



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 8CM4 / pdb_00008cm4
Title : W-formate dehydrogenase C872A from *Desulfovibrio vulgaris* - exposed to oxygen
Authors : Vilela-Alves, G.; Mota, C.; Klymanska, K.; Oliveira, A.R.; Manuel, R.R.; Pereira, I.C.; Romao, M.J.
Deposited on : 2023-02-17
Resolution : 2.30 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

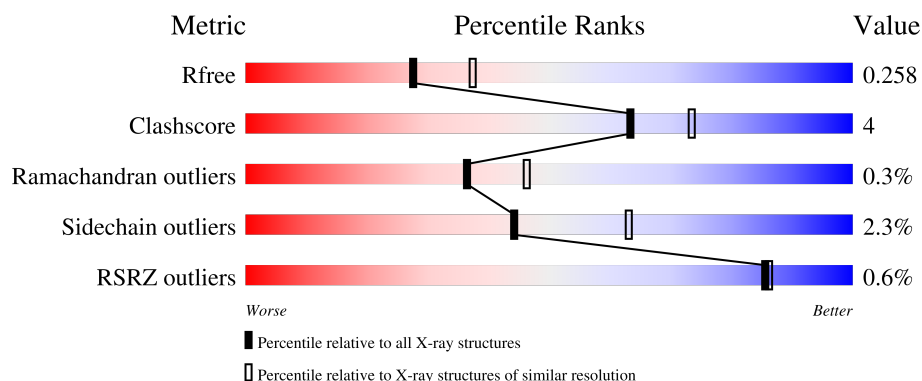
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	1013	% 86% 10% .
1	C	1013	% 84% 11% .
2	B	215	89% 10%
2	D	215	89% 10% .

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
9	PEG	D	304	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19187 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 Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	Se	0	0	0
			7621	4858	1328	1394	40	1			
1	C	970	Total	C	N	O	S	Se	0	0	0
			7591	4838	1322	1390	40	1			

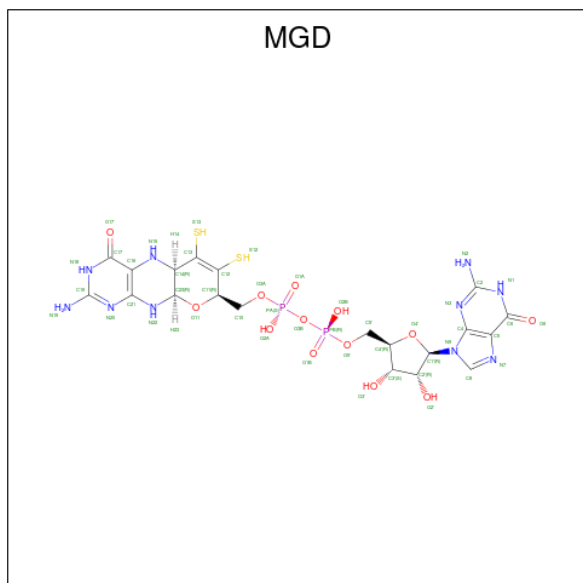
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	872	ALA	CYS	engineered mutation	UNP Q72EJ1
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
A	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
A	1012	GLU	-	expression tag	UNP Q72EJ1
A	1013	LYS	-	expression tag	UNP Q72EJ1
C	872	ALA	CYS	engineered mutation	UNP Q72EJ1
C	1006	TRP	-	expression tag	UNP Q72EJ1
C	1007	SER	-	expression tag	UNP Q72EJ1
C	1008	HIS	-	expression tag	UNP Q72EJ1
C	1009	PRO	-	expression tag	UNP Q72EJ1
C	1010	GLN	-	expression tag	UNP Q72EJ1
C	1011	PHE	-	expression tag	UNP Q72EJ1
C	1012	GLU	-	expression tag	UNP Q72EJ1
C	1013	LYS	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

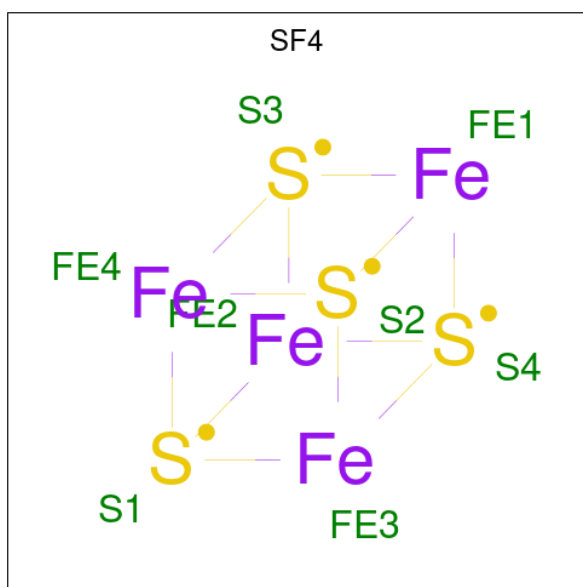
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			
2	D	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).



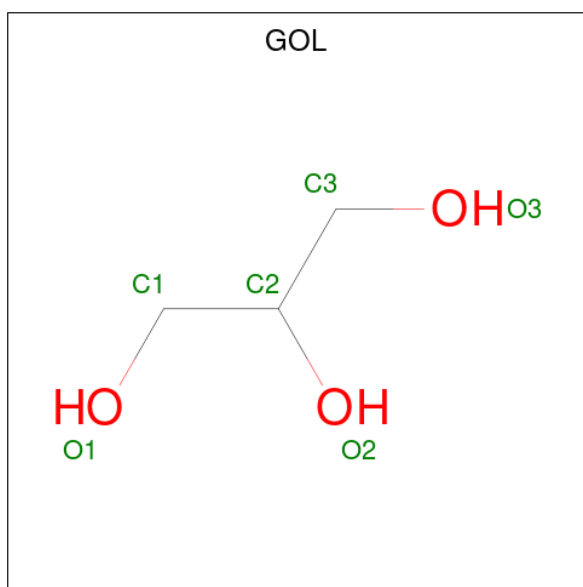
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		
3	A	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		
3	C	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		
3	C	1	Total	C	N	O	P S	0	0
			47	20	10	13	2 2		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

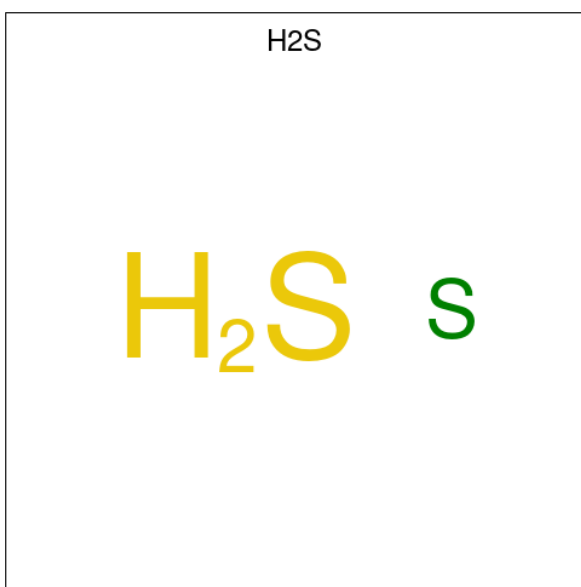


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

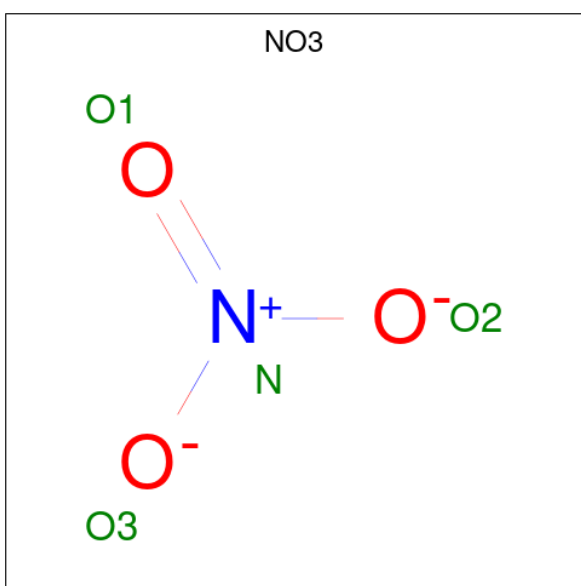
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	W	0	0
			1	1		
6	C	1	Total	W	0	0
			1	1		

- Molecule 7 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



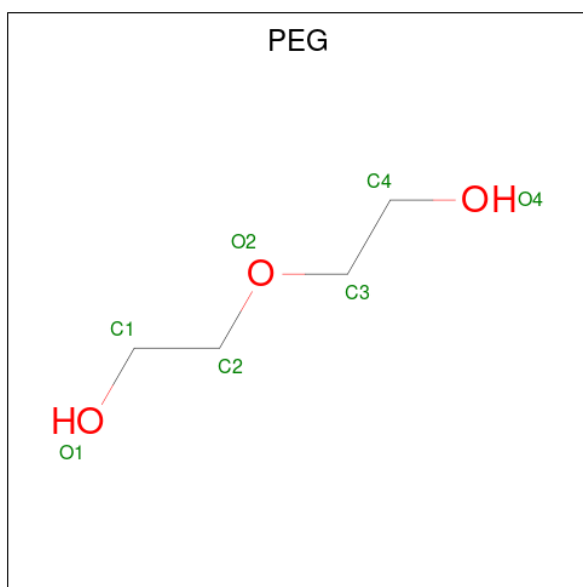
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	S	0	0
			1	1		
7	C	1	Total	S	0	0
			1	1		

- Molecule 8 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

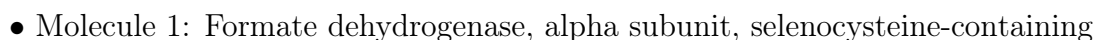


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	118	Total	O	0	0
			118	118		
10	B	60	Total	O	0	0
			60	60		
10	C	116	Total	O	0	0
			116	116		
10	D	62	Total	O	0	0
			62	62		

- Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing



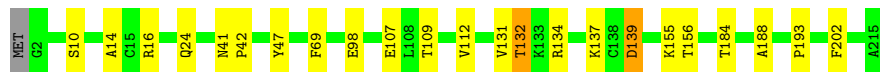
- Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain B:  89% 10%



- Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain D:  89% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.30Å 126.90Å 260.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.31 – 2.30 48.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.31-2.30) 99.8 (48.31-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.256 0.204 , 0.258	Depositor DCC
R_{free} test set	5427 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19187	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEC, MGD, H2S, W, GOL, PEG, NO3, SF4

