
1	A	547	VAL
1	A	606	LEU
2	B	96	GLU
2	B	146	GLN
2	B	257	TYR
2	B	334	GLU
2	B	363	GLU
2	B	384	ARG
2	B	474	GLU
2	B	576	LYS
2	B	598	CYS
2	B	601	PHE
2	B	696	ARG
2	B	697	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	HIS
2	B	146	GLN
2	B	579	GLN
2	B	680	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are modelled with single atom and 3 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	$\#\|Z\| > 2$
6	MPD	A	707	-	7,7,7	0.33	0	9,10,10	0.38	0
4	SF4	A	703	1	0,12,12	-	-	-		
3	RQM	A	701	1,5	0,12,12	-	-	-		
4	SF4	A	702	1	0,4,12	-	-	-		
4	SF4	B	802	2	0,12,12	-	-	-		
8	ACT	B	804	7	3,3,3	1.41	0	3,3,3	1.31	0
6	MPD	A	706	-	7,7,7	0.25	0	9,10,10	0.22	0
6	MPD	B	806	-	7,7,7	0.41	0	9,10,10	0.87	0

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
6	MPD	A	707	-	-	0/5/5/5	-
4	SF4	A	703	1	-	-	0/6/5/5
3	RQM	A	701	1,5	-	-	0/4/4/4
4	SF4	A	702	1	-	-	0/1/1/5
4	SF4	B	802	2	-	-	0/6/5/5
6	MPD	A	706	-	-	1/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	806	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	806	MPD	C2-C3-C4-O4
6	B	806	MPD	C2-C3-C4-C5
6	A	706	MPD	O2-C2-C3-C4

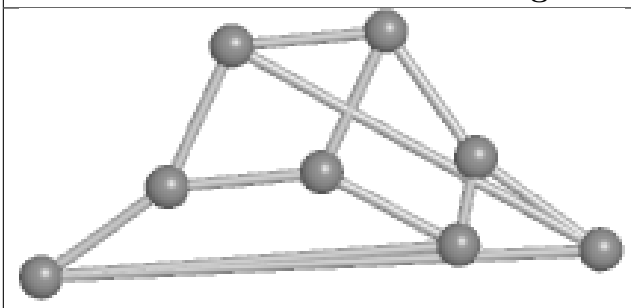
There are no ring outliers.

3 monomers are involved in 6 short contacts:

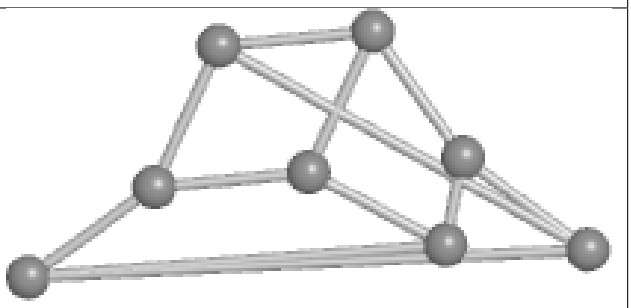
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	RQM	2	0
6	A	706	MPD	1	0
6	B	806	MPD	3	0

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.

