



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 AM UTC

PDB ID : 9QM1 / pdb_00009qm1
Title : W-formate dehydrogenase U192C from *Desulfovibrio vulgaris* - Soaked with Dithionite
Authors : Vilela-Alves, G.; Oliveira, A.R.; Pereira, I.C.; Romao, M.J.; Mota, C.
Deposited on : 2025-03-21
Resolution : 2.00 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

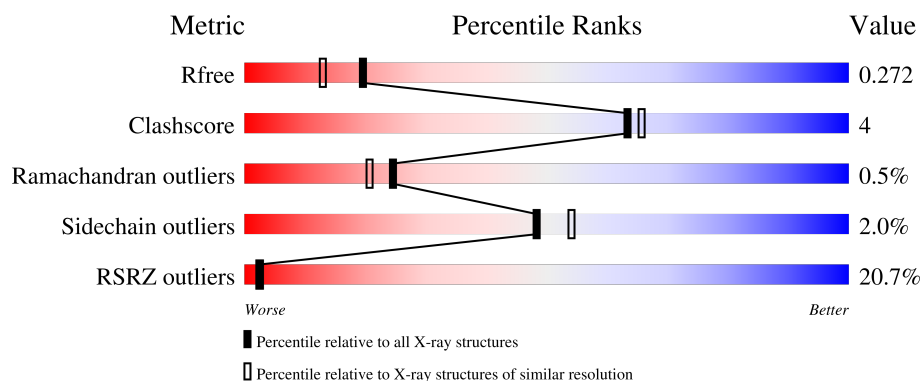
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	
2	B	214	

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
6	SO2	A	1209	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9828 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	967	Total	C	N	O	S	0	1	0
			7579	4832	1321	1384	42			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	CYS	SEC	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

- 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			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



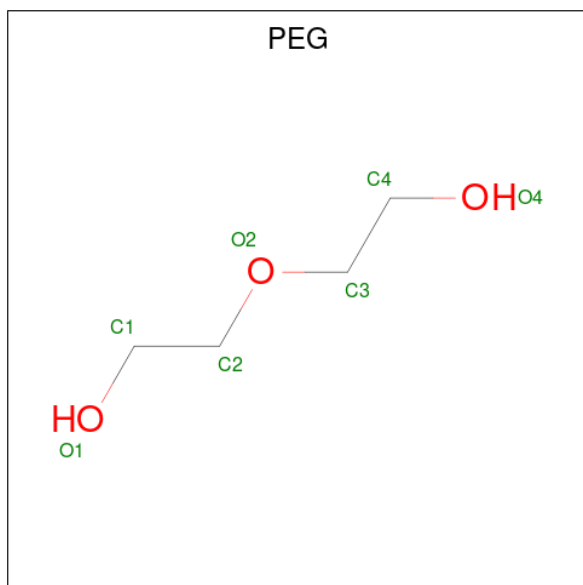
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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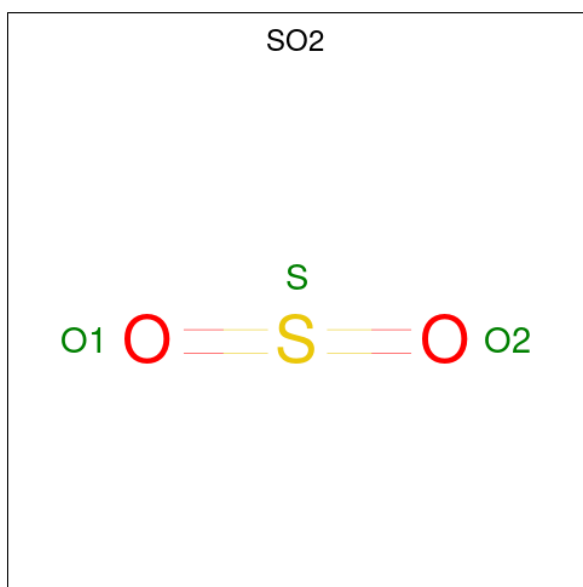
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



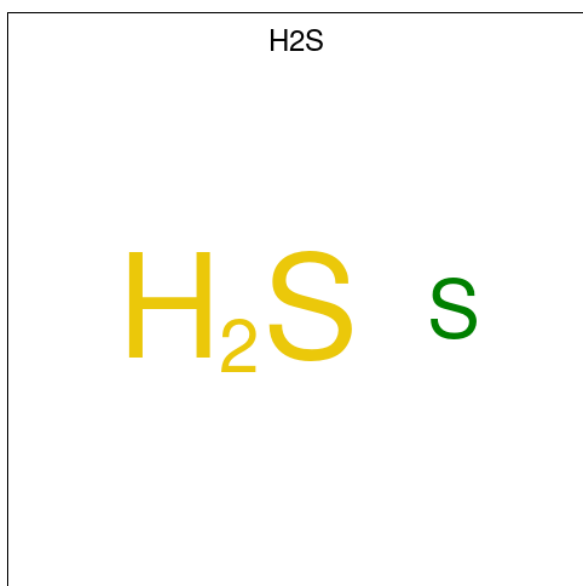
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is SULFUR DIOXIDE (CCD ID: SO2) (formula: O_2S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			3	2	1		