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	0.98	0/7826	1.39	4/10617 (0.0%)
1	C	1.00	0/7793	1.36	0/10571
2	B	0.96	0/1699	1.40	2/2302 (0.1%)
2	D	0.98	0/1699	1.38	2/2302 (0.1%)
All	All	0.99	0/19017	1.38	8/25792 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	GLN	CA-C-N	5.62	126.22	119.98
1	A	447	GLN	C-N-CA	5.62	126.22	119.98
2	D	139	ASP	CA-CB-CG	5.57	118.17	112.60
2	D	47	TYR	CA-C-O	-5.18	115.03	120.63
1	A	610	VAL	CA-C-N	5.06	127.31	120.38
1	A	610	VAL	C-N-CA	5.06	127.31	120.38
2	B	113	ASP	CA-C-N	5.01	125.50	119.94
2	B	113	ASP	C-N-CA	5.01	125.50	119.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7621	0	7447	56	0
1	C	7591	0	7425	69	0
2	B	1664	0	1633	16	0
2	D	1664	0	1633	14	0
3	A	94	0	44	5	0
3	C	94	0	44	5	0
4	A	8	0	0	0	0
4	B	24	0	0	1	0
4	C	8	0	0	1	0
4	D	24	0	0	0	0
5	A	18	0	24	0	0
5	C	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	4	0	0	0	0
9	D	7	0	10	4	0
10	A	118	0	0	0	0
10	B	60	0	0	0	0
10	C	116	0	0	0	0
10	D	62	0	0	0	0
All	All	19187	0	18268	149	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 (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:VAL:HG13	2:B:162:MET:CE	2.20	0.72
1:C:88:CYS:HB2	1:C:89:PRO:HD2	1.74	0.70
1:A:1008:HIS:ND1	1:A:1008:HIS:C	2.52	0.67
1:C:887:GLU:OE2	2:D:16:ARG:NH2	2.26	0.67
1:A:947:ILE:HG23	1:A:959:MET:HE3	1.76	0.67
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.36	0.65
1:C:161:GLY:HA3	1:C:551:TRP:O	1.98	0.63
2:B:7:VAL:HG13	2:B:162:MET:HE1	1.79	0.62
1:A:378:SER:OG	1:A:381:GLN:HG3	2.00	0.62
1:A:209:MET:HE3	1:A:212:HIS:HA	1.82	0.61
1:A:947:ILE:CG2	1:A:959:MET:HE3	2.32	0.60
2:D:139:ASP:HB3	9:D:304:PEG:H42	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:910:CYS:SG	1:C:960:VAL:HG13	2.43	0.59
1:C:195:PRO:HG3	1:C:992:ILE:HG21	1.84	0.58
1:A:565:ASN:O	1:A:569:MET:HG3	2.04	0.58
1:A:883:TYR:O	1:A:963:PRO:HA	2.03	0.57
1:C:76:GLY:O	2:D:155:LYS:NZ	2.38	0.57
1:A:206:ARG:HB2	1:A:773:TYR:OH	2.05	0.57
1:C:476:TYR:HE1	1:C:499:VAL:HG21	1.70	0.57
1:C:947:ILE:HG23	1:C:959:MET:CE	2.34	0.57
1:A:947:ILE:HG23	1:A:959:MET:CE	2.35	0.57
1:A:413:GLY:O	1:A:417:ILE:HD12	2.04	0.57
1:A:177:LEU:HD22	1:A:182:LEU:HD22	1.87	0.55
1:C:177:LEU:HD22	1:C:182:LEU:HD22	1.88	0.54
2:D:139:ASP:HB3	9:D:304:PEG:C4	2.38	0.53
2:D:132:THR:HG23	2:D:134:ARG:HG3	1.89	0.53
1:C:234:PRO:HD2	4:C:1103:SF4:S3	2.49	0.53
2:B:132:THR:HG22	2:B:134:ARG:H	1.74	0.53
2:B:129:ASP:OD2	2:B:132:THR:HB	2.08	0.53
1:C:779:ASP:HB2	1:C:780:LYS:HE3	1.91	0.52
1:C:947:ILE:HD12	1:C:959:MET:HE3	1.90	0.52
1:C:224:ILE:HG12	1:C:402:MET:HE3	1.92	0.52
1:C:337:LEU:HD12	1:C:337:LEU:N	2.24	0.52
2:D:41:ASN:HA	2:D:42:PRO:C	2.34	0.52
1:C:210:THR:HG22	1:C:773:TYR:HE2	1.75	0.52
1:C:401:ILE:HG12	1:C:420:MET:HG2	1.92	0.52
1:A:986:GLY:HA3	1:A:992:ILE:O	2.10	0.51
2:B:7:VAL:HG13	2:B:162:MET:HE2	1.90	0.51
1:A:918:LYS:HE3	2:D:193:PRO:HD2	1.91	0.51
1:C:80:HIS:NE2	1:C:626:GLN:OE1	2.33	0.51
1:C:894:MET:SD	3:C:1102:MGD:H2'	2.50	0.51
1:C:190:ARG:HG2	1:C:533:TRP:HB2	1.93	0.50
1:C:714:PHE:CE2	1:C:767:VAL:HG13	2.46	0.50
1:C:225:MET:HE3	1:C:253:VAL:HG11	1.93	0.50
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.47	0.50
1:C:224:ILE:HG12	1:C:402:MET:CE	2.42	0.50
1:C:500:ALA:O	1:C:504:LYS:HG2	2.12	0.50
1:A:54:ALA:O	1:A:620:ASN:HB2	2.12	0.50
1:C:699:GLU:HA	1:C:703:LYS:O	2.12	0.50
2:B:188:ALA:HA	2:B:202:PHE:O	2.12	0.49
1:A:162:SER:HB2	1:A:551:TRP:O	2.13	0.49
1:C:469:LYS:HG2	1:C:524:ALA:CB	2.43	0.49
1:A:127:THR:HG22	1:A:651:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:O	1:C:301:THR:OG1	2.25	0.49
1:C:883:TYR:O	1:C:963:PRO:HA	2.12	0.49
2:B:47:TYR:HA	2:B:136:SER:OG	2.13	0.49
1:C:405:MET:HG2	3:C:1101:MGD:H101	1.95	0.49
1:A:125:ALA:O	1:A:129:ILE:HG13	2.13	0.48
1:C:233:HIS:N	1:C:234:PRO:HD3	2.28	0.48
1:C:698:THR:HG21	1:C:722:SER:OG	2.13	0.48
1:C:404:ALA:HB3	3:C:1101:MGD:O2A	2.13	0.48
2:B:7:VAL:CG1	2:B:162:MET:HE1	2.44	0.48
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.54	0.48
1:C:209:MET:HE2	1:C:438:ASN:HB3	1.96	0.48
1:C:743:ARG:HB3	1:C:760:ASN:O	2.14	0.48
1:A:861:ALA:HA	1:A:988:PRO:HG3	1.95	0.47
1:A:197:VAL:HB	1:A:198:PRO:CD	2.44	0.47
1:C:625:MET:HE3	1:C:763:PHE:CD2	2.49	0.47
1:C:909:PHE:CE2	1:C:963:PRO:HG3	2.50	0.47
1:A:845:CYS:SG	1:A:871:VAL:HG13	2.55	0.47
2:B:161:THR:HG22	2:B:162:MET:HE2	1.96	0.47
2:D:107:GLU:HG2	2:D:134:ARG:CZ	2.45	0.47
1:A:161:GLY:HA3	1:A:551:TRP:O	2.15	0.46
1:A:278:PHE:HZ	1:A:385:VAL:HG11	1.79	0.46
1:A:57:CYS:SG	1:A:83:ASN:HB3	2.56	0.46
1:A:714:PHE:CE2	1:A:767:VAL:HG13	2.51	0.46
1:C:225:MET:HE3	1:C:253:VAL:CG1	2.46	0.46
1:C:769:ARG:HD3	1:C:805:ASP:HA	1.96	0.46
2:D:137:LYS:O	9:D:304:PEG:H32	2.15	0.46
1:C:53:CYS:SG	1:C:55:VAL:HG23	2.55	0.46
2:B:41:ASN:HA	2:B:42:PRO:C	2.41	0.45
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.98	0.45
1:A:937:LEU:C	1:A:937:LEU:HD12	2.41	0.45
1:C:197:VAL:HA	1:C:207:GLY:HA3	1.98	0.45
1:A:443:GLU:HB2	1:A:446:VAL:HB	1.97	0.45
1:A:914:LYS:HE2	1:A:945:GLU:HG3	1.97	0.45
1:C:900:TRP:CH2	2:D:24:GLN:HA	2.52	0.45
1:A:940:VAL:HG11	2:B:35:ASN:HB3	1.99	0.45
1:C:160:PHE:HA	1:C:186:GLU:O	2.17	0.44
1:C:88:CYS:CB	1:C:89:PRO:HD2	2.46	0.44
2:B:162:MET:HE3	4:B:301:SF4:S3	2.57	0.44
1:C:401:ILE:HB	1:C:420:MET:HE2	2.00	0.44
1:A:297:VAL:HA	1:A:301:THR:HG23	2.00	0.44
1:A:282:LEU:O	1:A:286:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:860:VAL:O	1:C:988:PRO:HB3	2.18	0.44
1:A:617:SER:HA	1:A:626:GLN:O	2.18	0.43
1:C:272:SER:HA	3:C:1101:MGD:O6	2.18	0.43
1:A:194:SER:OG	1:A:195:PRO:HD3	2.18	0.43
1:C:459:TRP:HB3	1:C:460:PRO:HD2	2.01	0.43
1:C:380:GLU:H	1:C:380:GLU:CD	2.26	0.43
1:C:758:PHE:O	1:C:770:ARG:NH1	2.52	0.43
1:A:910:CYS:SG	1:A:960:VAL:CG1	3.05	0.43
2:B:54:ARG:NE	2:B:72:GLU:OE1	2.40	0.43
1:C:858:ASN:HB3	1:C:861:ALA:HB2	1.99	0.43
1:A:50:CYS:HA	1:A:59:LEU:HD11	2.00	0.43
1:A:41:GLN:HB3	1:A:42:TRP:CE3	2.54	0.43
1:C:162:SER:HB2	1:C:551:TRP:O	2.19	0.42
1:C:910:CYS:SG	1:C:960:VAL:CG1	3.07	0.42
1:A:665:ALA:HB3	1:A:666:PRO:HD3	2.01	0.42
1:A:233:HIS:O	1:A:236:ALA:HB3	2.19	0.42
1:A:442:GLY:HA3	3:A:1101:MGD:C13	2.49	0.42
1:A:893:LEU:HD13	3:A:1102:MGD:O3'	2.20	0.42
1:A:757:LEU:HD22	1:A:770:ARG:HB2	2.00	0.42
1:C:256:ARG:HG2	1:C:947:ILE:CD1	2.49	0.42
1:A:896:ARG:HD3	1:A:966:TYR:HA	2.02	0.42
2:B:181:VAL:HG11	2:B:201:LEU:HD21	2.02	0.42
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.54	0.42
1:C:926:ASP:OD2	1:C:1004:LYS:HE2	2.19	0.42
1:C:98:GLY:O	1:C:103:ARG:NH1	2.44	0.42
1:C:696:LYS:HE2	1:C:698:THR:HG21	2.01	0.42
1:C:806:GLY:HA3	1:C:817:ILE:HG21	2.02	0.42
1:A:188:GLN:HB3	3:A:1102:MGD:S12	2.60	0.42
1:C:173:TYR:CE2	1:C:177:LEU:HD11	2.54	0.42
1:A:937:LEU:HD12	1:A:937:LEU:O	2.20	0.41
2:D:137:LYS:H	9:D:304:PEG:H32	1.85	0.41
2:D:188:ALA:HA	2:D:202:PHE:O	2.20	0.41
1:C:457:HIS:CD2	1:C:458:ILE:HG23	2.56	0.41
1:C:587:SER:HB2	1:C:969:MET:HE1	2.03	0.41
1:C:615:GLU:HA	1:C:628:ARG:O	2.20	0.41
1:A:194:SER:N	1:A:195:PRO:CD	2.84	0.41
1:A:186:GLU:CD	1:A:190:ARG:HE	2.28	0.41
1:C:240:VAL:HG21	1:C:402:MET:HE1	2.03	0.41
1:C:947:ILE:HD12	1:C:959:MET:CE	2.49	0.41
1:C:959:MET:HB3	1:C:959:MET:HE2	1.78	0.41
1:A:561:ASN:CG	1:A:934:ARG:HG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:TRP:CH2	1:A:969:MET:HE3	2.55	0.41
1:A:194:SER:O	1:A:198:PRO:HD2	2.21	0.41
2:D:14:ALA:HB2	2:D:69:PHE:CG	2.56	0.41
1:A:502:TYR:O	1:A:505:ALA:HB3	2.22	0.41
1:C:232:ASN:HA	3:C:1101:MGD:N20	2.36	0.41
1:C:315:ASP:C	1:C:853:SER:HB2	2.46	0.41
1:C:620:ASN:OD1	1:C:620:ASN:C	2.63	0.41
1:C:959:MET:HG2	1:C:960:VAL:N	2.36	0.41
1:C:194:SER:N	1:C:195:PRO:CD	2.84	0.40
1:C:374:ILE:HD12	1:C:374:ILE:HA	1.89	0.40
2:D:109:THR:O	2:D:112:VAL:HG22	2.21	0.40
1:A:403:TYR:CD1	1:A:403:TYR:C	3.00	0.40
1:A:405:MET:HG2	3:A:1101:MGD:H101	2.03	0.40
1:A:846:PRO:HG3	1:A:879:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	970/1013 (96%)	936 (96%)	31 (3%)	3 (0%)	36	46
1	C	967/1013 (96%)	918 (95%)	45 (5%)	4 (0%)	30	38
2	B	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
2	D	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
All	All	2361/2456 (96%)	2264 (96%)	90 (4%)	7 (0%)	36	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	TRP

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Mol	Chain	Res	Type
1	C	325	ASN
1	C	872	ALA
1	A	404	ALA
1	C	533	TRP
1	A	756	GLY
1	C	663	TYR

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	790/818 (97%)	774 (98%)	16 (2%)	48	67
1	C	787/818 (96%)	767 (98%)	20 (2%)	42	60
2	B	185/186 (100%)	183 (99%)	2 (1%)	65	81
2	D	185/186 (100%)	179 (97%)	6 (3%)	34	51
All	All	1947/2008 (97%)	1903 (98%)	44 (2%)	44	63

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	154	THR
1	A	237	PHE
1	A	301	THR
1	A	314	LYS
1	A	468	SER
1	A	658	LYS
1	A	698	THR
1	A	700	VAL
1	A	722	SER
1	A	780	LYS
1	A	781	THR
1	A	863	GLN
1	A	940	VAL
1	A	970	VAL

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Mol	Chain	Res	Type
1	A	1008	HIS
2	B	132	THR
2	B	156	THR
1	C	36	GLU
1	C	66	ASP
1	C	154	THR
1	C	235	ILE
1	C	237	PHE
1	C	282	LEU
1	C	315	ASP
1	C	528	LEU
1	C	672	ILE
1	C	696	LYS
1	C	713	SER
1	C	780	LYS
1	C	800	VAL
1	C	831	ARG
1	C	849	LYS
1	C	886	THR
1	C	970	VAL
1	C	972	LYS
1	C	984	SER
1	C	989	ASN
2	D	10	SER
2	D	98	GLU
2	D	131	VAL
2	D	132	THR
2	D	156	THR
2	D	184	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	A	383	GLN
1	A	447	GLN
1	A	863	GLN
1	C	68	GLN
1	C	362	HIS
1	C	814	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 18 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
4	SF4	B	303	2	0,12,12	-	-	-		
3	MGD	A	1101	6	47,52,52	0.54	0	58,81,81	0.93	2 (3%)
4	SF4	D	301	2	0,12,12	-	-	-		
4	SF4	D	302	2	0,12,12	-	-	-		
4	SF4	C	1103	1	0,12,12	-	-	-		
4	SF4	B	301	2	0,12,12	-	-	-		
5	GOL	A	1104	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	C	1104	-	5,5,5	0.09	0	5,5,5	0.32	0
8	NO3	B	304	-	1,3,3	0.05	0	0,3,3	-	-
4	SF4	A	1103	1	0,12,12	-	-	-		
4	SF4	D	303	2	0,12,12	-	-	-		
5	GOL	A	1107	-	5,5,5	0.11	0	5,5,5	0.28	0
4	SF4	B	302	2	0,12,12	-	-	-		
3	MGD	C	1102	6	47,52,52	0.82	1 (2%)	58,81,81	1.04	4 (6%)
3	MGD	A	1102	6	47,52,52	0.75	1 (2%)	58,81,81	0.99	4 (6%)
9	PEG	D	304	-	6,6,6	0.49	0	5,5,5	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	1106	-	5,5,5	0.08	0	5,5,5	0.26	0
3	MGD	C	1101	6	47,52,52	0.62	1 (2%)	58,81,81	0.85	1 (1%)

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
4	SF4	B	303	2	-	-	0/6/5/5
3	MGD	A	1101	6	-	2/22/66/66	0/6/6/6
4	SF4	D	301	2	-	-	0/6/5/5
4	SF4	D	302	2	-	-	0/6/5/5
4	SF4	C	1103	1	-	-	0/6/5/5
5	GOL	C	1104	-	-	2/4/4/4	-
5	GOL	A	1104	-	-	2/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
4	SF4	A	1103	1	-	-	0/6/5/5
5	GOL	A	1107	-	-	2/4/4/4	-
4	SF4	D	303	2	-	-	0/6/5/5
4	SF4	B	302	2	-	-	0/6/5/5
3	MGD	C	1102	6	-	5/22/66/66	0/6/6/6
3	MGD	A	1102	6	-	5/22/66/66	0/6/6/6
9	PEG	D	304	-	-	4/4/4/4	-
5	GOL	A	1106	-	-	2/4/4/4	-
3	MGD	C	1101	6	-	2/22/66/66	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1102	MGD	C23-C14	4.59	1.57	1.53
3	A	1102	MGD	C23-C14	3.68	1.56	1.53
3	C	1101	MGD	C23-C14	2.30	1.55	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	MGD	O11-C23-C14	2.93	110.92	108.96
3	C	1102	MGD	C19-N20-C21	2.89	118.45	113.36
3	A	1101	MGD	C19-N20-C21	2.85	118.39	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	MGD	C19-N20-C21	2.85	118.38	113.36
3	A	1102	MGD	C19-N20-C21	2.58	117.92	113.36
3	A	1102	MGD	O11-C23-C14	2.42	110.58	108.96
3	A	1102	MGD	C23-C14-N15	2.29	110.12	107.87
3	C	1102	MGD	O4'-C1'-C2'	-2.21	101.90	106.62
3	C	1102	MGD	O3'-C3'-C4'	-2.15	104.89	111.08
3	A	1102	MGD	O3B-PA-O1A	-2.08	104.44	110.70
3	A	1101	MGD	C17-C16-N15	2.08	121.94	116.27

There are no chirality outliers.