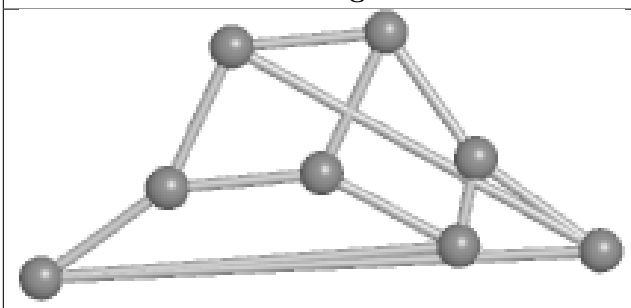
Ligand SF4 A 703



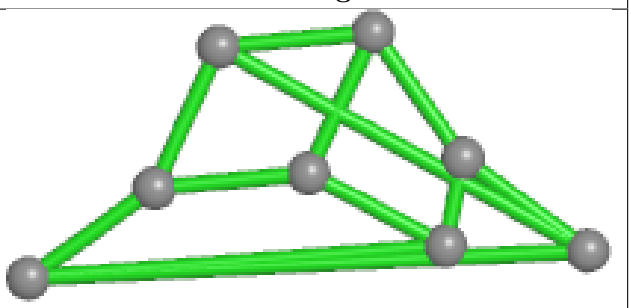
Bond lengths



Bond angles

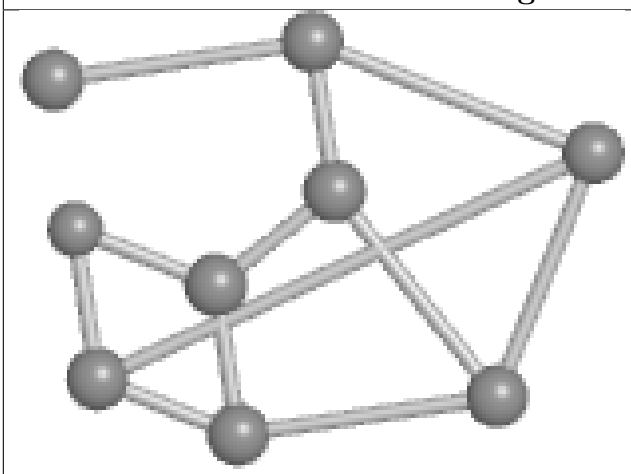


Torsions

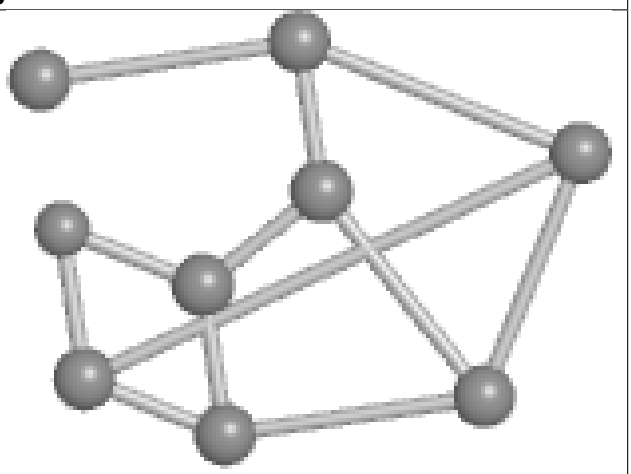


Rings

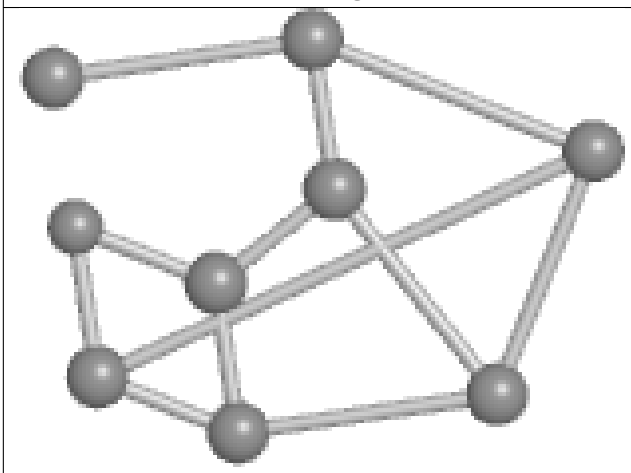
Ligand RQM A 701



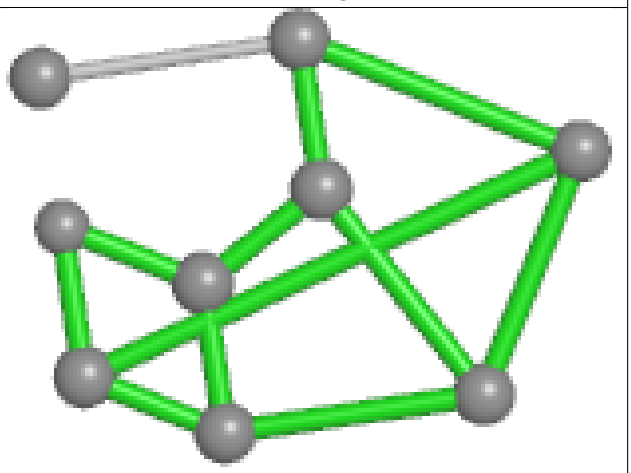
Bond lengths



Bond angles

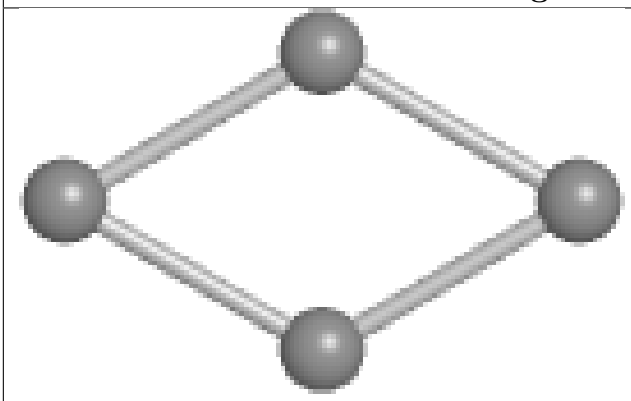


Torsions

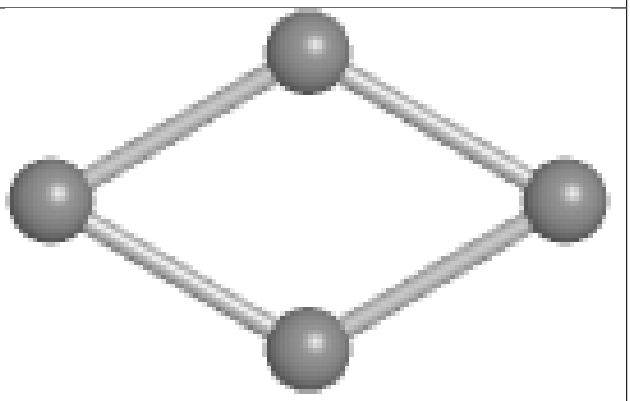


Rings

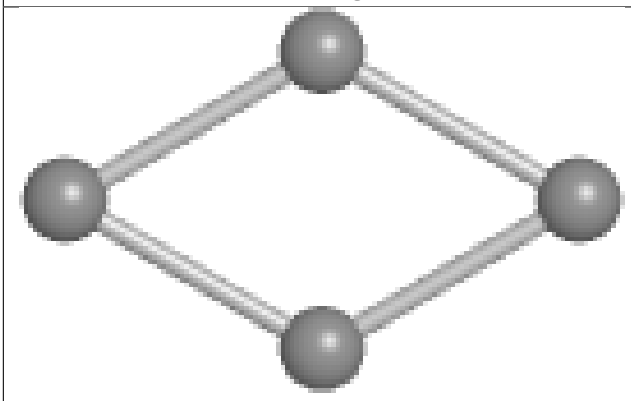
Ligand SF4 A 702



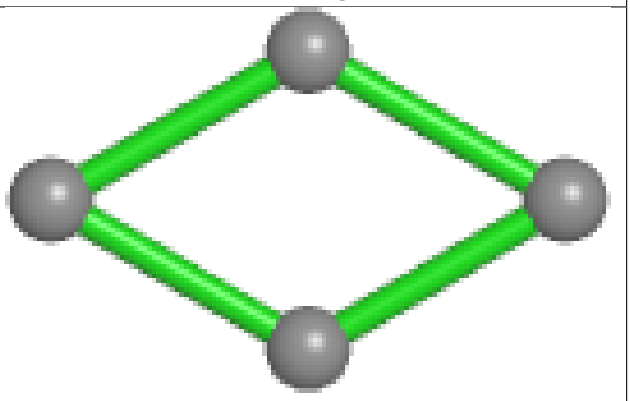
Bond lengths



Bond angles

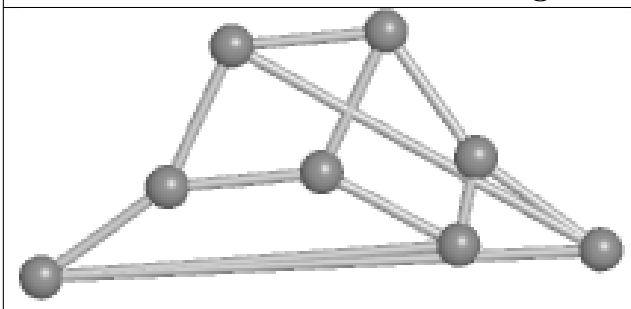


Torsions

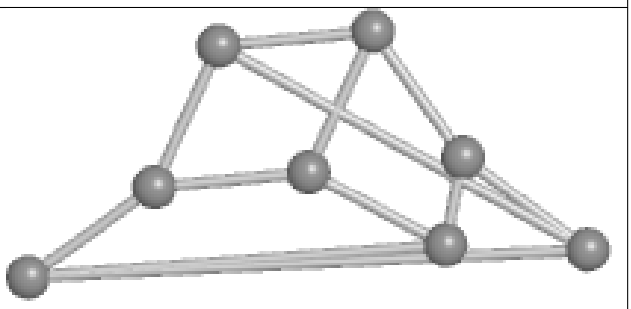