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

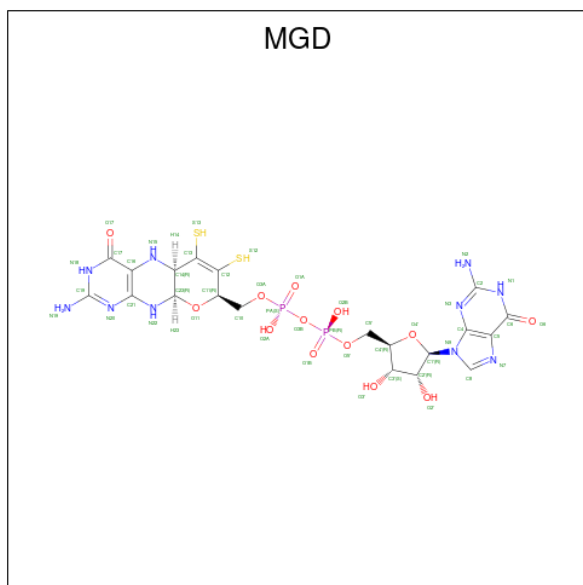


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	S	0	0
			1	1		

- Molecule 8 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

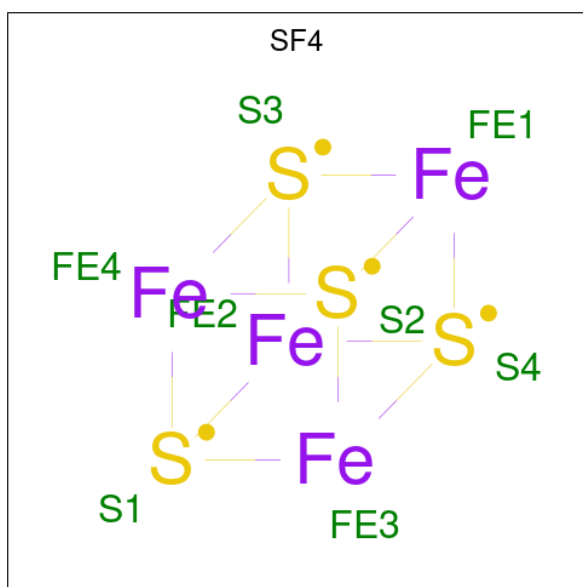
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total W 1 1	0	0

- Molecule 9 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: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



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

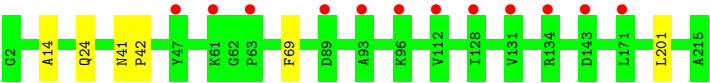
- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	296	Total	O	0	0
			296	296		
11	B	119	Total	O	0	0
			119	119		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.80Å 122.51Å 146.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.93 – 2.00 62.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (62.93-2.00) 99.3 (62.93-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.267 0.221 , 0.272	Depositor DCC
R_{free} test set	3696 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9828	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: PEG, W, GOL, MGD, H2S, EDO, SO2, 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	0.99	0/7790	1.37	0/10566
2	B	0.99	0/1699	1.38	0/2302
All	All	0.99	0/9489	1.37	0/12868