All (26) torsion outliers are listed below:

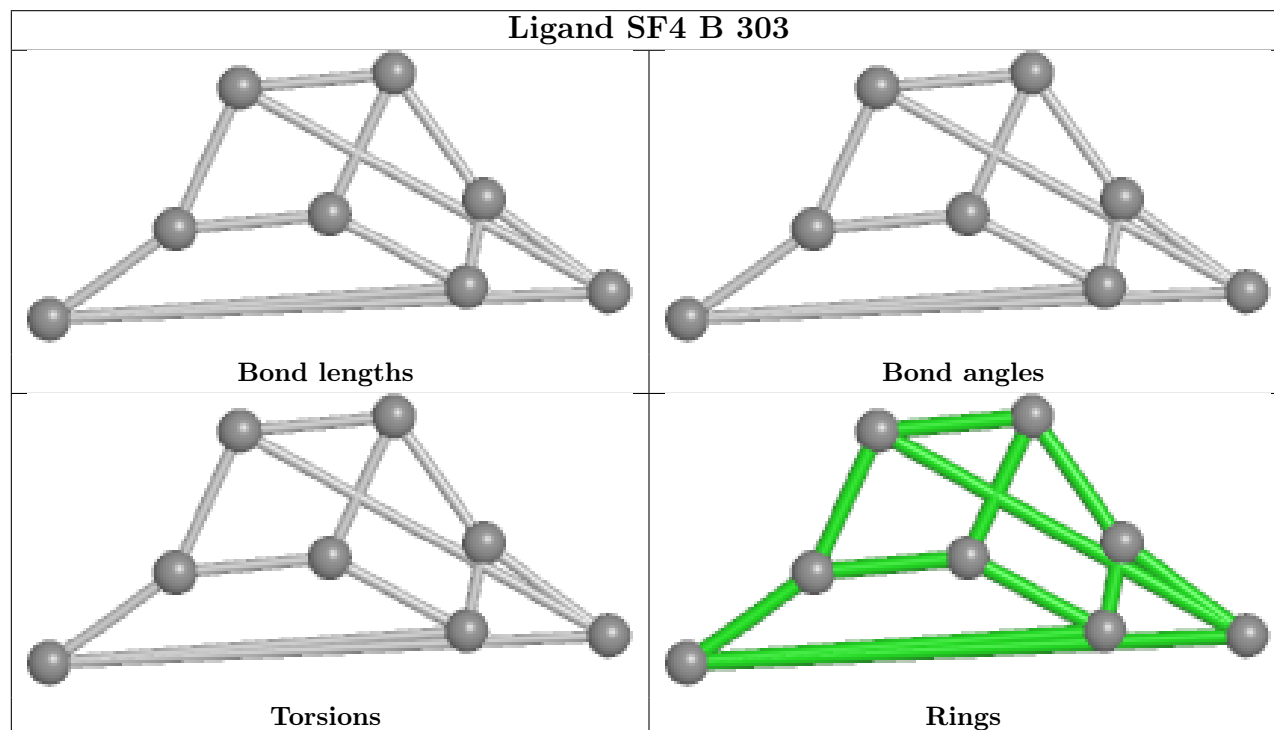
Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C4'-C5'-O5'-PB
3	C	1102	MGD	C4'-C5'-O5'-PB
5	A	1104	GOL	O1-C1-C2-C3
5	A	1107	GOL	C1-C2-C3-O3
5	C	1104	GOL	C1-C2-C3-O3
5	A	1104	GOL	O1-C1-C2-O2
3	C	1102	MGD	O4'-C4'-C5'-O5'
3	A	1102	MGD	O4'-C4'-C5'-O5'
5	A	1106	GOL	O1-C1-C2-C3
9	D	304	PEG	O2-C3-C4-O4
5	A	1107	GOL	O2-C2-C3-O3
5	C	1104	GOL	O2-C2-C3-O3
9	D	304	PEG	O1-C1-C2-O2
3	A	1102	MGD	C3'-C4'-C5'-O5'
3	C	1102	MGD	C3'-C4'-C5'-O5'
3	C	1102	MGD	PA-O3B-PB-O1B
3	A	1101	MGD	PA-O3B-PB-O5'
3	C	1101	MGD	PA-O3B-PB-O5'
9	D	304	PEG	C4-C3-O2-C2
3	C	1102	MGD	PA-O3B-PB-O2B
5	A	1106	GOL	O1-C1-C2-O2
3	A	1102	MGD	PA-O3B-PB-O1B
3	A	1102	MGD	PA-O3B-PB-O2B
3	C	1101	MGD	PA-O3B-PB-O2B
9	D	304	PEG	C1-C2-O2-C3
3	A	1101	MGD	PA-O3B-PB-O2B

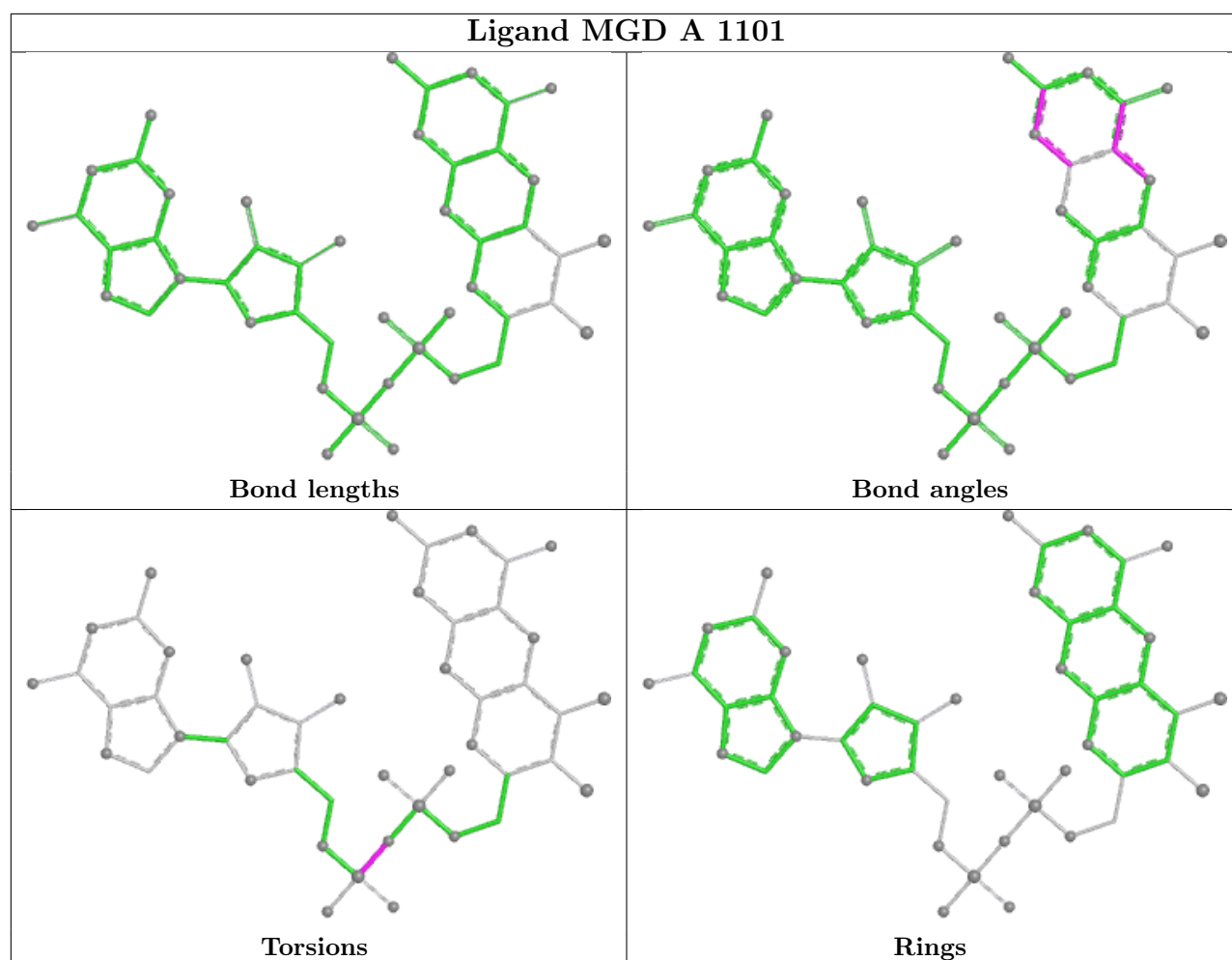
There are no ring outliers.

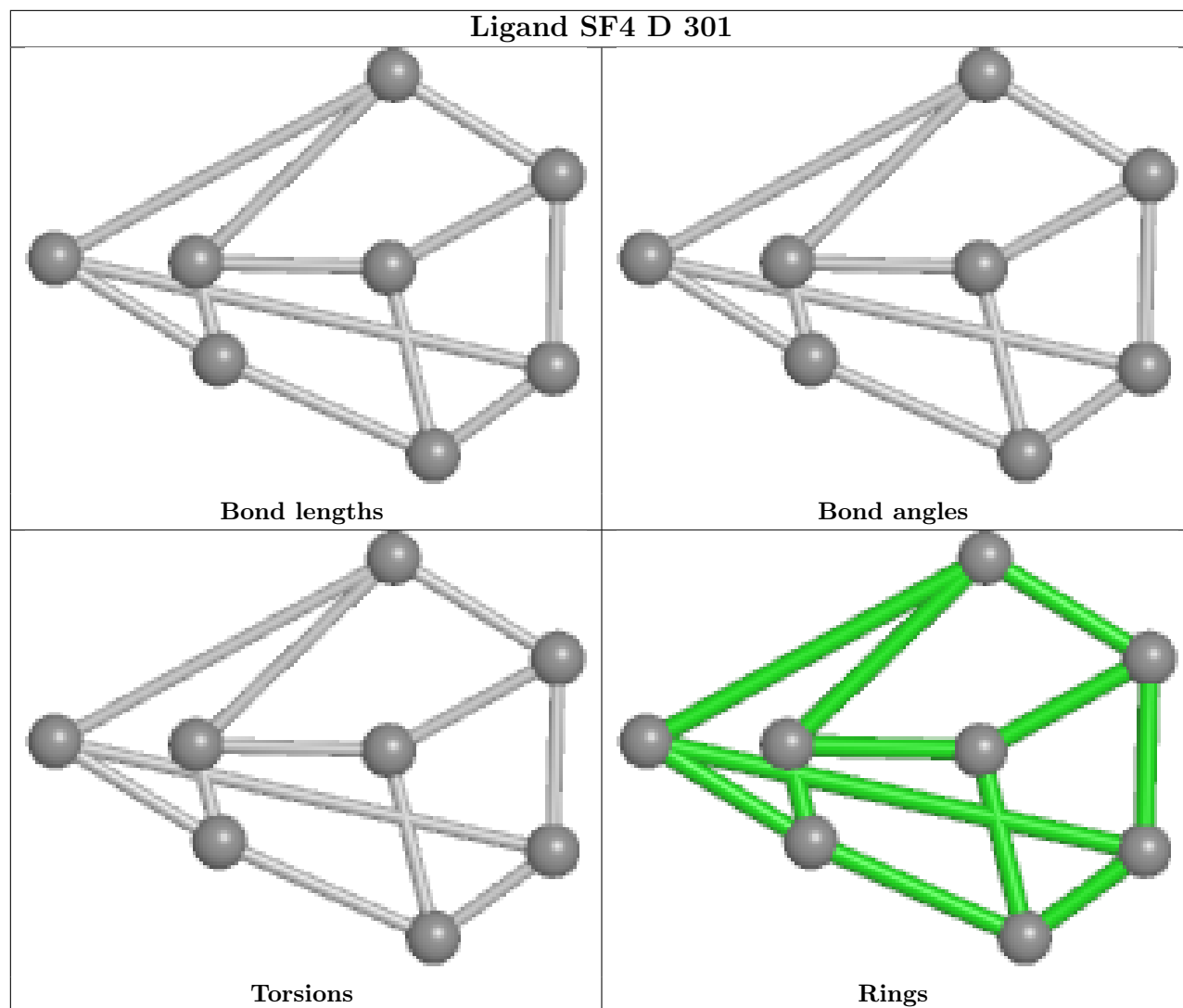
7 monomers are involved in 16 short contacts:

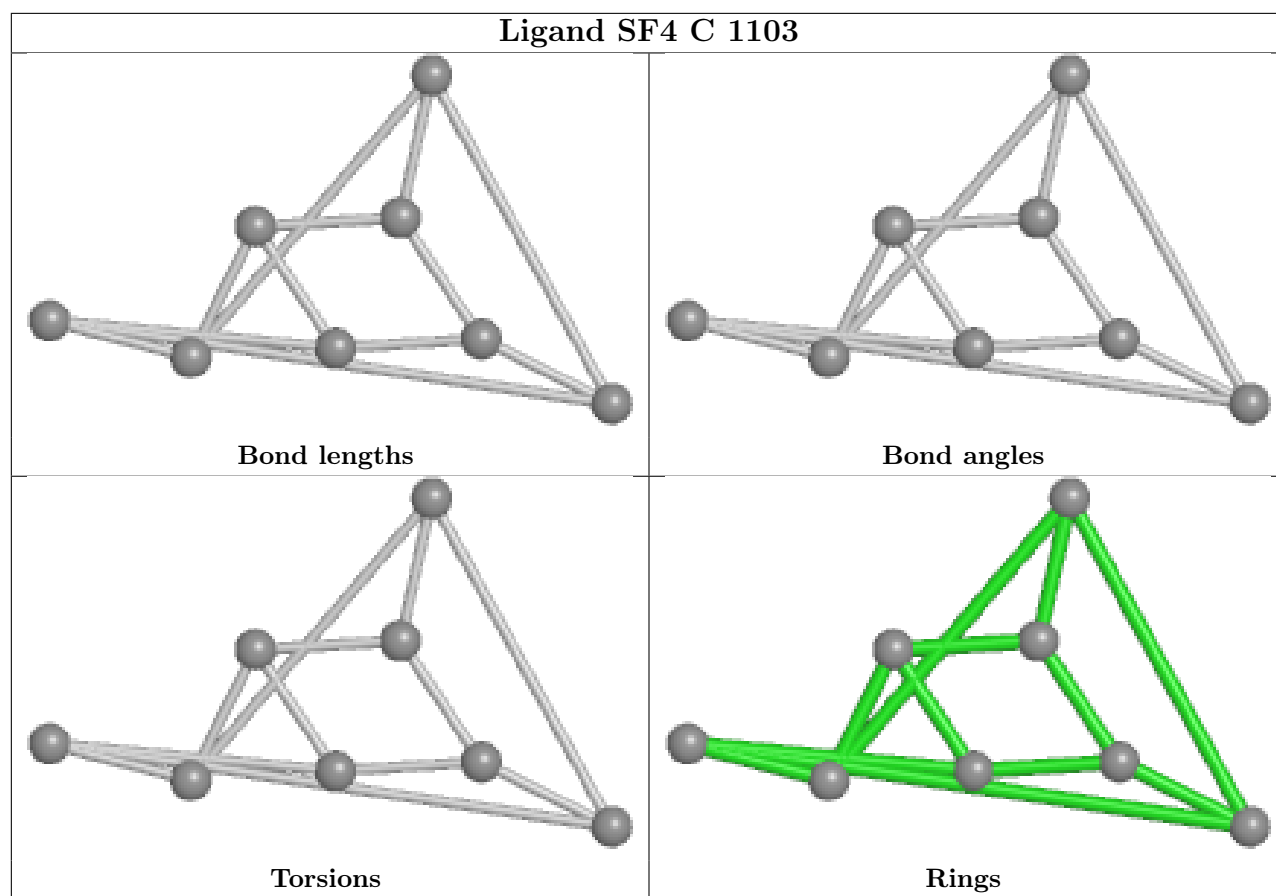
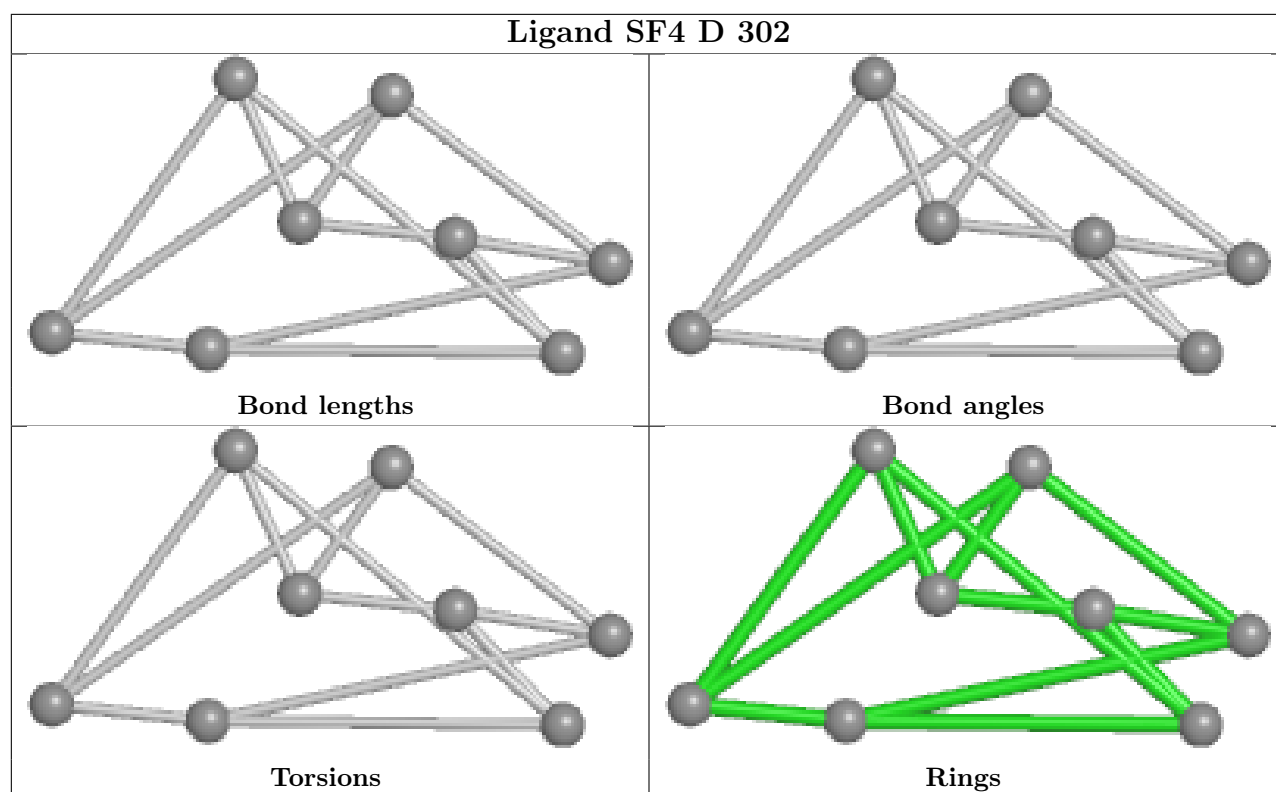
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	MGD	2	0
4	C	1103	SF4	1	0
4	B	301	SF4	1	0
3	C	1102	MGD	1	0
3	A	1102	MGD	3	0
9	D	304	PEG	4	0
3	C	1101	MGD	4	0