Rings

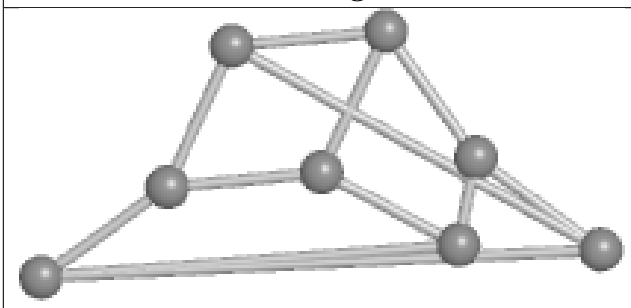
Ligand SF4 B 802



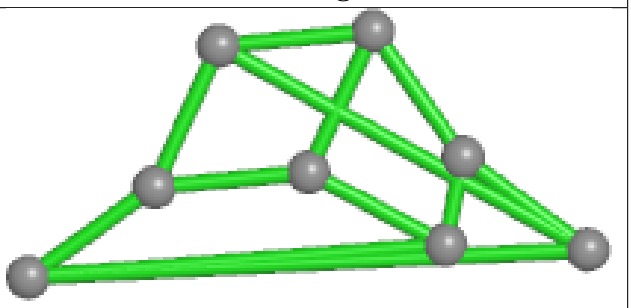
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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, 95^{th} 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	669/676 (98%)	-0.61	4 (0%)	89	88	18, 30, 49, 68	0
2	B	730/730 (100%)	-0.81	3 (0%)	92	92	18, 30, 47, 84	0
All	All	1399/1406 (99%)	-0.72	7 (0%)	91	90	18, 30, 48, 84	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	HIS	3.3
1	A	305	GLY	2.7
2	B	580	ARG	2.5
1	A	303	ALA	2.2
1	A	414	PRO	2.2
2	B	576	LYS	2.0
2	B	363	GLU	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 monosaccharides in this entry.