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	7579	0	7425	71	0
2	B	1664	0	1633	4	0
3	A	12	0	16	1	0
4	A	20	0	30	0	0
5	A	7	0	10	0	0
6	A	3	0	0	3	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
9	A	94	0	44	5	0
10	A	8	0	0	0	0
10	B	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	296	0	0	1	0
11	B	119	0	0	0	0
All	All	9828	0	9158	74	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 (74) 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:168:GLU:HA	1:A:690:MET:HE1	1.51	0.91
1:A:171:TRP:CB	1:A:690:MET:HE2	2.11	0.79
1:A:171:TRP:HB3	1:A:690:MET:HE2	1.73	0.69
1:A:171:TRP:HB3	1:A:690:MET:CE	2.25	0.66
1:A:775:ARG:O	3:A:1201:GOL:O2	2.14	0.66
1:A:595:ASN:N	1:A:595:ASN:OD1	2.31	0.63
1:A:105:THR:O	1:A:106:GLN:O	2.18	0.62
1:A:192:CYS:SG	6:A:1209:SO2:S	2.98	0.61
1:A:132:ARG:O	1:A:136:THR:OG1	2.21	0.59
1:A:591:GLY:O	1:A:593:GLY:N	2.36	0.59
1:A:565:ASN:O	1:A:569:MET:HG3	2.03	0.59
1:A:105:THR:HG22	1:A:636:ALA:CB	2.34	0.57
1:A:193:HIS:HB2	6:A:1209:SO2:S	2.45	0.56
1:A:129:ILE:CG2	1:A:648:MET:HE2	2.38	0.54
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.89	0.54
1:A:121:THR:HG23	1:A:124:PHE:H	1.73	0.54
1:A:586:SER:O	1:A:589:TRP:CZ3	2.62	0.53
1:A:588:PHE:O	1:A:594:MET:HG3	2.09	0.53
1:A:894:MET:SD	9:A:1213:MGD:H2'	2.48	0.53
1:A:173:TYR:HB2	1:A:645:MET:HE1	1.90	0.53
1:A:129:ILE:HG21	1:A:648:MET:HE2	1.90	0.52
1:A:858:ASN:HB3	1:A:861:ALA:HB2	1.91	0.52
1:A:607:PRO:O	1:A:638:THR:OG1	2.27	0.51
1:A:131:LYS:O	1:A:135:LYS:HG2	2.11	0.50
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.46	0.50
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.51	0.50
1:A:63:THR:HG21	1:A:632:PRO:HA	1.94	0.49
1:A:996:LYS:HD2	9:A:1212:MGD:C8	2.42	0.49
1:A:795:LYS:HE3	1:A:796:ASP:H	1.78	0.48
2:B:41:ASN:HA	2:B:42:PRO:C	2.38	0.48
1:A:226:GLY:HA2	1:A:406:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HD12	1:A:606:LEU:N	2.28	0.48
1:A:107:PRO:HA	1:A:607:PRO:HD3	1.96	0.48
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.48	0.48
1:A:171:TRP:CG	1:A:690:MET:HE2	2.49	0.47
1:A:750:PRO:O	1:A:754:ARG:HG2	2.15	0.47
1:A:410:HIS:HA	1:A:994:GLU:HG3	1.97	0.47
1:A:476:TYR:HE1	1:A:499:VAL:HG21	1.78	0.47
1:A:582:GLU:HG2	1:A:969:MET:HE1	1.96	0.46
1:A:476:TYR:CE1	1:A:499:VAL:HG21	2.51	0.46
1:A:446:VAL:HG21	6:A:1209:SO2:S	2.55	0.46
1:A:284:LYS:NZ	1:A:288:ASP:OD2	2.48	0.46
1:A:194:SER:N	1:A:195:PRO:CD	2.78	0.46
1:A:404:ALA:HB3	9:A:1212:MGD:O2A	2.16	0.46
1:A:569:MET:HE1	1:A:585:THR:HG23	1.97	0.45
1:A:132:ARG:NH2	1:A:602:GLU:OE2	2.50	0.45
1:A:355:VAL:HG13	1:A:827:TYR:HB2	1.99	0.45
1:A:129:ILE:HG21	1:A:648:MET:CE	2.47	0.45
1:A:475:LEU:HD23	1:A:475:LEU:HA	1.86	0.44
1:A:643:ASP:OD1	1:A:680:GLU:HB2	2.18	0.44
1:A:157:ILE:HG22	1:A:182:LEU:HD21	2.00	0.43
1:A:896:ARG:HD2	1:A:970:VAL:O	2.18	0.43
1:A:168:GLU:HA	1:A:690:MET:CE	2.35	0.43
1:A:547:GLY:HA3	1:A:574:TRP:CE2	2.54	0.43
1:A:549:PHE:HE1	1:A:648:MET:HE1	1.83	0.43
1:A:195:PRO:HA	1:A:990:THR:HG21	2.01	0.42
1:A:110:ARG:HD2	1:A:589:TRP:CZ3	2.55	0.42
1:A:232:ASN:HA	9:A:1212:MGD:N20	2.34	0.42
1:A:209:MET:HG3	1:A:438:ASN:HA	2.00	0.42
1:A:508:PRO:HD3	1:A:671:ASN:HB2	2.01	0.42
1:A:585:THR:O	1:A:588:PHE:HD2	2.03	0.42
1:A:623:ARG:O	1:A:764:CYS:HA	2.20	0.42
1:A:108:LEU:HB3	1:A:117:TRP:HB3	2.01	0.41
1:A:206:ARG:HB2	1:A:773:TYR:OH	2.20	0.41
1:A:860:VAL:O	1:A:988:PRO:HB3	2.20	0.41
1:A:591:GLY:O	1:A:592:PRO:C	2.63	0.41
1:A:882:THR:HA	1:A:962:LEU:O	2.20	0.41
1:A:272:SER:HA	9:A:1212:MGD:O6	2.20	0.41
2:B:201:LEU:HD23	2:B:201:LEU:C	2.46	0.41
1:A:754:ARG:NH1	1:A:787:PRO:O	2.52	0.41
1:A:930:VAL:HG11	1:A:962:LEU:HD11	2.02	0.41
1:A:108:LEU:CB	1:A:117:TRP:CE3	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HB2	1:A:117:TRP:CE3	2.56	0.40
1:A:446:VAL:HG11	11:A:1301:HOH:O	2.21	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	964/1013 (95%)	919 (95%)	39 (4%)	6 (1%)	21	17
2	B	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	1176/1227 (96%)	1123 (96%)	47 (4%)	6 (0%)	24	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	592	PRO
1	A	678	HIS
1	A	636	ALA
1	A	533	TRP
1	A	663	TYR

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	788/820 (96%)	769 (98%)	19 (2%)	43	47
2	B	185/185 (100%)	185 (100%)	0	100	100
All	All	973/1005 (97%)	954 (98%)	19 (2%)	48	54

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	122	TRP
1	A	136	THR
1	A	237	PHE
1	A	361	LYS
1	A	528	LEU
1	A	595	ASN
1	A	599	ILE
1	A	633	LYS
1	A	638	THR
1	A	648	MET
1	A	672	ILE
1	A	674	ASP
1	A	684	THR
1	A	696	LYS
1	A	697	ASP
1	A	754	ARG
1	A	795	LYS
1	A	969	MET