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.

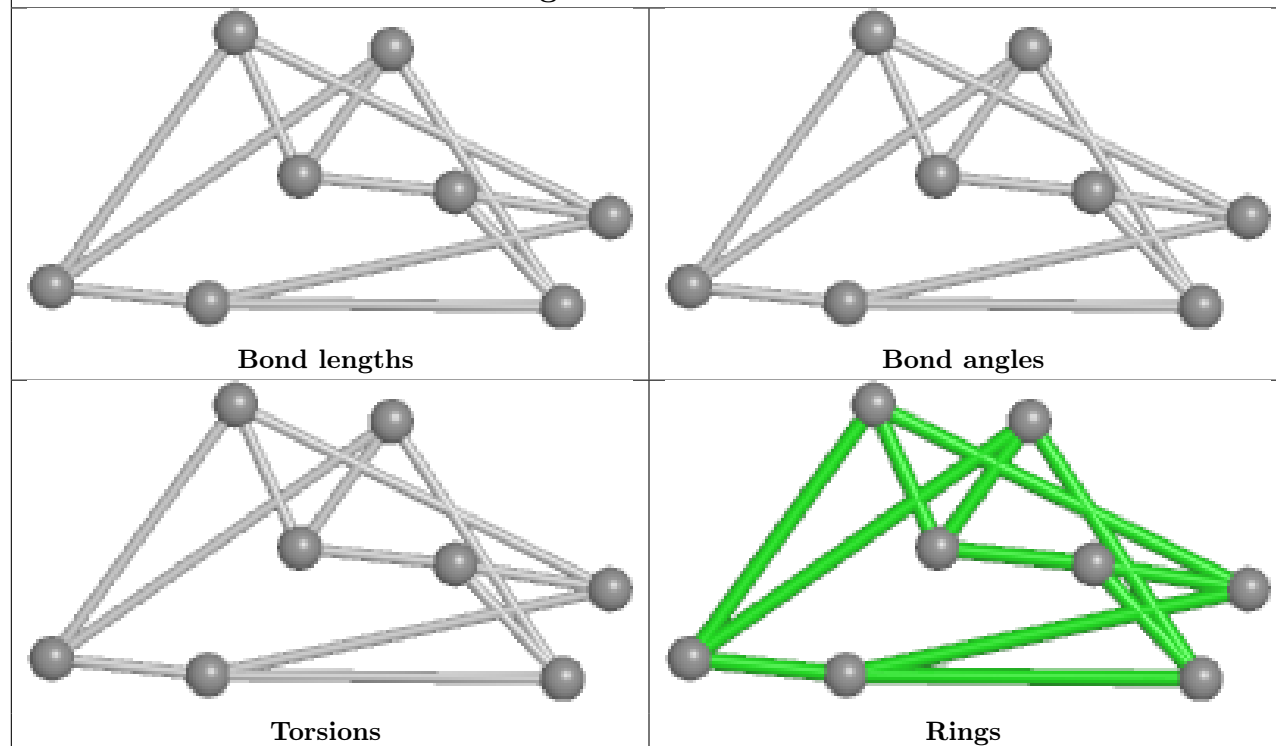




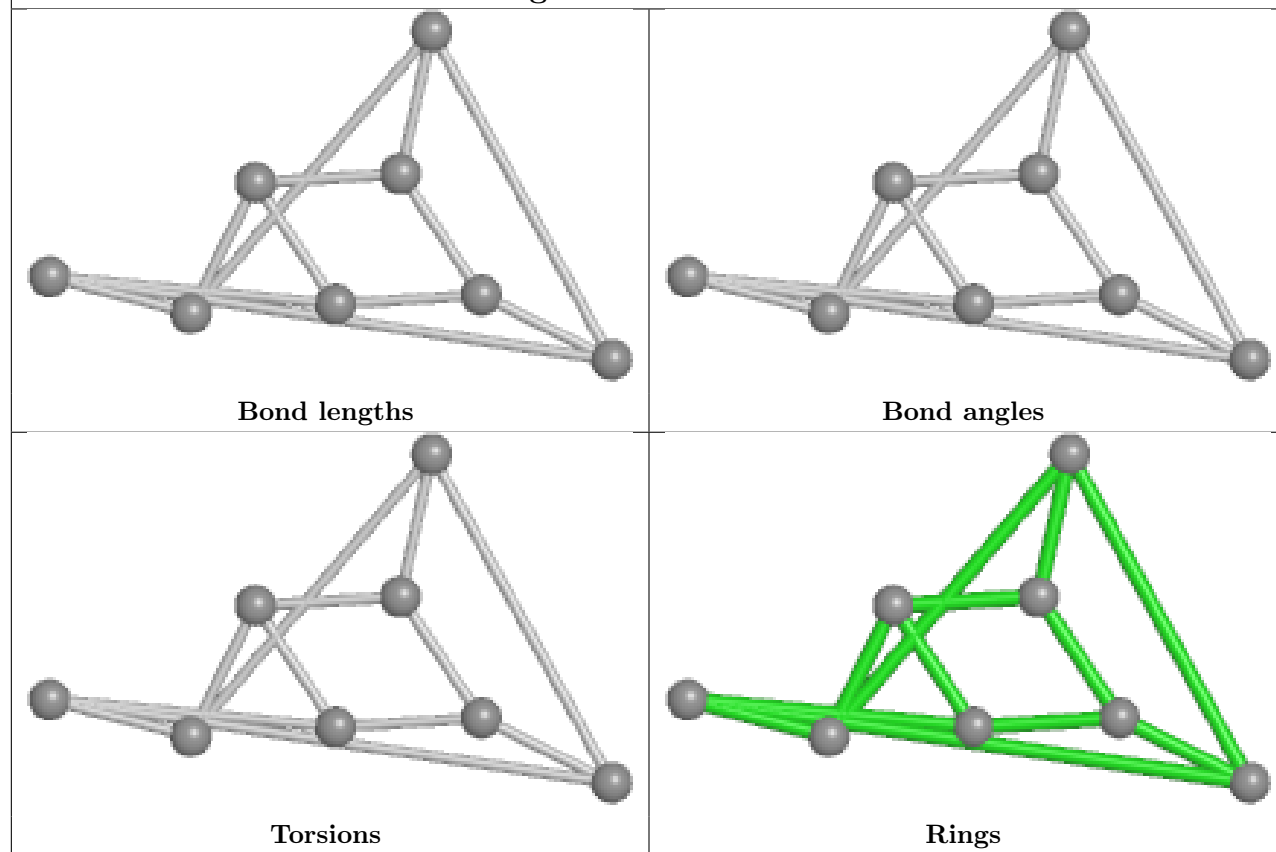




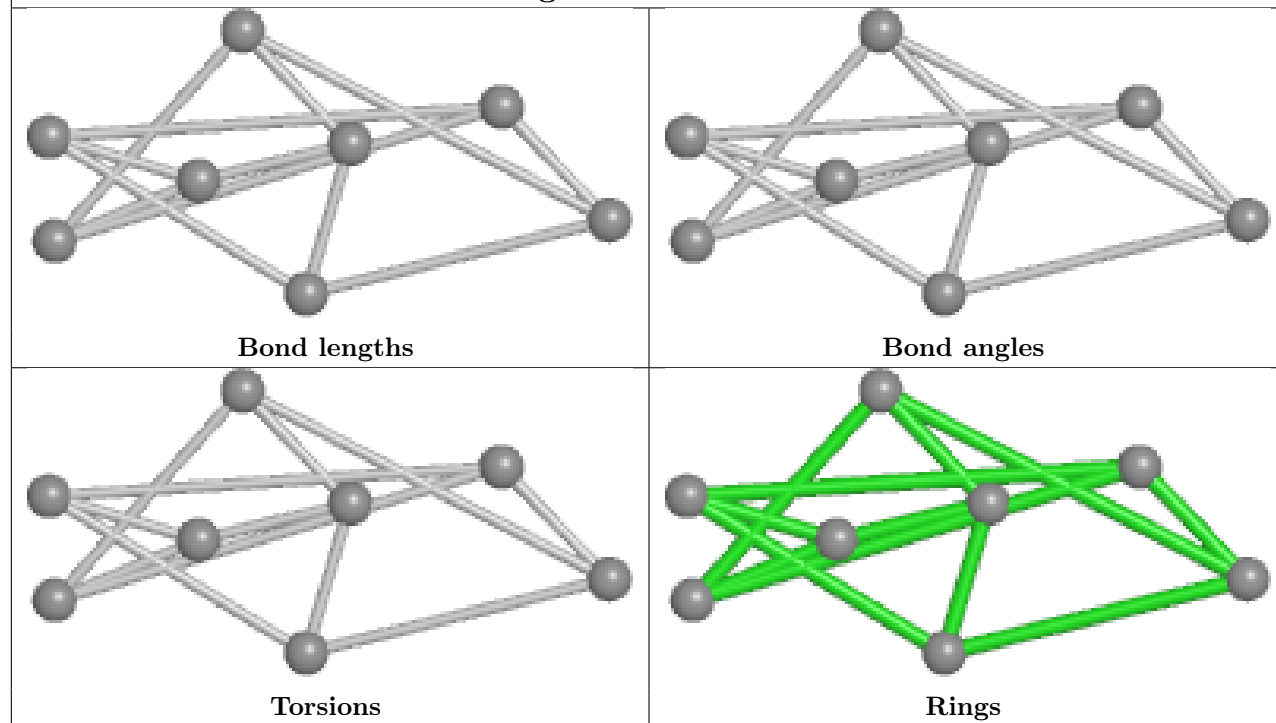
Ligand SF4 B 301



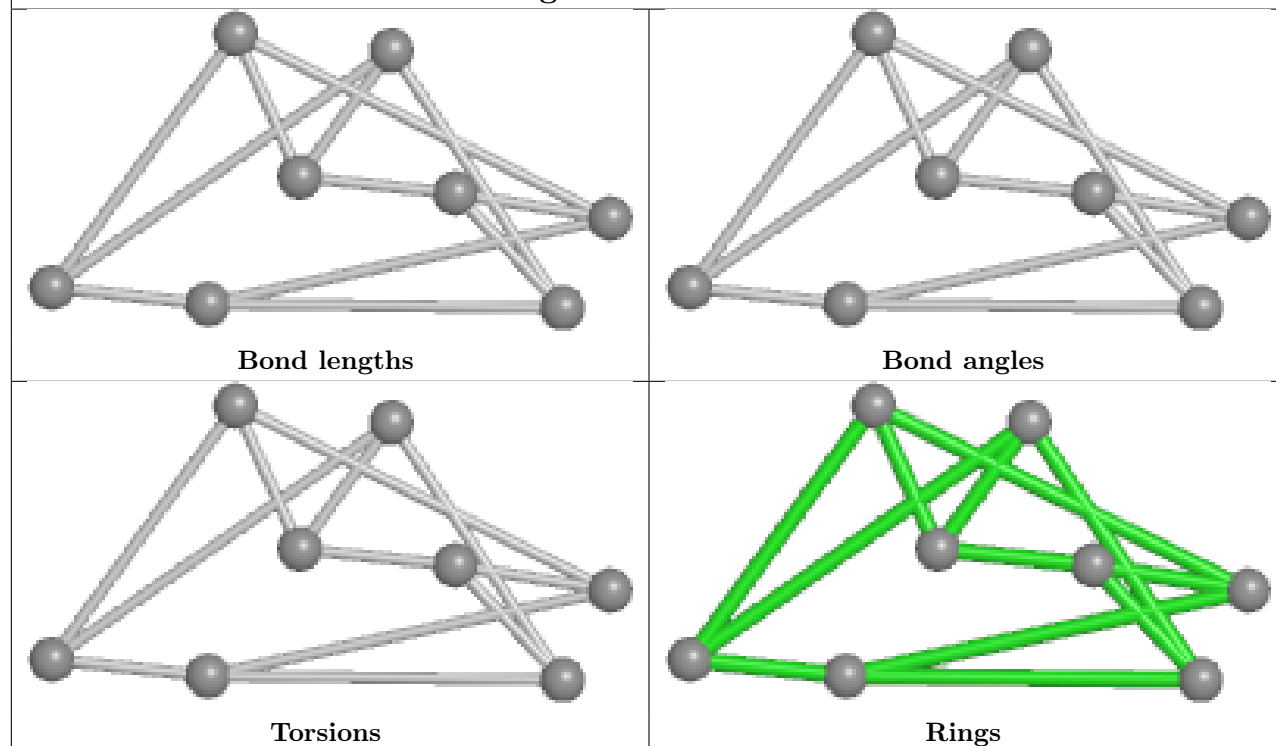
Ligand SF4 A 1103

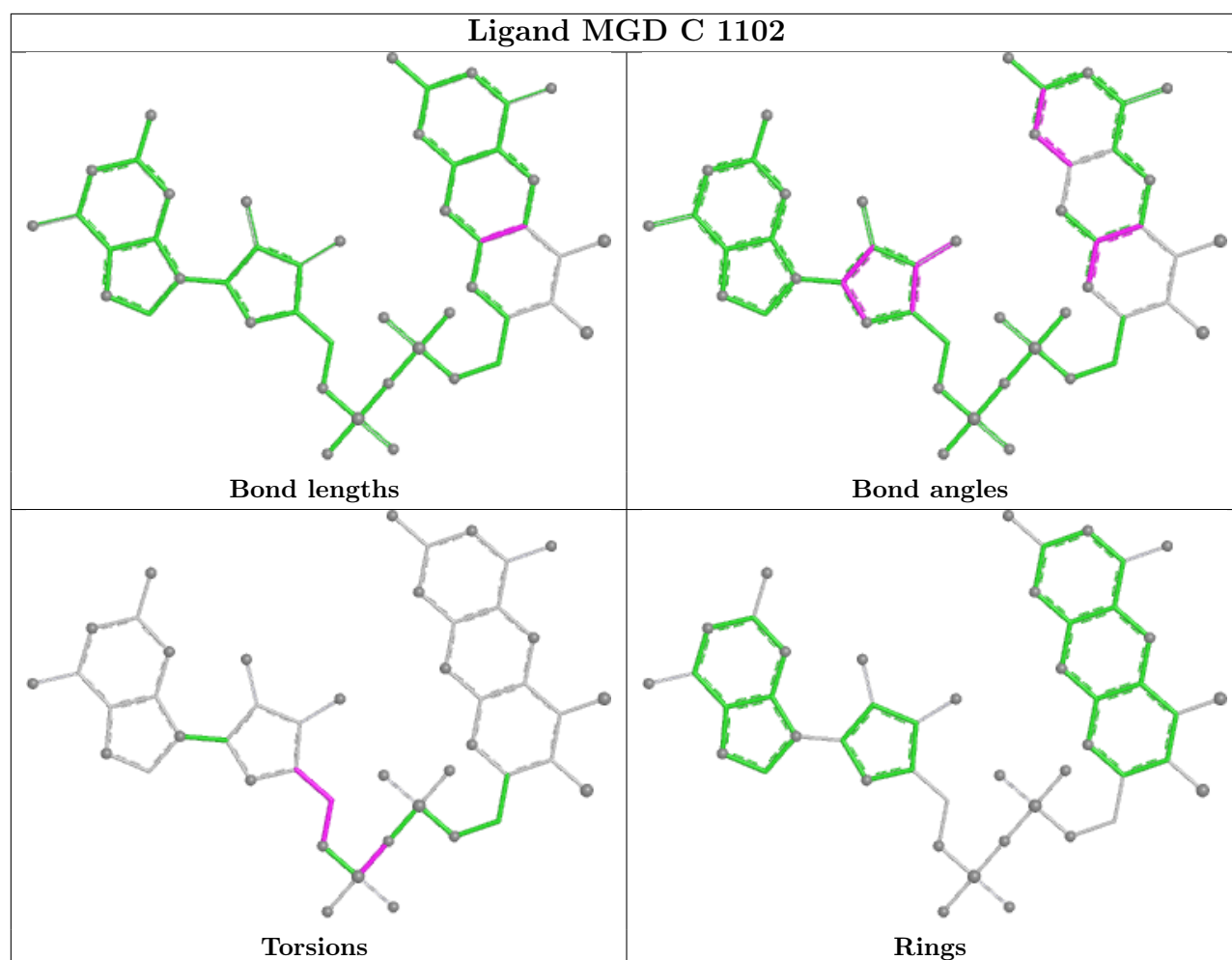


Ligand SF4 D 303

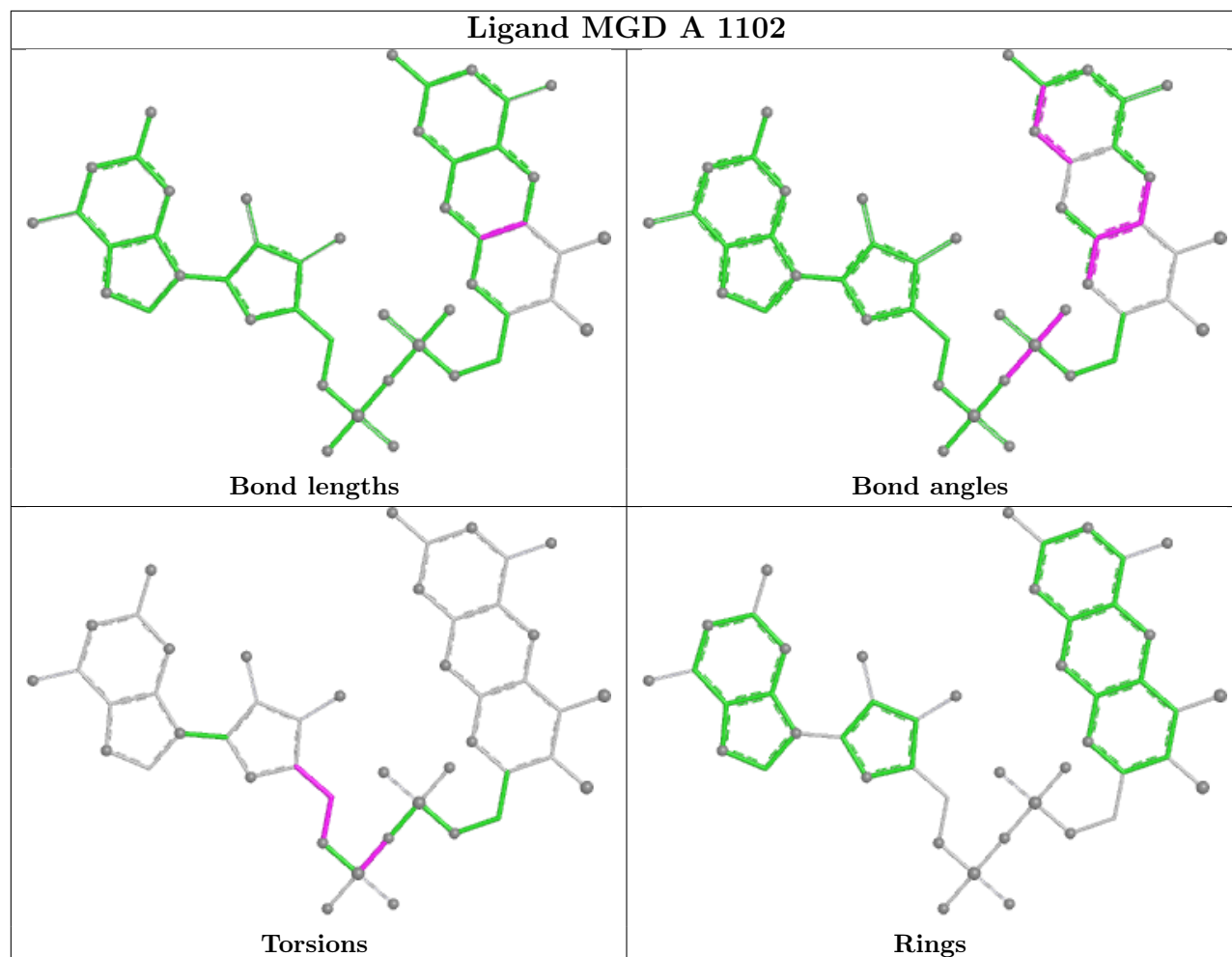


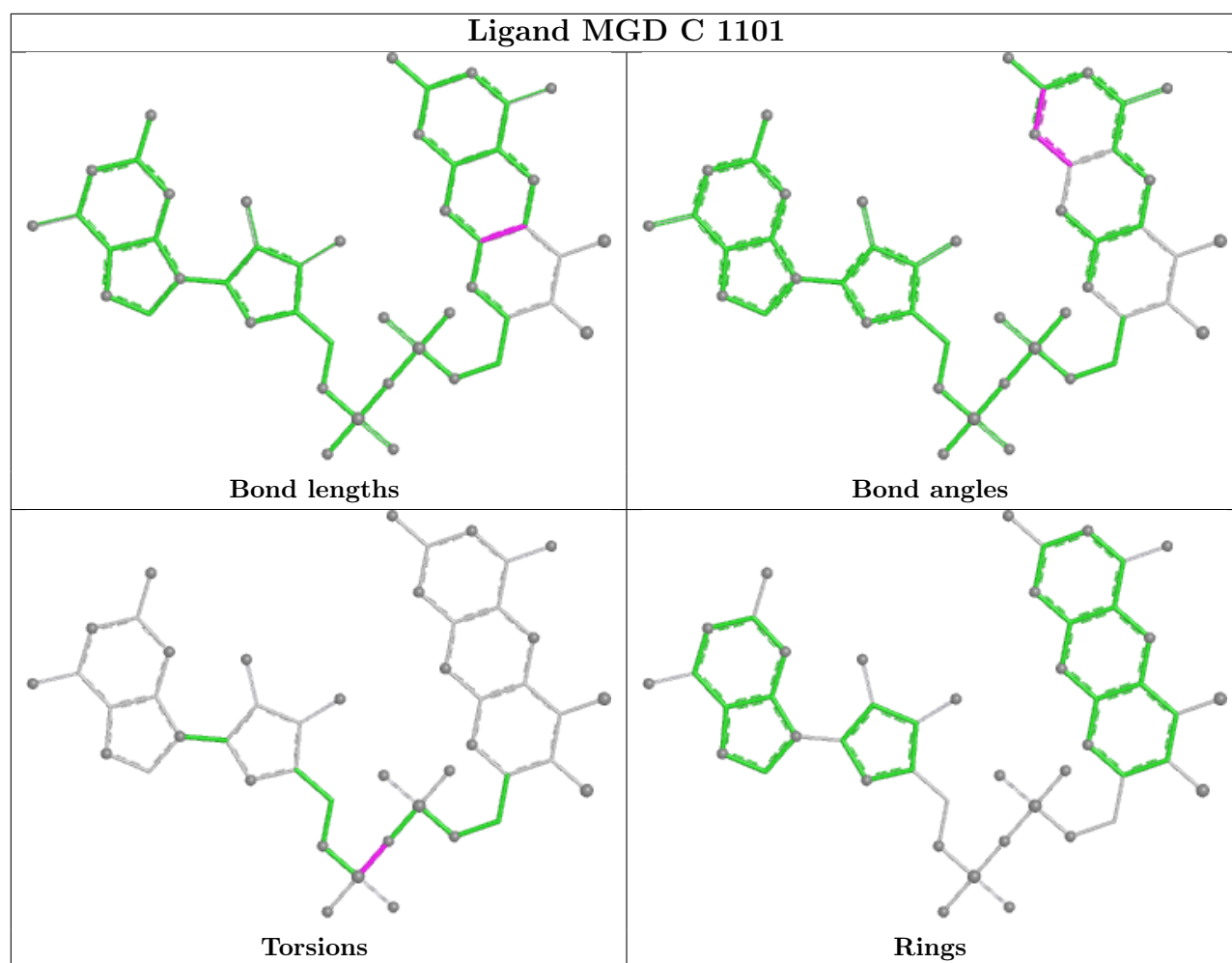
Ligand SF4 B 302





Ligand MGD A 1102





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	972/1013 (95%)	0.17	6 (0%) 85 86	25, 44, 68, 86	0
1	C	969/1013 (95%)	0.22	9 (0%) 81 82	26, 46, 75, 115	0
2	B	214/215 (99%)	-0.15	0 100 100	25, 34, 52, 65	0
2	D	214/215 (99%)	-0.18	0 100 100	26, 35, 52, 80	0
All	All	2369/2456 (96%)	0.13	15 (0%) 85 86	25, 43, 72, 115	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	871	VAL	3.3
1	A	42	TRP	3.1
1	C	339	ALA	2.7
1	C	657	ALA	2.7
1	A	701	GLY	2.3
1	A	719	ALA	2.3
1	A	1008	HIS	2.3
1	A	314	LYS	2.2
1	A	694	PHE	2.2
1	C	505	ALA	2.2
1	C	42	TRP	2.1
1	C	146	ALA	2.1
1	C	736	ASP	2.1
1	C	695	LEU	2.1
1	C	870	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