6.4 Ligands

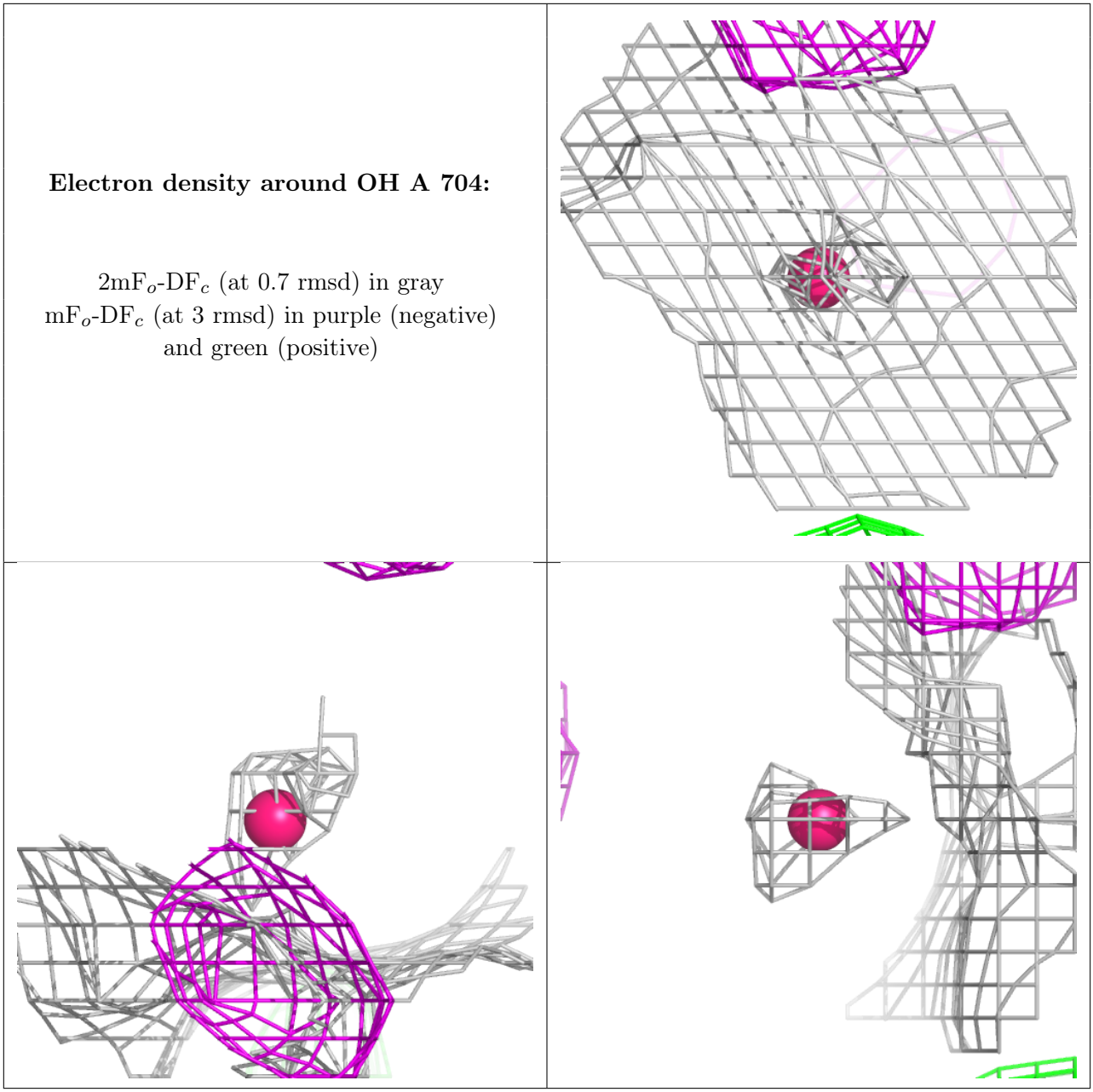
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	OH	A	704	1/1	0.87	0.15	39,39,39,39	0
6	MPD	B	806	8/8	0.89	0.28	40,42,46,46	0
6	MPD	A	707	8/8	0.90	0.23	39,53,56,60	0
6	MPD	A	706	8/8	0.91	0.14	39,47,57,61	0
3	RQM	A	701	9/9	0.96	0.09	28,36,44,49	8
5	OH	A	705	1/1	0.97	0.20	28,28,28,28	0
4	SF4	A	702	4/8	0.98	0.06	24,24,25,26	0
8	ACT	B	804	4/4	0.98	0.12	35,37,37,41	0
4	SF4	A	703	8/8	0.99	0.07	21,22,23,24	0
7	NI	B	801	1/1	0.99	0.06	25,25,25,25	0
4	SF4	B	802	8/8	0.99	0.05	24,26,27,29	0
9	NA	B	805	1/1	0.99	0.06	26,26,26,26	0
7	NI	B	803	1/1	1.00	0.04	39,39,39,39	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.

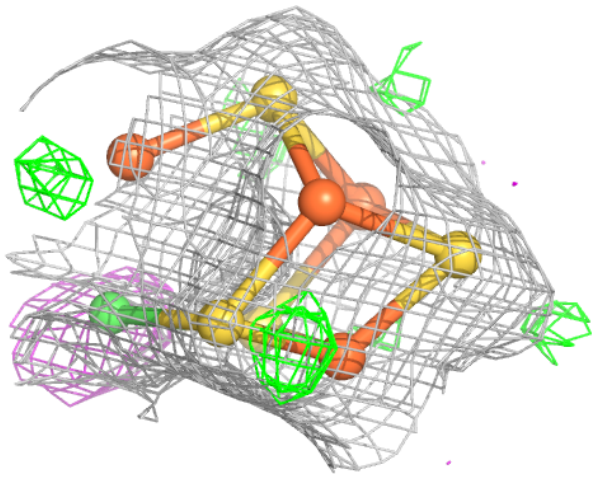
Electron density around OH A 704:

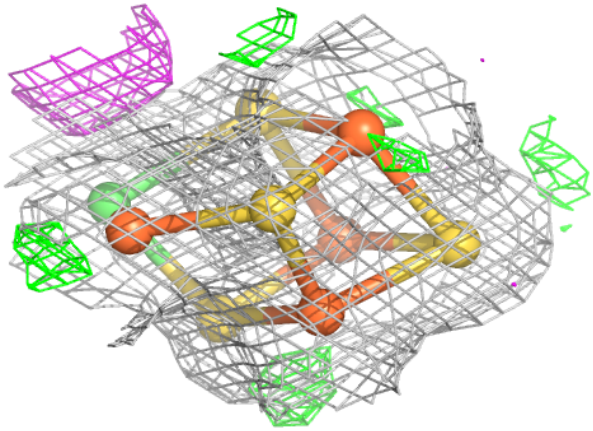
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