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	73	ASN
1	A	704	GLN
2	B	24	GLN
2	B	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 15 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	$\# Z > 2$
10	SF4	A	1214	1	0,12,12	-	-	-		
3	GOL	A	1203	-	5,5,5	0.10	0	5,5,5	0.27	0
10	SF4	B	302	2	0,12,12	-	-	-		
4	EDO	A	1207	-	3,3,3	0.07	0	2,2,2	0.13	0
4	EDO	A	1208	-	3,3,3	0.07	0	2,2,2	0.09	0
9	MGD	A	1212	8	47,52,52	0.49	0	58,81,81	0.99	4 (6%)
3	GOL	A	1201	-	5,5,5	0.10	0	5,5,5	0.21	0
10	SF4	B	301	2	0,12,12	-	-	-		
10	SF4	B	303	2	0,12,12	-	-	-		
4	EDO	A	1205	-	3,3,3	0.07	0	2,2,2	0.13	0
6	SO2	A	1209	-	2,2,2	0.26	0	1,1,1	0.02	0
5	PEG	A	1206	-	6,6,6	0.17	0	5,5,5	0.11	0
9	MGD	A	1213	8	47,52,52	0.80	1 (2%)	58,81,81	1.03	4 (6%)
4	EDO	A	1204	-	3,3,3	0.09	0	2,2,2	0.13	0
4	EDO	A	1202	-	3,3,3	0.05	0	2,2,2	0.14	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
10	SF4	A	1214	1	-	-	0/6/5/5
3	GOL	A	1203	-	-	2/4/4/4	-
10	SF4	B	302	2	-	-	0/6/5/5
4	EDO	A	1207	-	-	1/1/1/1	-
4	EDO	A	1208	-	-	0/1/1/1	-
9	MGD	A	1212	8	-	1/22/66/66	0/6/6/6
3	GOL	A	1201	-	-	2/4/4/4	-
10	SF4	B	301	2	-	-	0/6/5/5
10	SF4	B	303	2	-	-	0/6/5/5
4	EDO	A	1205	-	-	1/1/1/1	-
5	PEG	A	1206	-	-	2/4/4/4	-
9	MGD	A	1213	8	-	3/22/66/66	0/6/6/6
4	EDO	A	1204	-	-	1/1/1/1	-
4	EDO	A	1202	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1213	MGD	C23-C14	4.12	1.56	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1213	MGD	O11-C23-C14	3.59	111.36	108.96
9	A	1212	MGD	C19-N20-C21	3.02	118.69	113.36
9	A	1213	MGD	C19-N20-C21	2.91	118.50	113.36
9	A	1212	MGD	C23-C14-N15	2.83	110.64	107.87
9	A	1213	MGD	C23-C14-N15	2.61	110.43	107.87
9	A	1212	MGD	O11-C23-N22	2.43	110.81	108.61
9	A	1213	MGD	C17-C16-N15	2.26	122.43	116.27
9	A	1212	MGD	C17-C16-N15	2.00	121.73	116.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	GOL	O1-C1-C2-O2
3	A	1201	GOL	O1-C1-C2-C3
9	A	1213	MGD	C4'-C5'-O5'-PB
9	A	1213	MGD	O4'-C4'-C5'-O5'
4	A	1204	EDO	O1-C1-C2-O2

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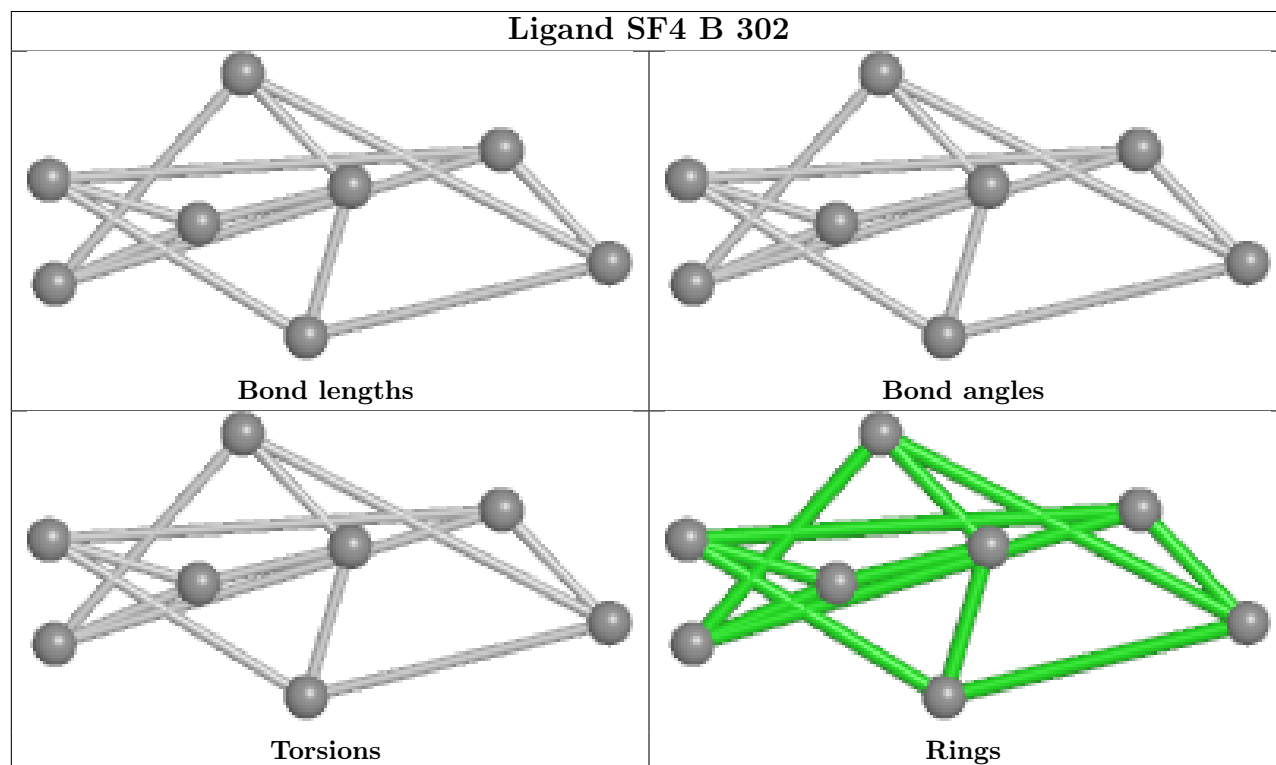
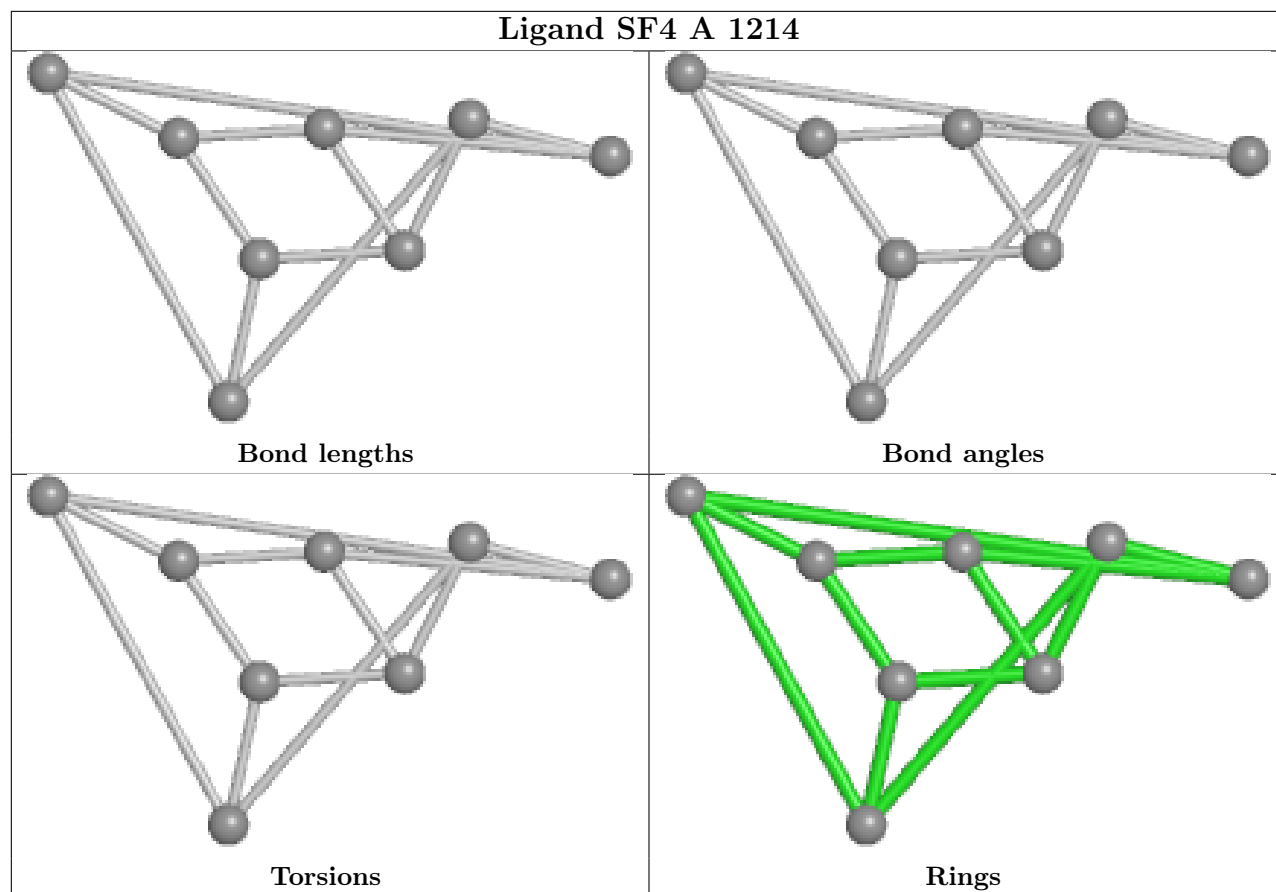
Mol	Chain	Res	Type	Atoms
3	A	1203	GOL	C1-C2-C3-O3
4	A	1202	EDO	O1-C1-C2-O2
9	A	1213	MGD	C3'-C4'-C5'-O5'
5	A	1206	PEG	O1-C1-C2-O2
4	A	1205	EDO	O1-C1-C2-O2
3	A	1203	GOL	O2-C2-C3-O3
9	A	1212	MGD	PA-O3B-PB-O5'
4	A	1207	EDO	O1-C1-C2-O2
5	A	1206	PEG	O2-C3-C4-O4