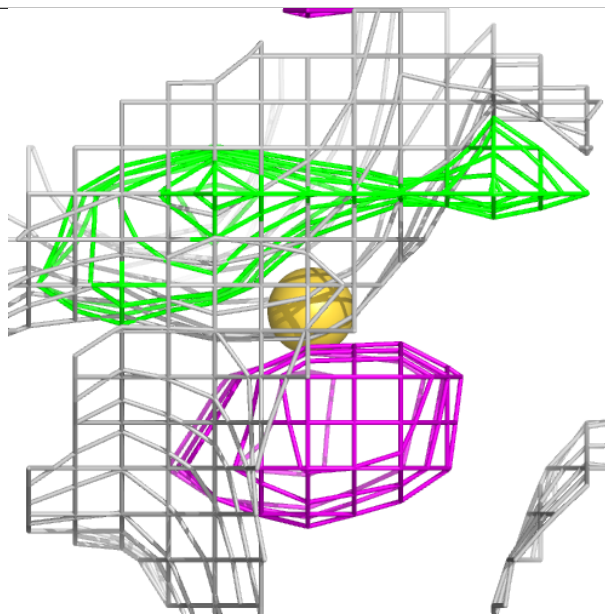
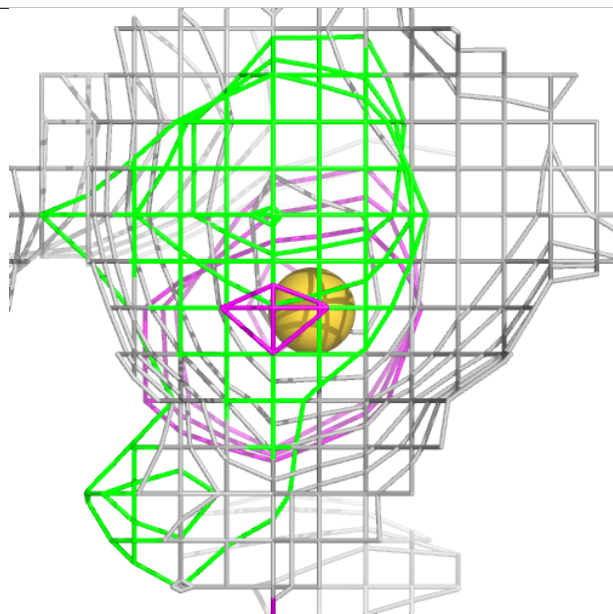
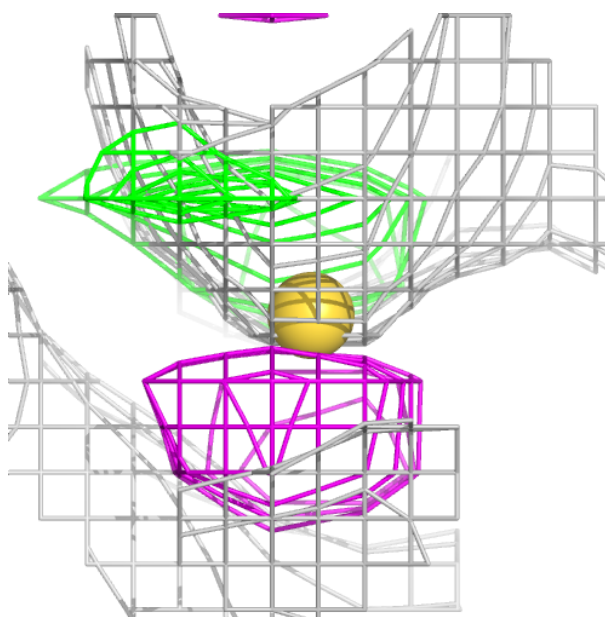
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NO3	B	304	4/4	0.80	0.11	38,45,45,51	0
5	GOL	A	1106	6/6	0.82	0.11	64,65,68,69	0
5	GOL	A	1107	6/6	0.85	0.11	57,62,63,64	0
9	PEG	D	304	7/7	0.88	0.15	22,35,46,47	0
5	GOL	A	1104	6/6	0.89	0.14	52,57,59,63	0
7	H2S	A	1108	1/1	0.93	0.29	29,29,29,29	1
5	GOL	C	1104	6/6	0.94	0.10	58,60,61,65	0
3	MGD	C	1102	47/47	0.97	0.07	22,33,39,43	0
3	MGD	A	1101	47/47	0.97	0.07	28,31,36,37	0
3	MGD	A	1102	47/47	0.97	0.06	24,35,41,43	0
3	MGD	C	1101	47/47	0.97	0.06	27,32,37,40	0
7	H2S	C	1106	1/1	0.98	0.18	30,30,30,30	1
4	SF4	A	1103	8/8	0.99	0.03	27,29,31,32	0
4	SF4	B	301	8/8	0.99	0.03	26,26,28,28	0
4	SF4	B	302	8/8	0.99	0.03	29,30,31,33	0
4	SF4	B	303	8/8	0.99	0.02	27,29,31,32	0
6	W	A	1105	1/1	0.99	0.02	33,33,33,33	0
4	SF4	C	1103	8/8	0.99	0.03	28,29,31,34	0
4	SF4	D	301	8/8	0.99	0.03	26,27,29,30	0
4	SF4	D	302	8/8	0.99	0.03	27,28,30,30	0
4	SF4	D	303	8/8	0.99	0.03	30,31,34,35	0
6	W	C	1105	1/1	1.00	0.01	34,34,34,34	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.