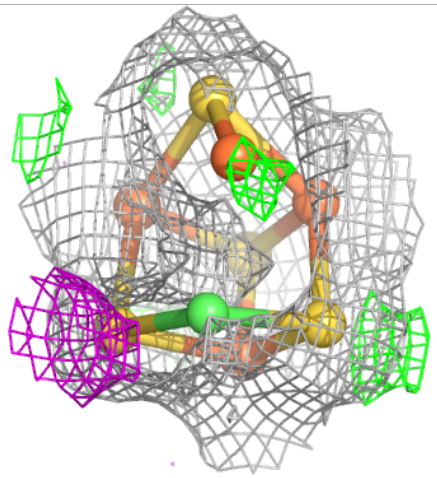


Electron density around RQM A 701:

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

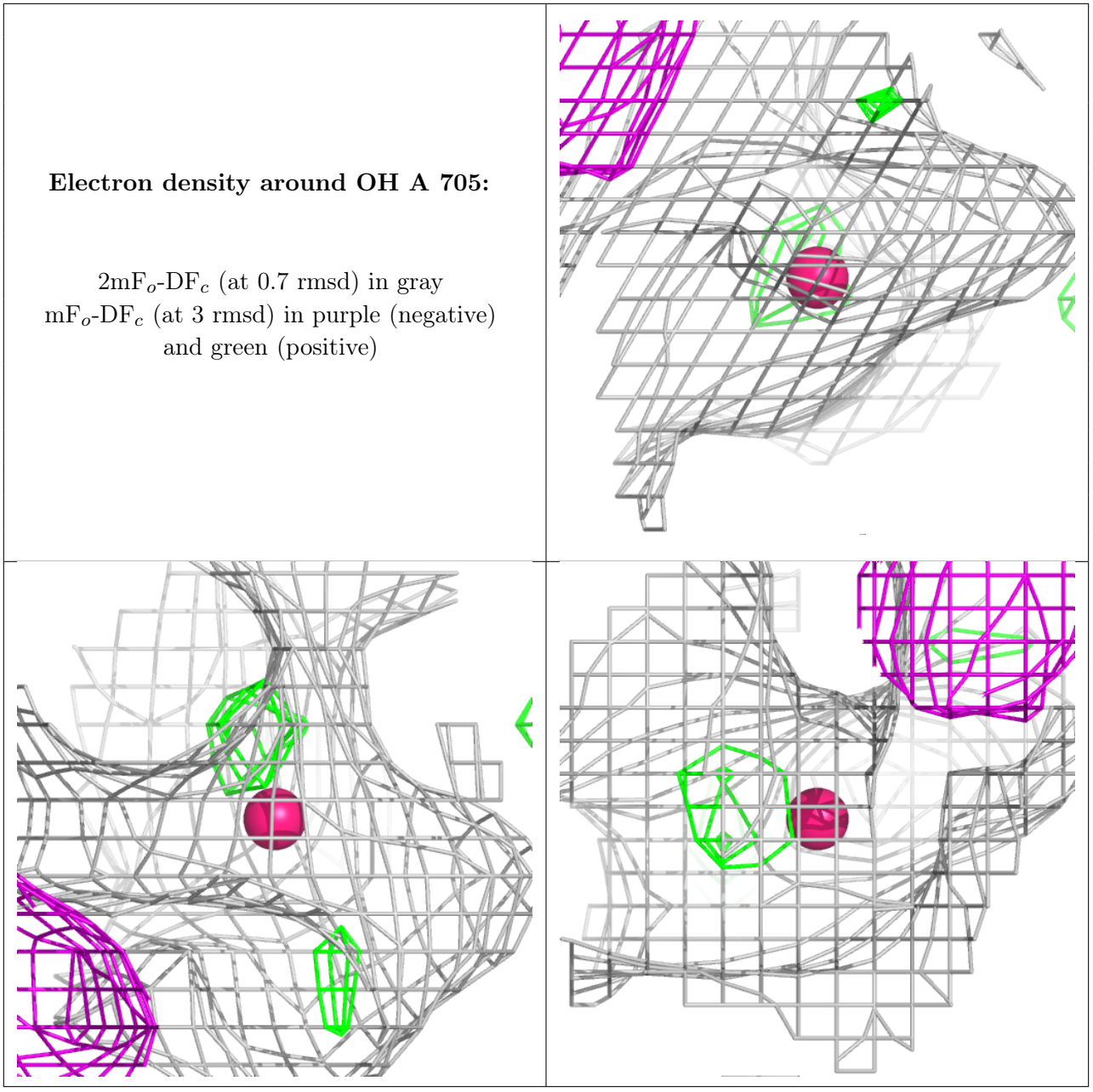






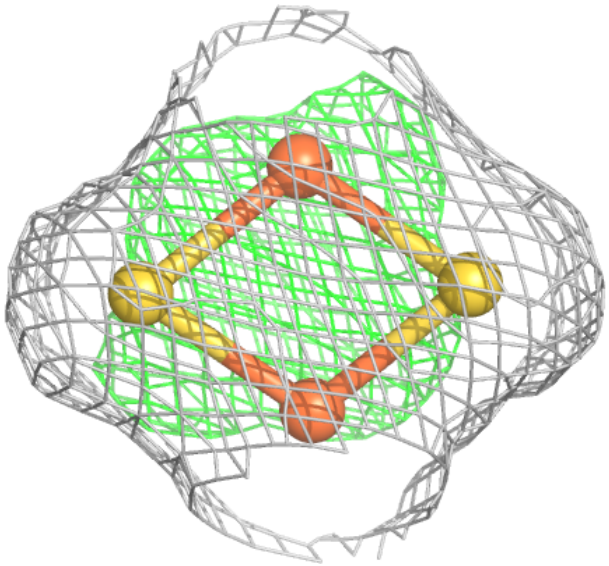
Electron density around OH A 705:

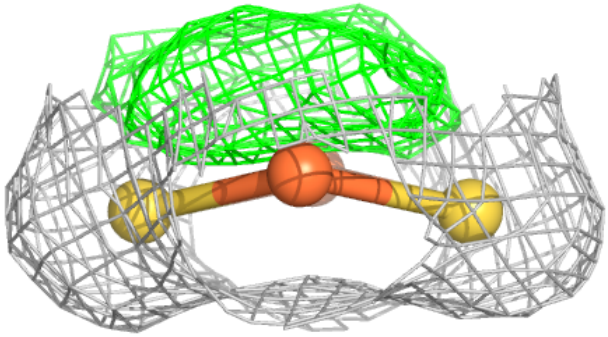
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

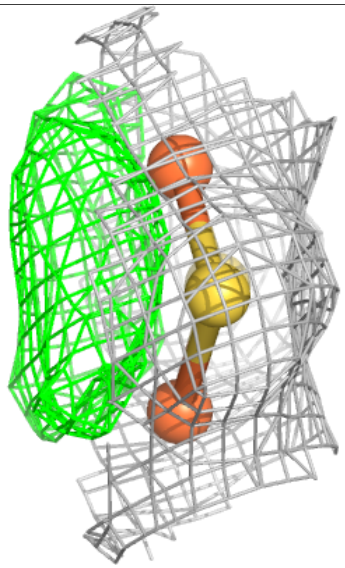


Electron density around SF4 A 702:

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

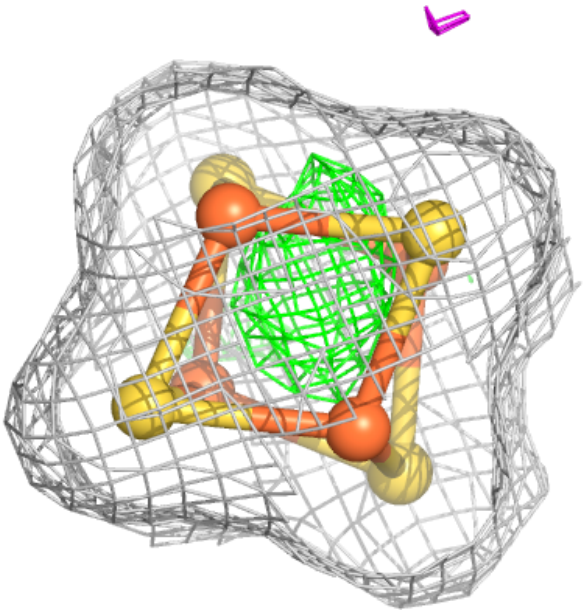


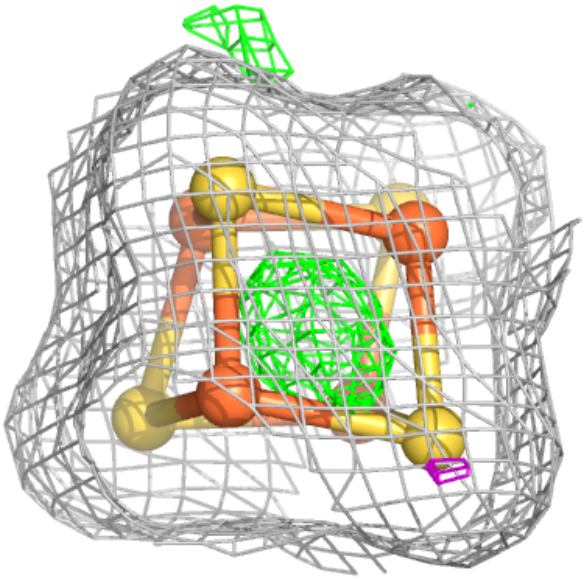


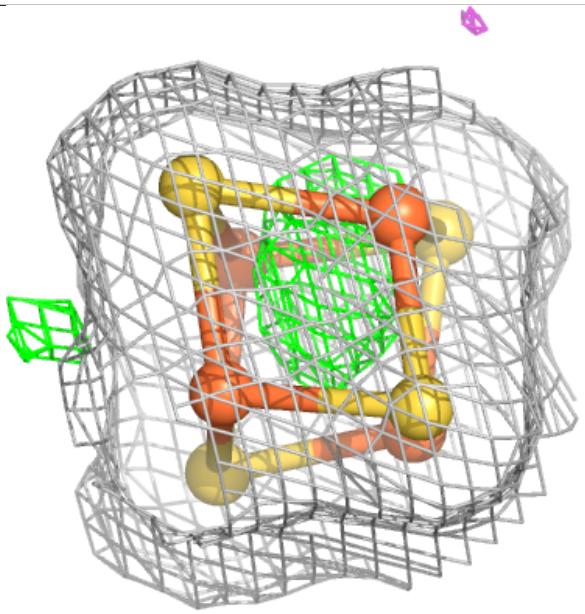


Electron density around SF4 A 703:

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

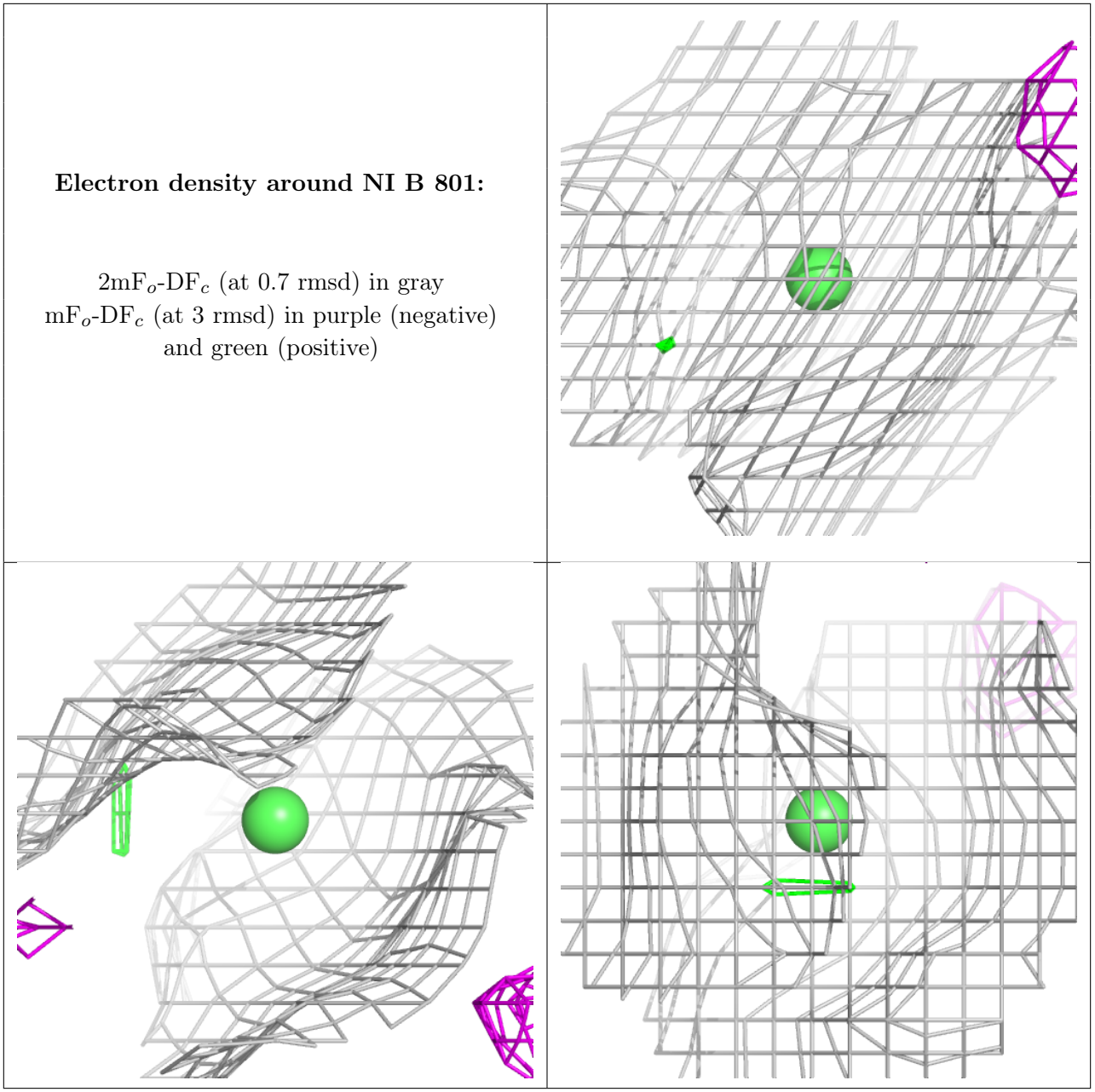






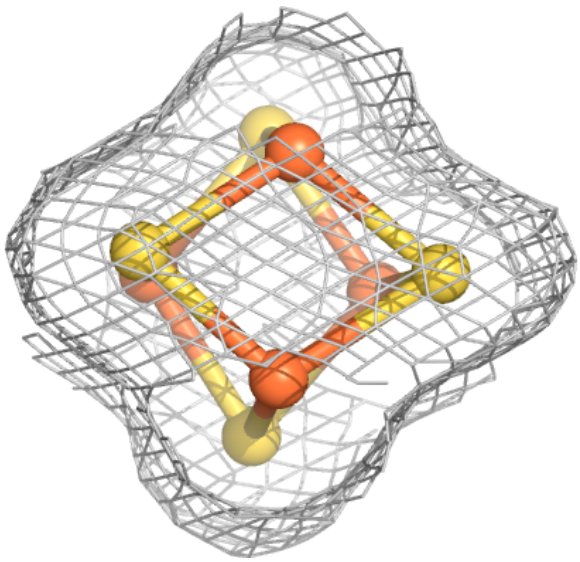
Electron density around NI B 801:

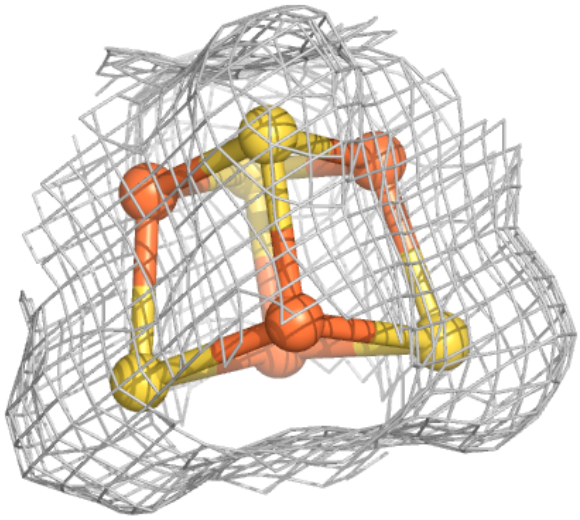
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