There are no ring outliers.

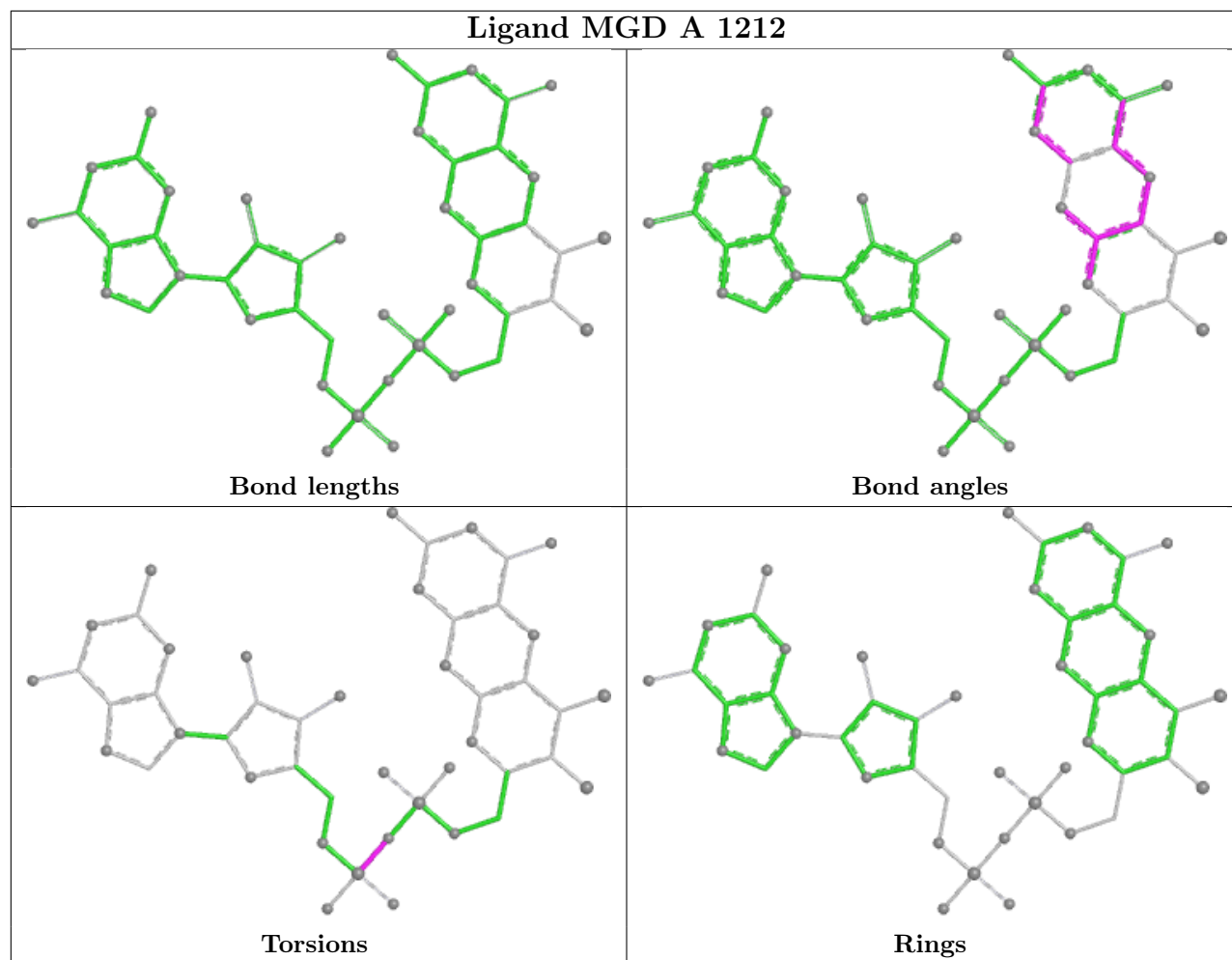
4 monomers are involved in 9 short contacts:

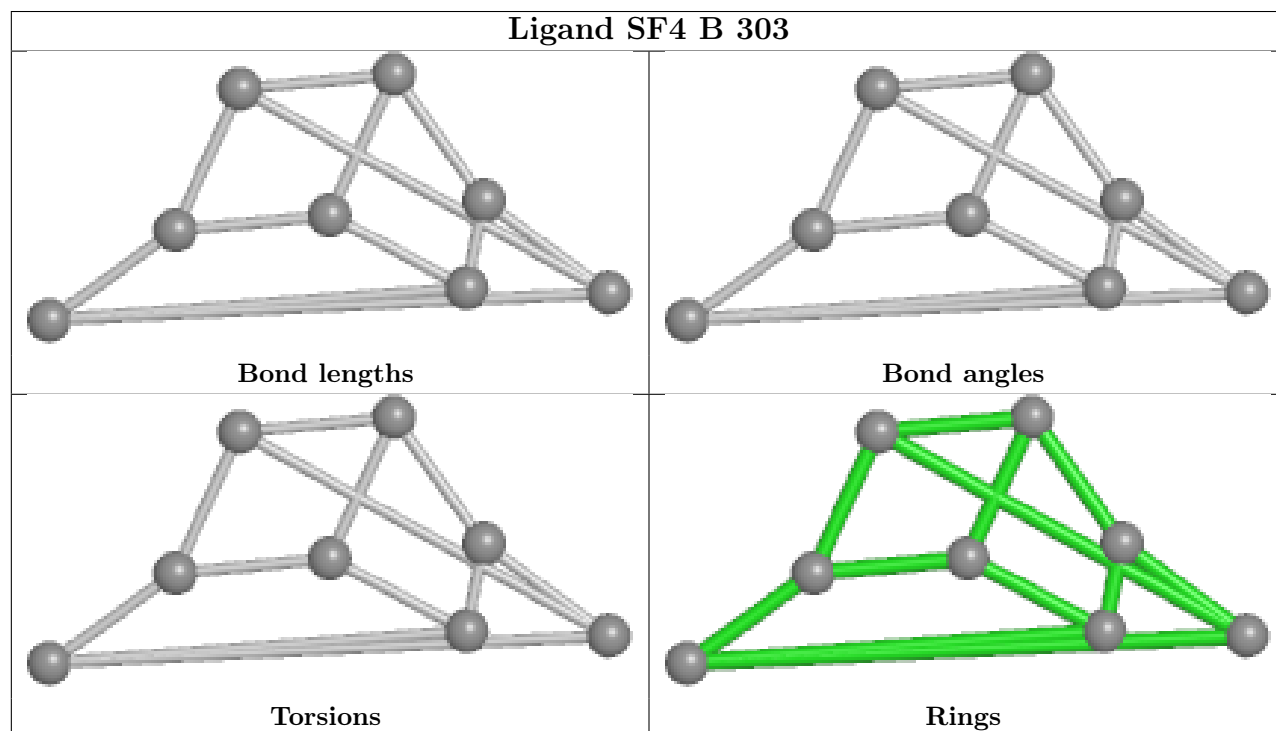
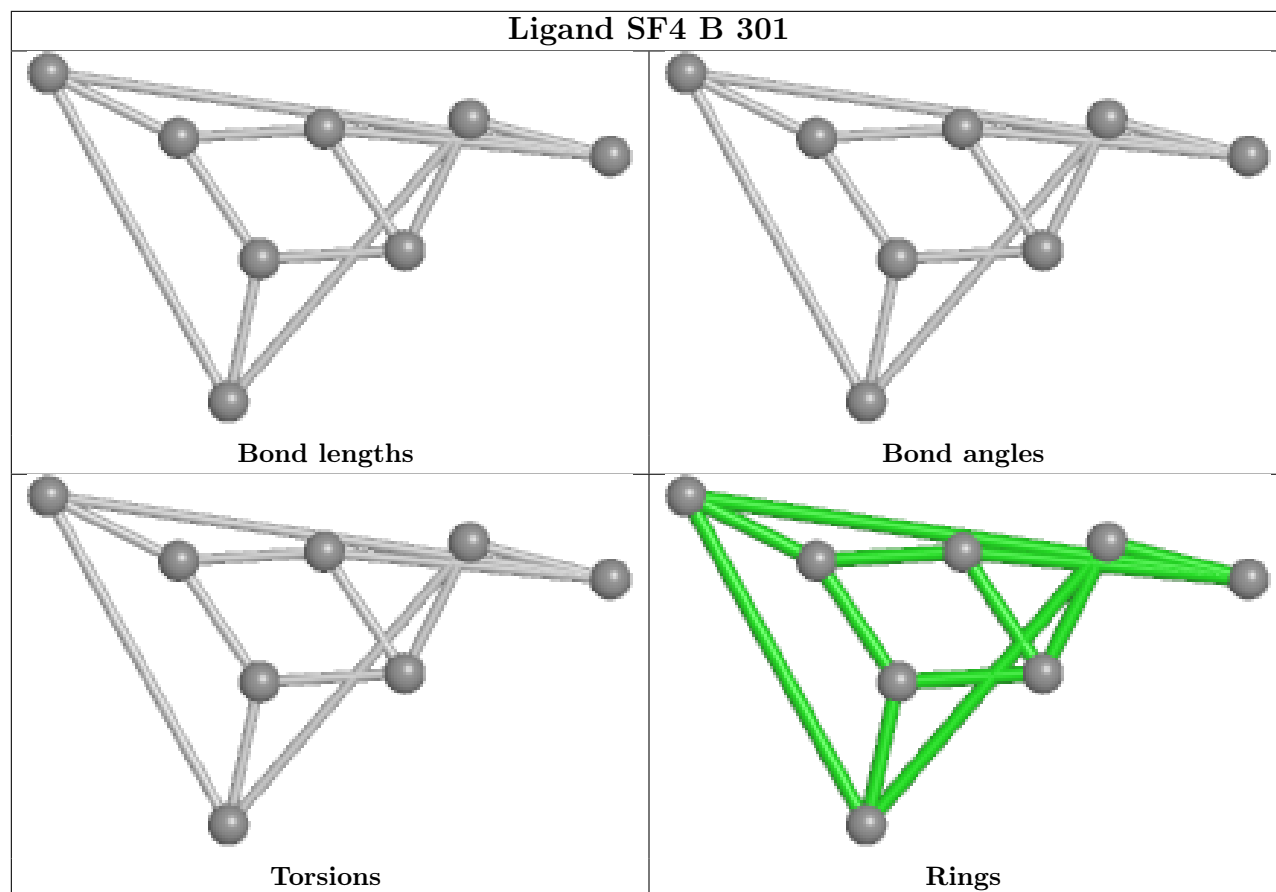
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1212	MGD	4	0
3	A	1201	GOL	1	0
6	A	1209	SO2	3	0
9	A	1213	MGD	1	0