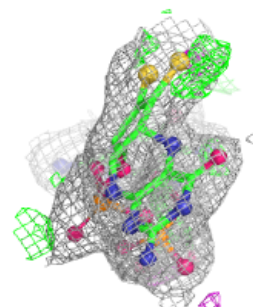
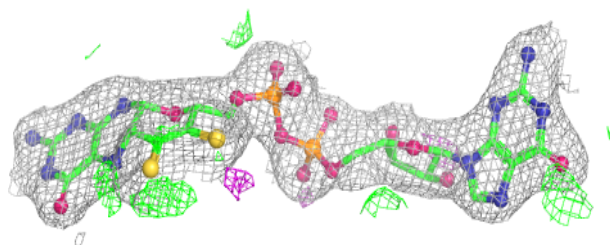
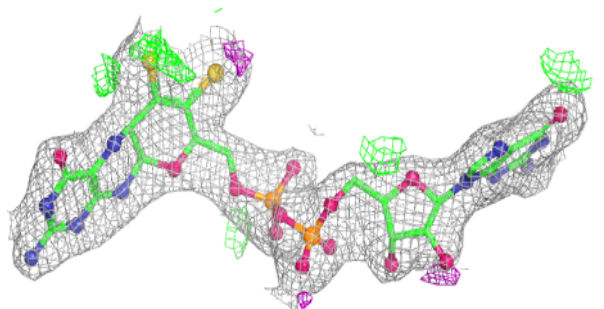
Electron density around H2S A 1108:

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

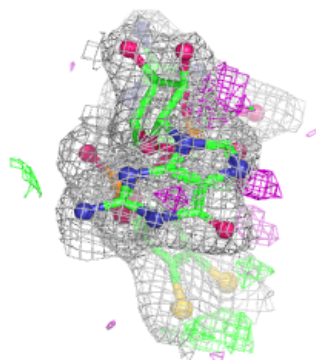
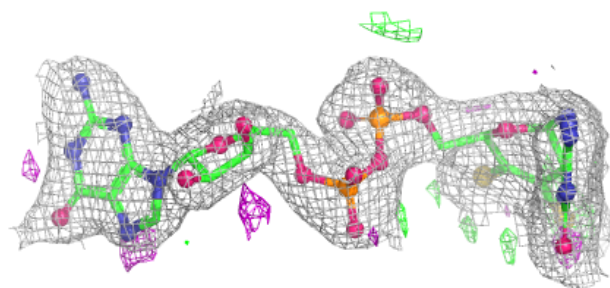
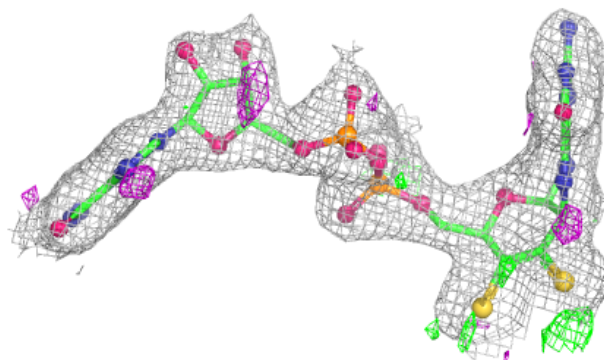


Electron density around MGD C 1102:

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

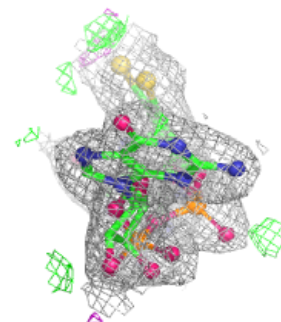
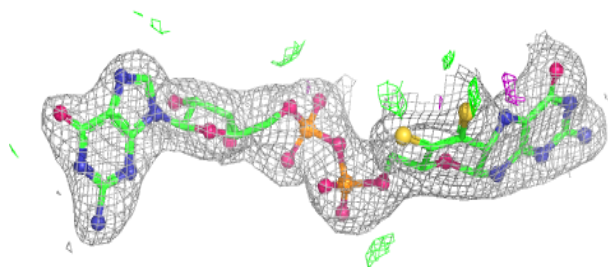
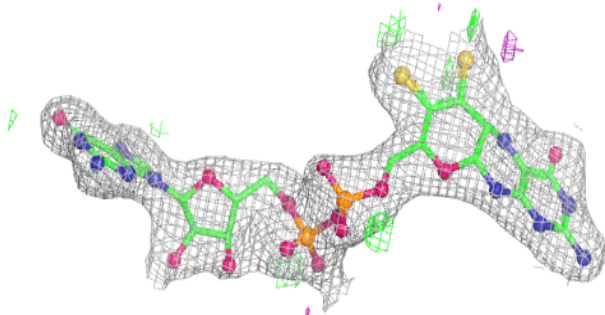
**Electron density around MGD A 1101:**

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

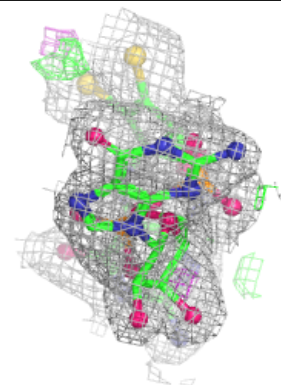
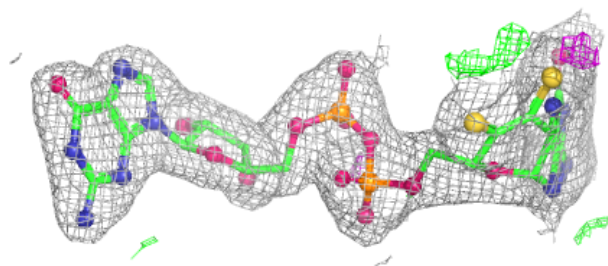
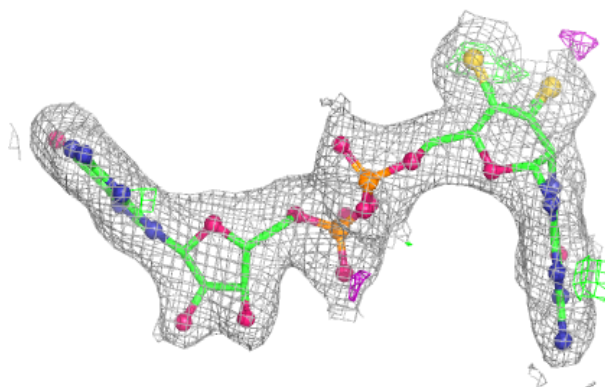


Electron density around MGD A 1102:

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

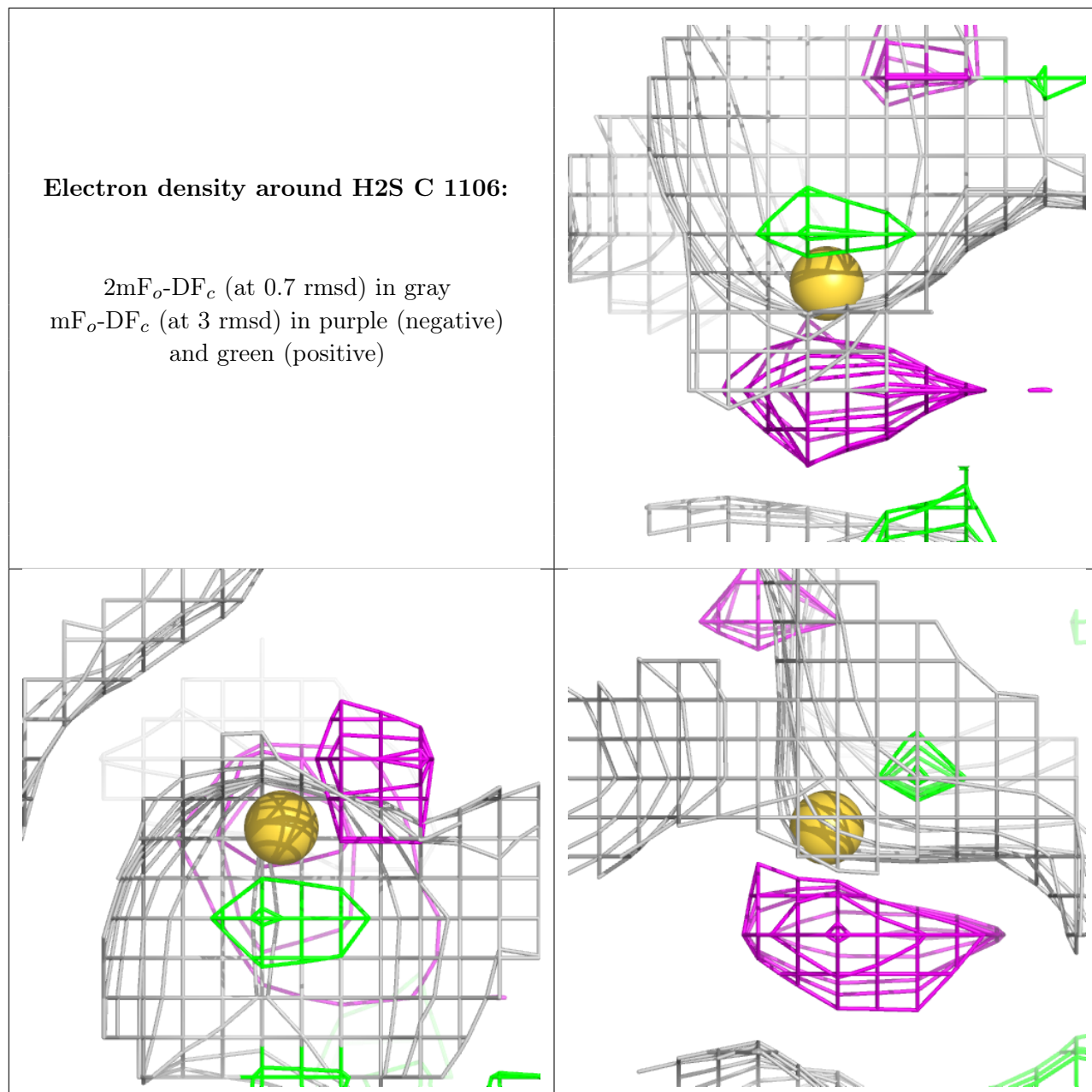
**Electron density around MGD C 1101:**

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



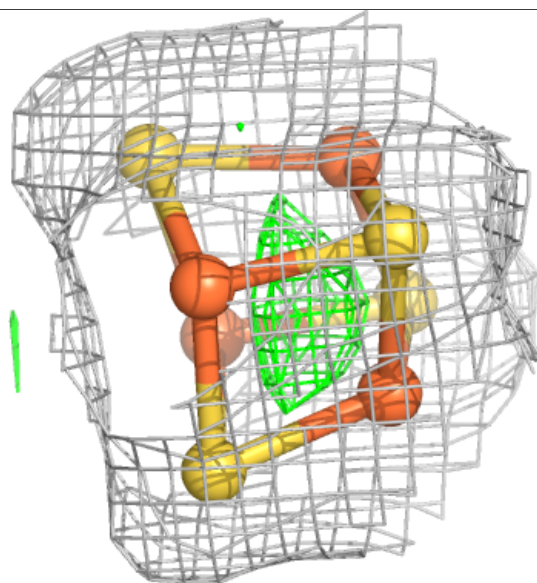
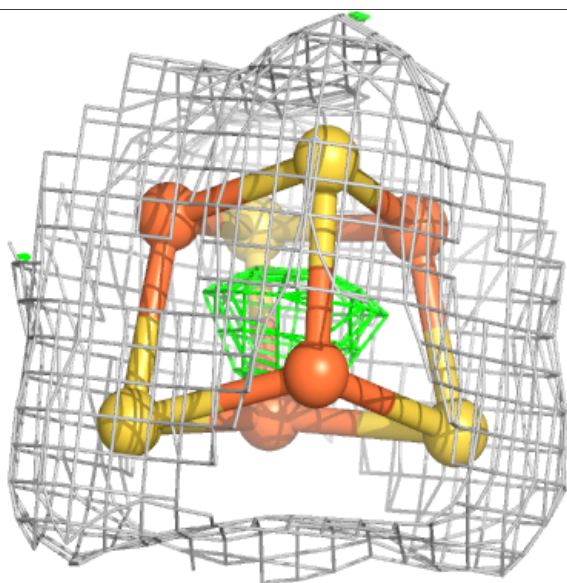
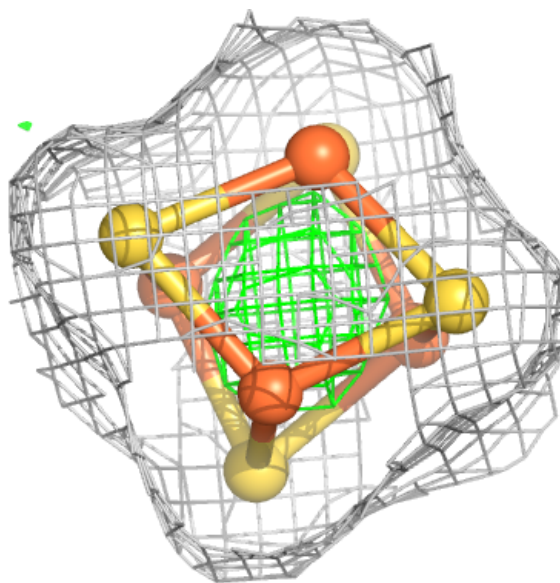
Electron density around H2S C 1106:

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



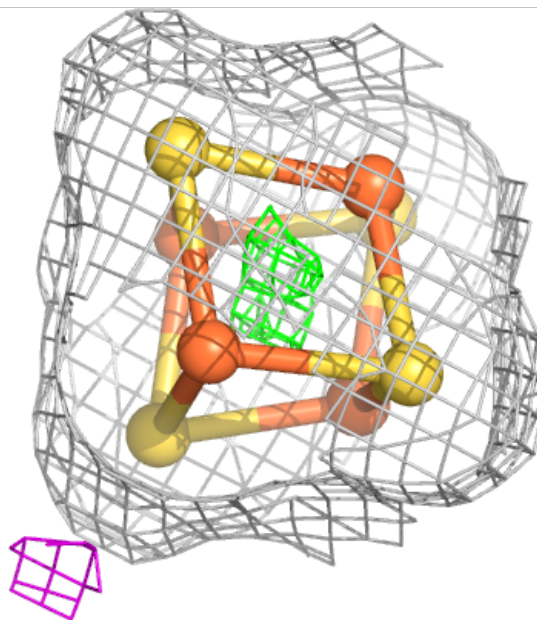
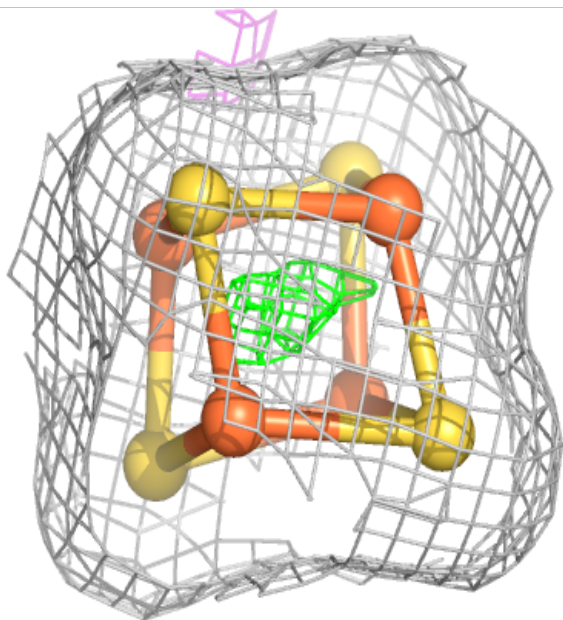
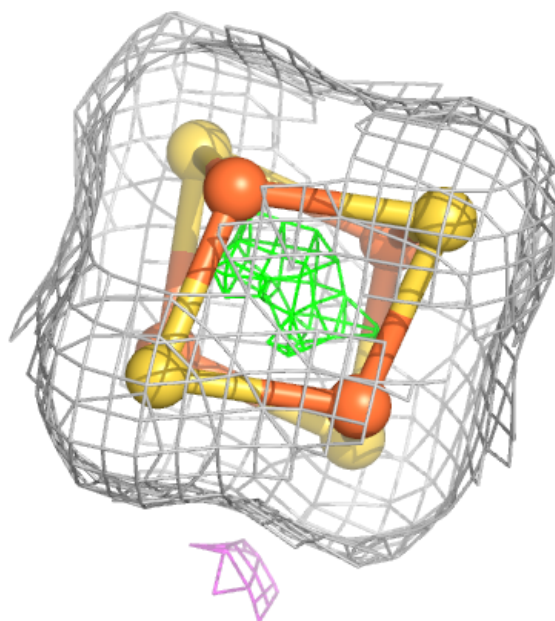
Electron density around SF4 A 1103:

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



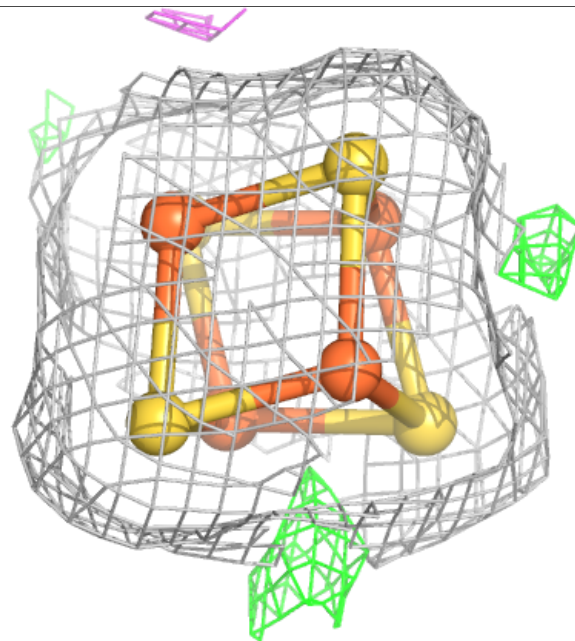
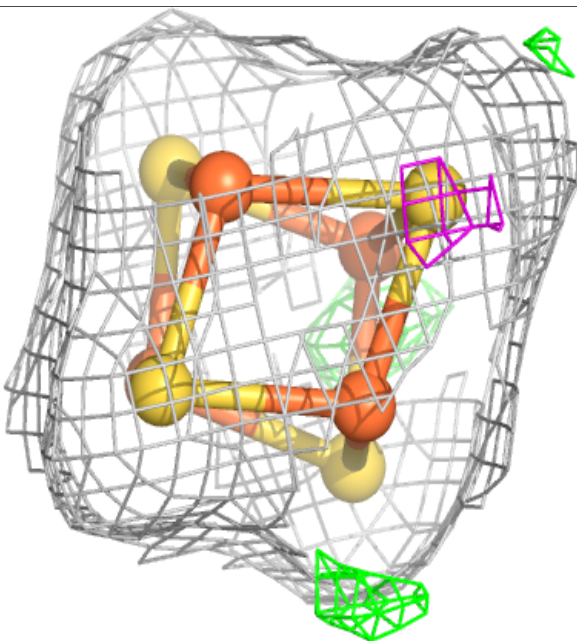
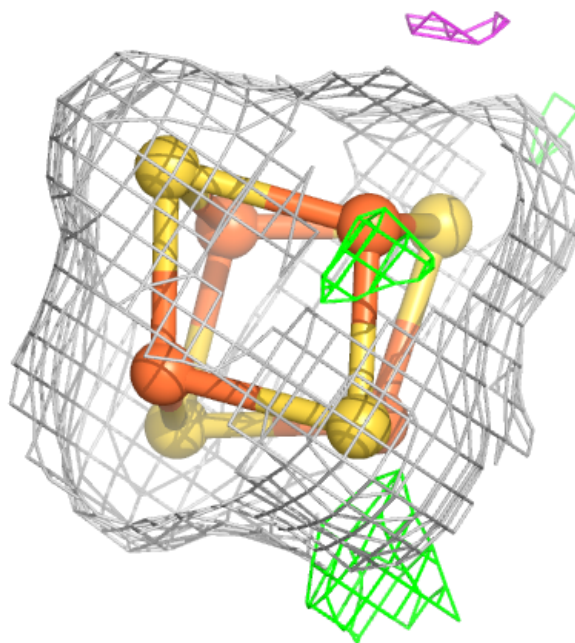
Electron density around SF4 B 301:

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



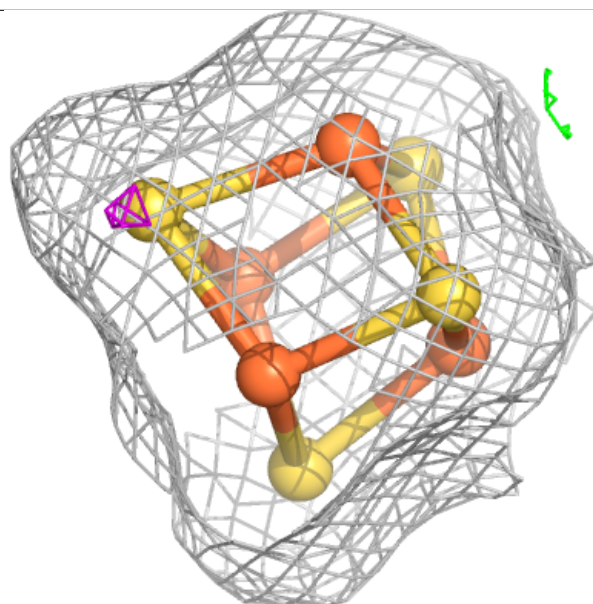
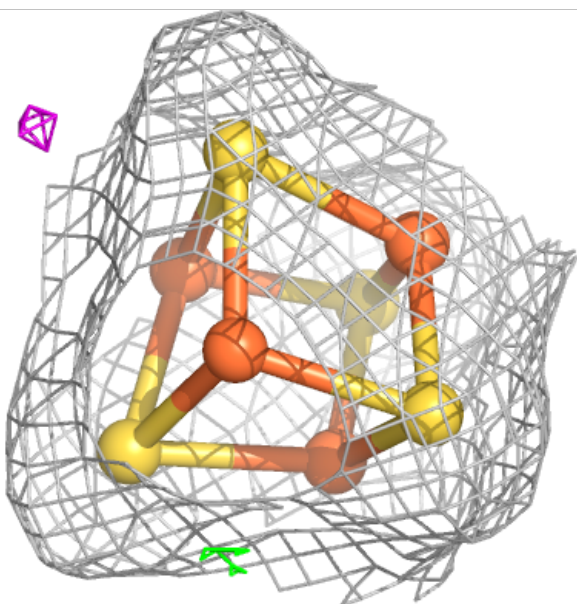
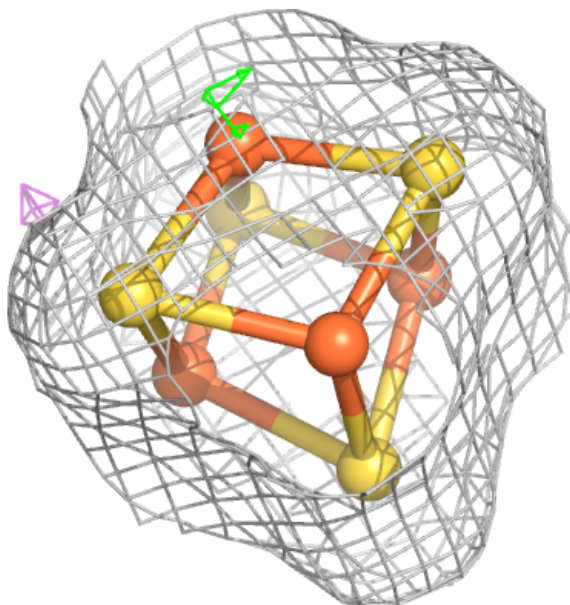
Electron density around SF4 B 302:

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



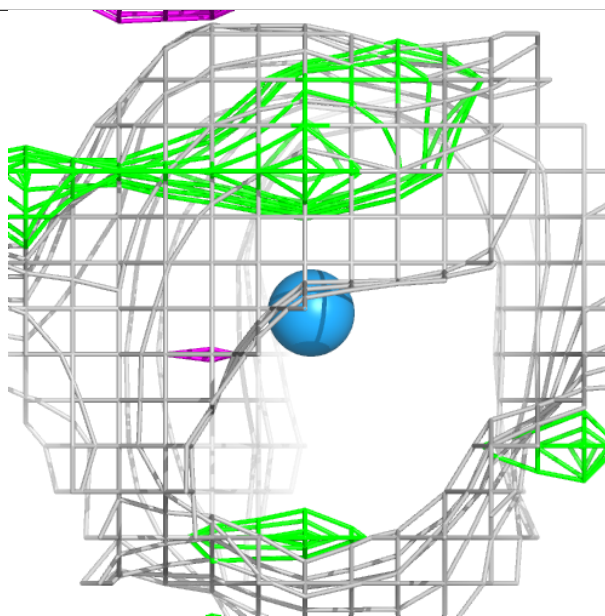
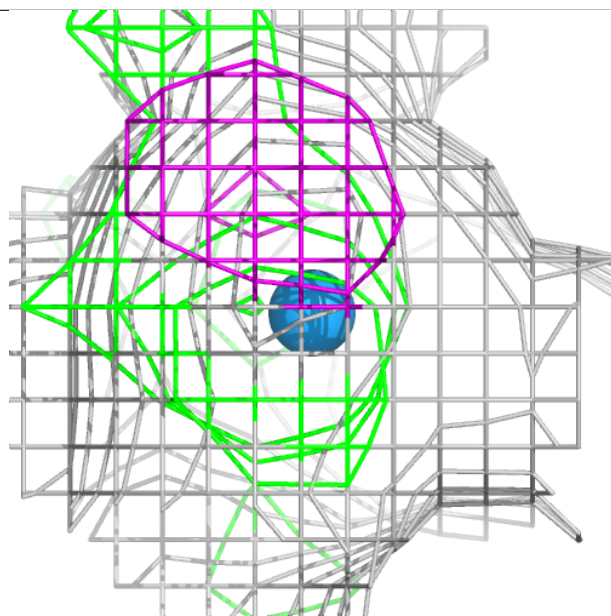
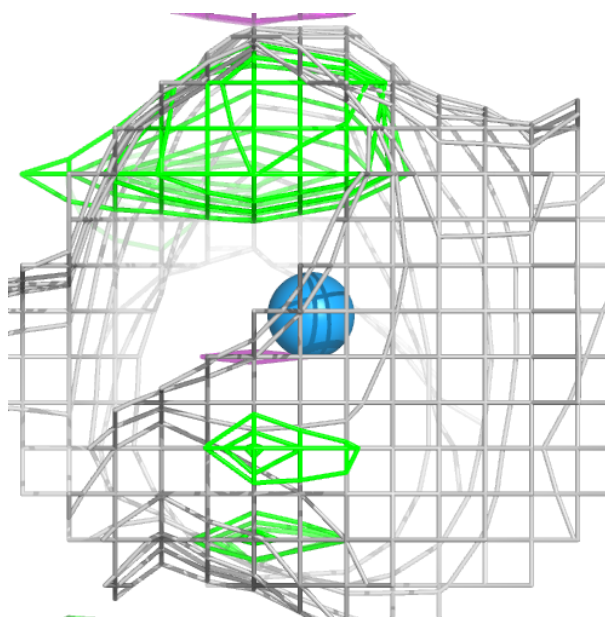
Electron density around SF4 B 303:

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



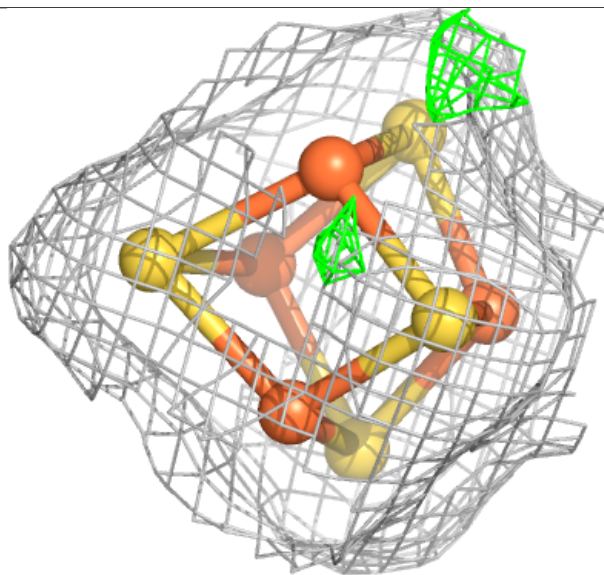
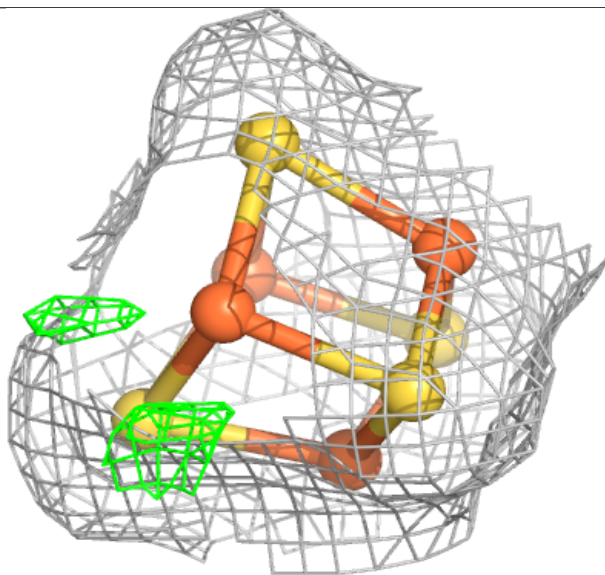
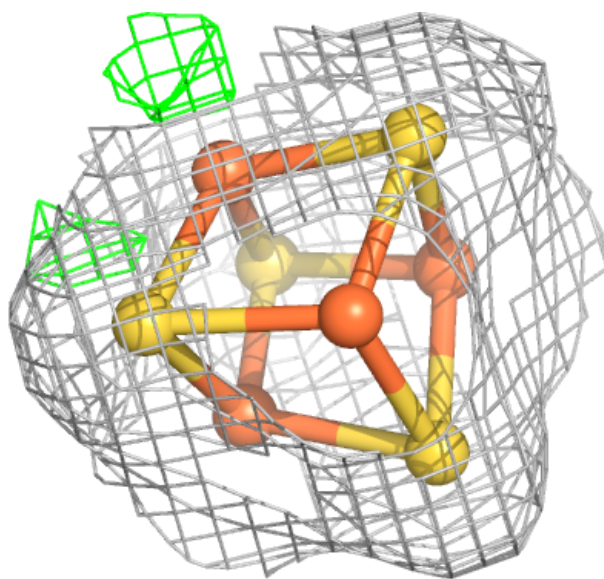
Electron density around W A 1105:

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



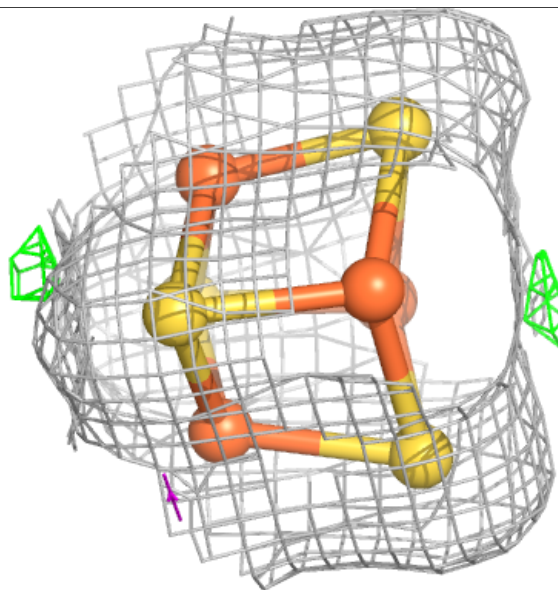
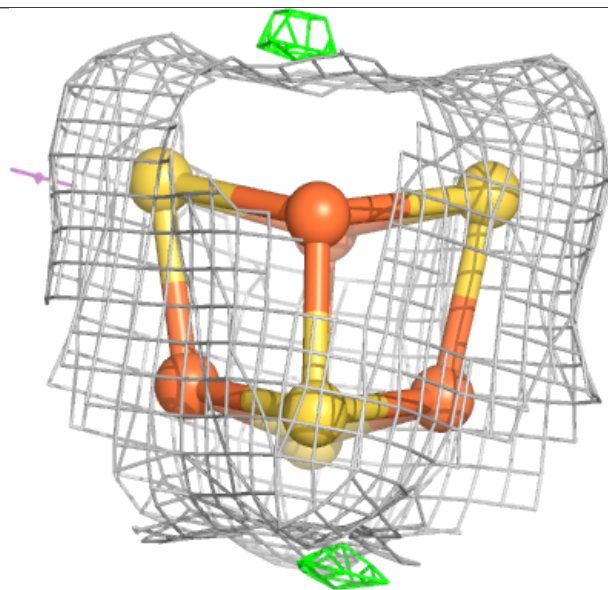
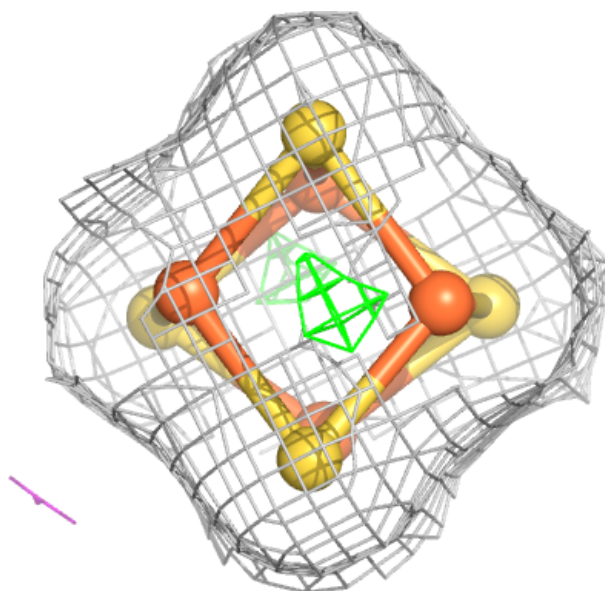
Electron density around SF4 C 1103:

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



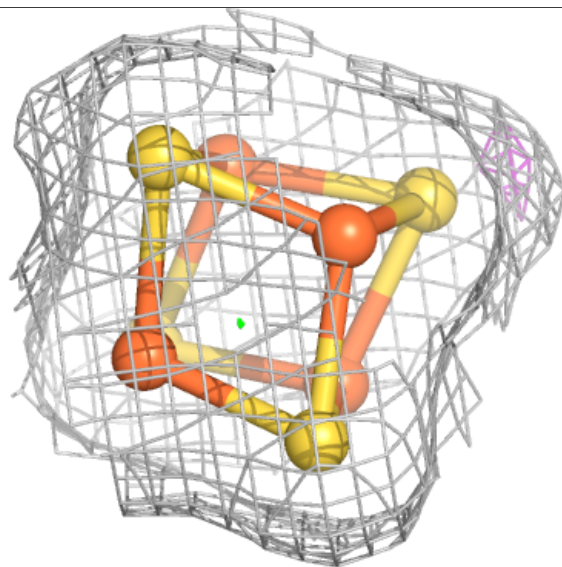
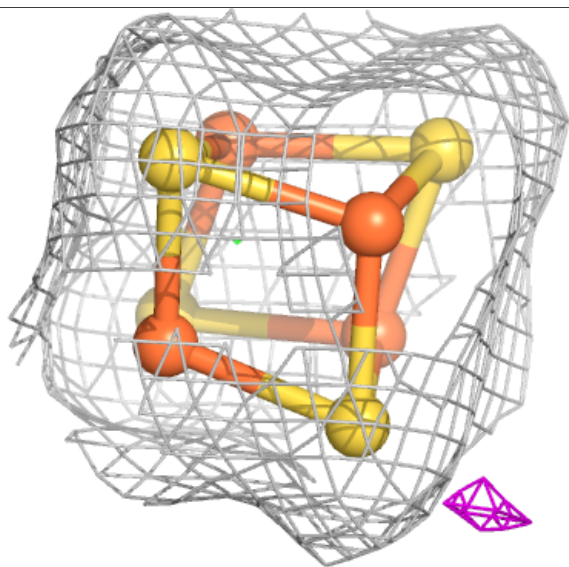
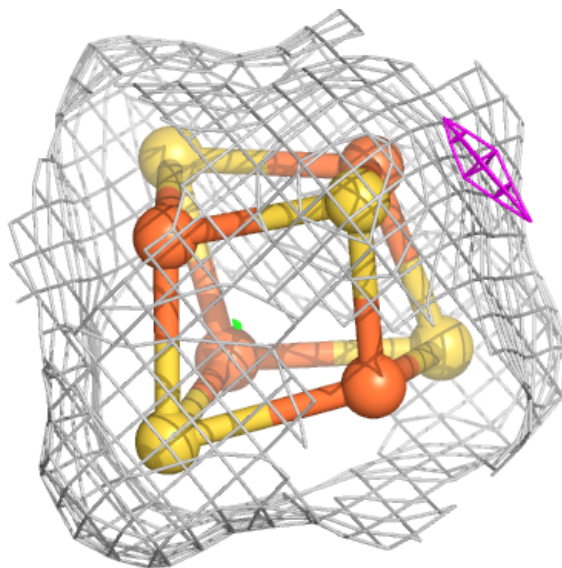
Electron density around SF4 D 301:

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



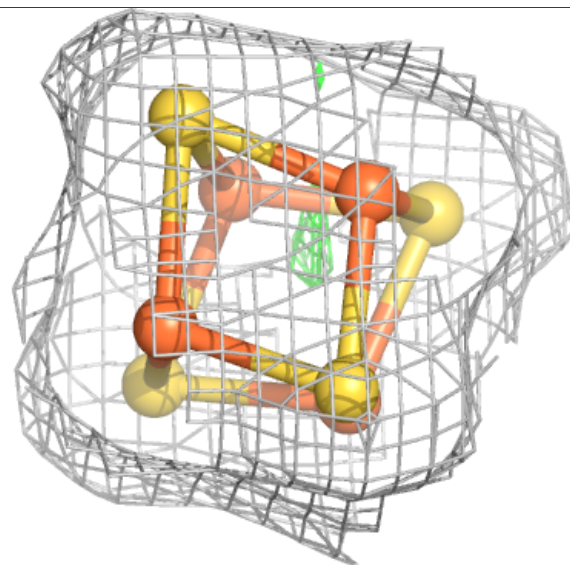
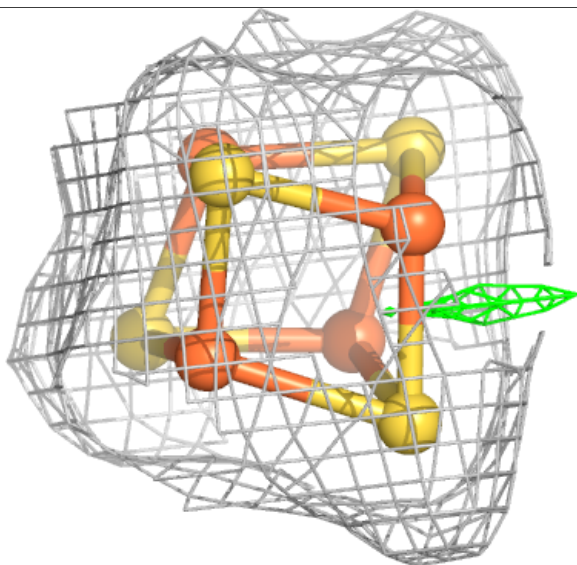
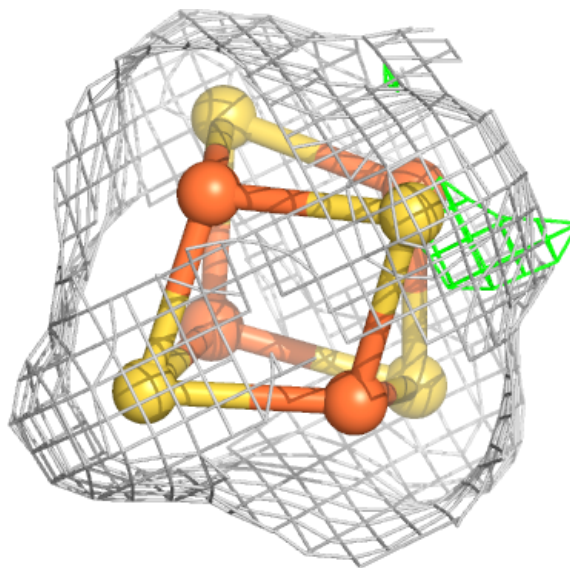
Electron density around SF4 D 302:

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



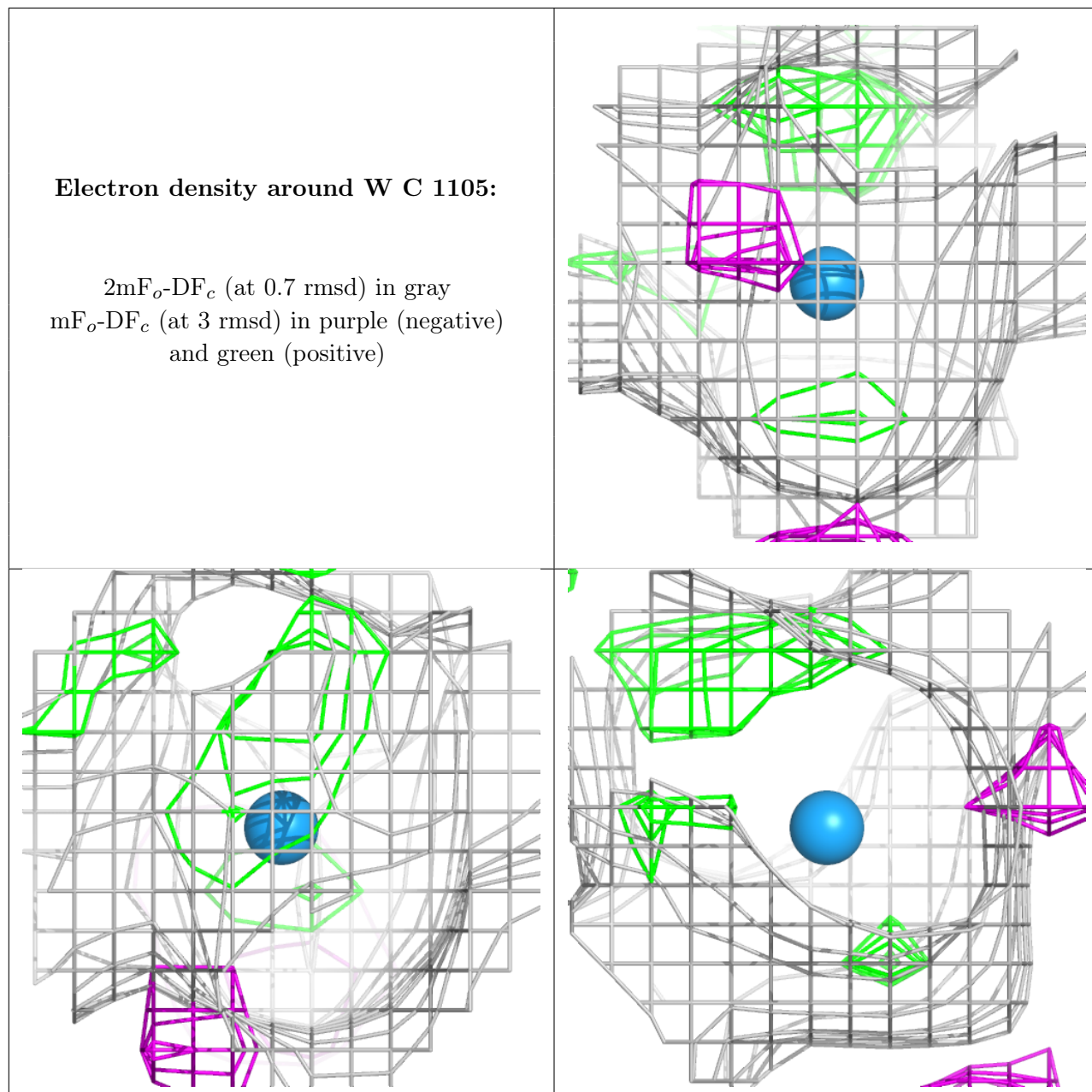
Electron density around SF4 D 303:

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



Electron density around W C 1105:

$2mF_o-DF_c$ (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.