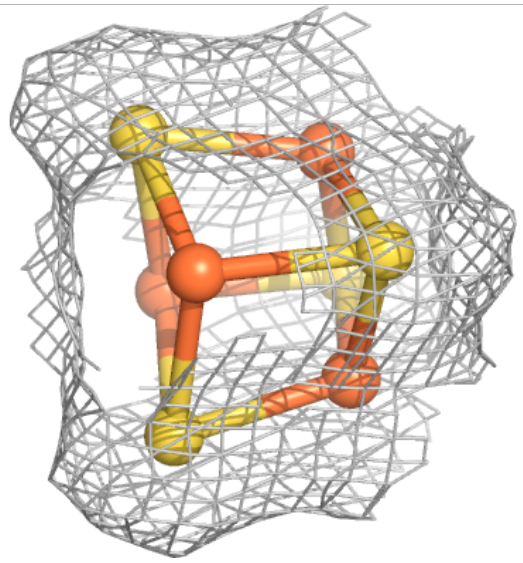


Electron density around SF4 B 802:

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

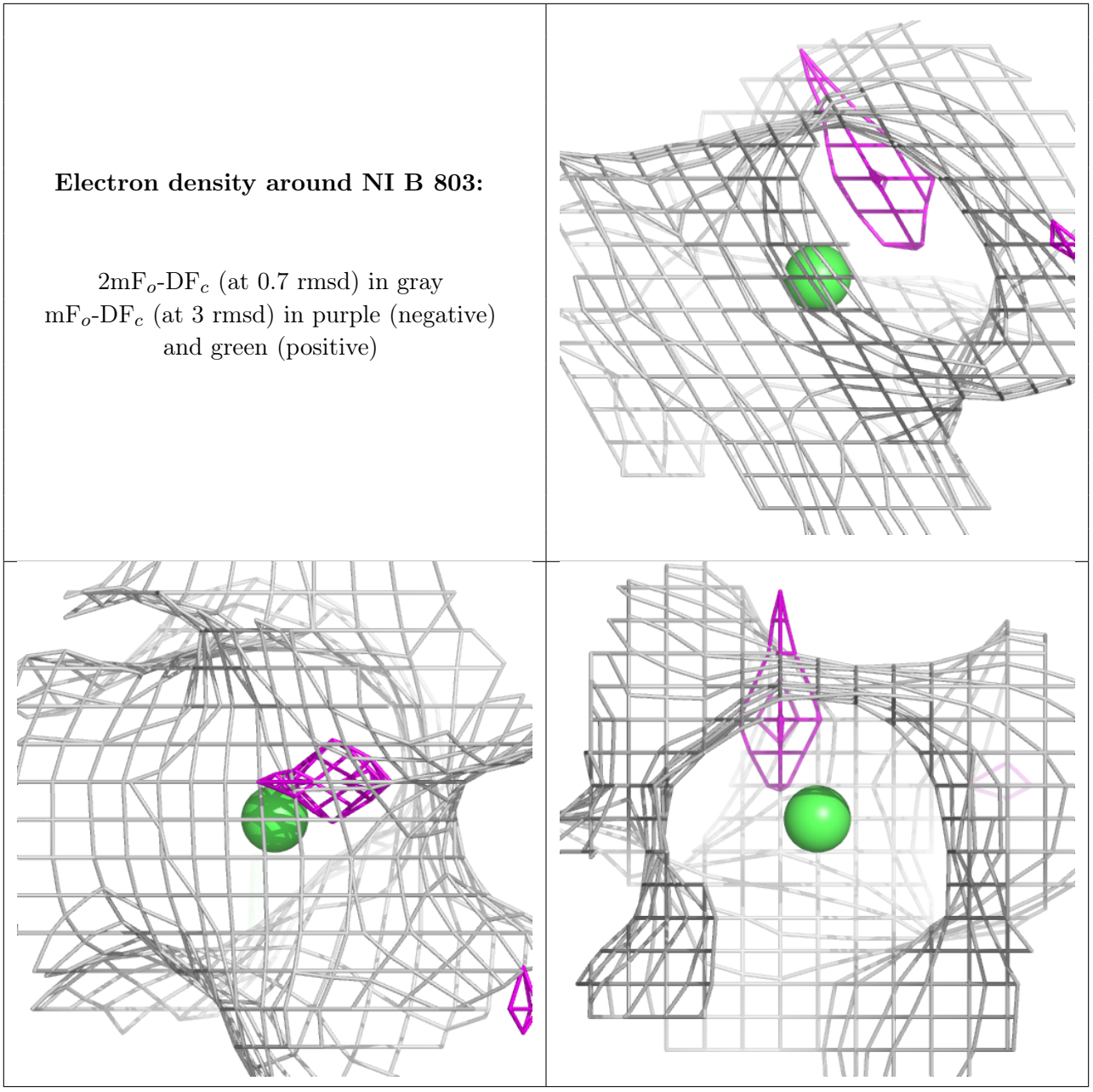






Electron density around NI B 803:

$2mF_o$-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 (i)

There are no such residues in this entry.