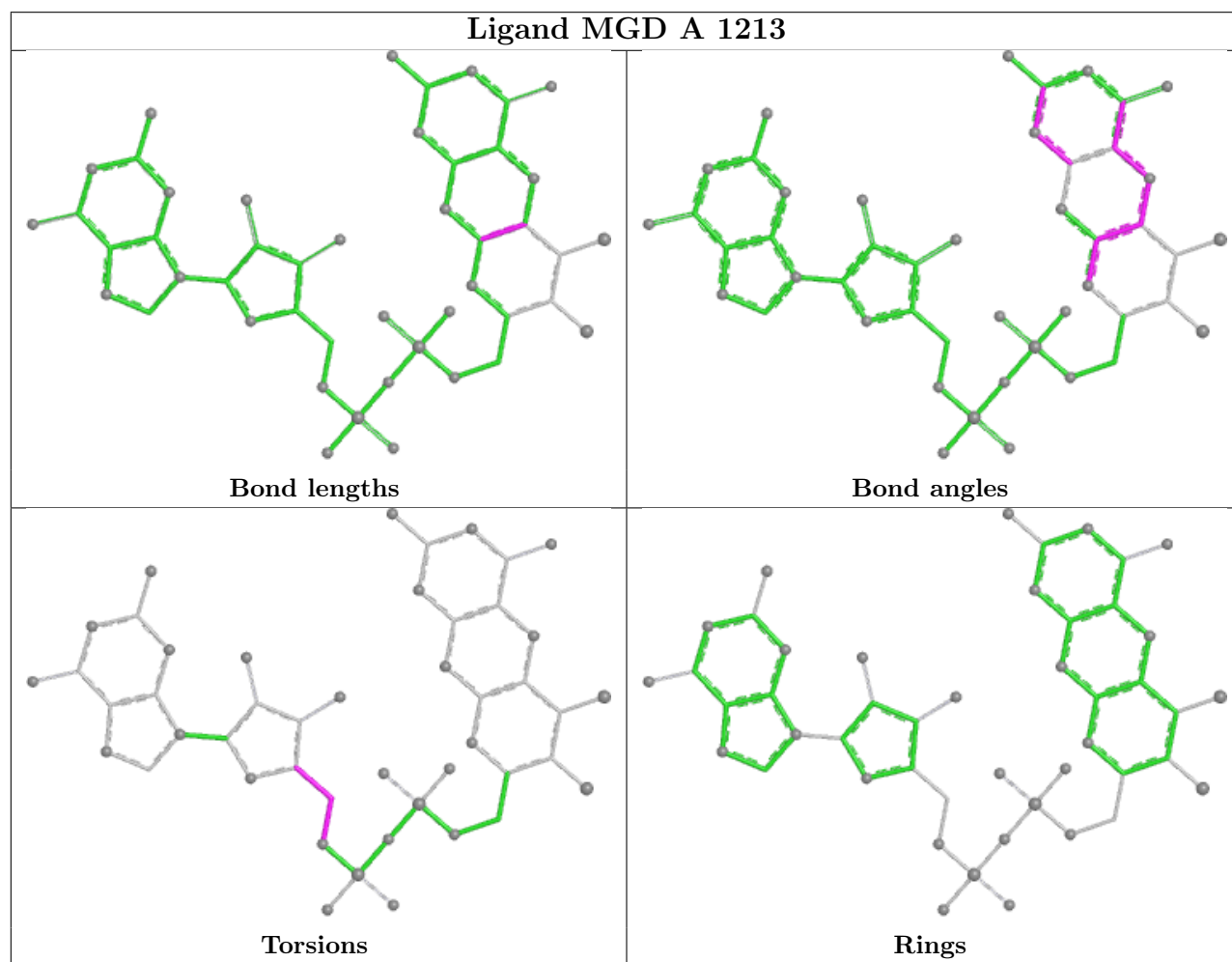
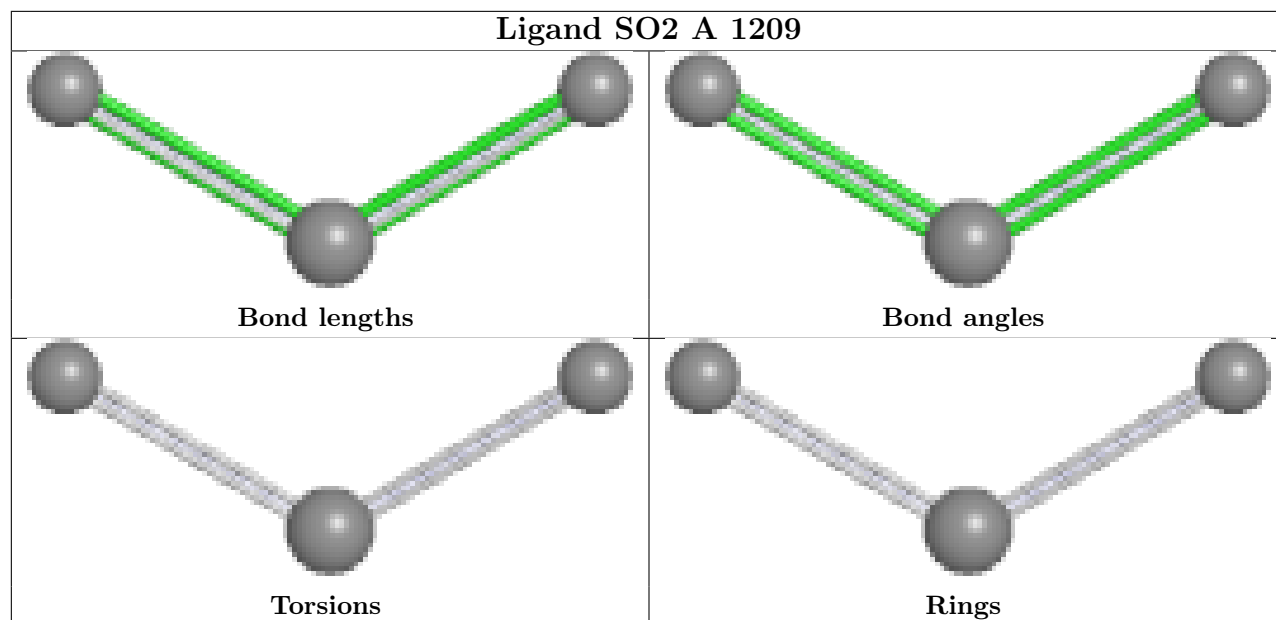
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 MGD A 1212







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	967/1013 (95%)	1.23	232 (23%) 2 2	10, 31, 62, 100	1 (0%)
2	B	214/214 (100%)	0.51	12 (5%) 30 29	14, 25, 52, 83	0
All	All	1181/1227 (96%)	1.10	244 (20%) 2 2	10, 30, 60, 100	1 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	PRO	8.8
1	A	117	TRP	8.0
1	A	122	TRP	7.9
1	A	672	ILE	6.3
1	A	109	TYR	6.3
1	A	574	TRP	5.9
1	A	866	GLY	5.7
1	A	116	THR	5.6
1	A	127	THR	5.5
1	A	660	GLY	5.5
1	A	113	PHE	5.4
1	A	737	ALA	5.4
1	A	597	ALA	5.3
1	A	596	PRO	5.2
1	A	606	LEU	5.2
1	A	108	LEU	5.2
1	A	599	ILE	5.1
1	A	589	TRP	5.0
1	A	652	VAL	4.9
1	A	129	ILE	4.8
1	A	112	PRO	4.8
1	A	69	GLY	4.7
1	A	43	ALA	4.6
1	A	139	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	604	PHE	4.6
1	A	120	VAL	4.5
1	A	105	THR	4.5
1	A	568	ALA	4.5
1	A	639	LYS	4.4
1	A	740	LEU	4.4
2	B	47	TYR	4.4
1	A	968	TRP	4.3
1	A	673	ALA	4.3
1	A	662	ALA	4.2
1	A	605	PHE	4.2
1	A	104	GLY	4.1
1	A	562	ALA	4.1
1	A	646	LEU	4.1
1	A	636	ALA	4.1
1	A	586	SER	4.0
1	A	101	ASP	4.0
1	A	151	VAL	4.0
1	A	156	ALA	4.0
1	A	603	VAL	4.0
1	A	1005	VAL	4.0
1	A	607	PRO	4.0
1	A	543	GLY	3.9
1	A	661	GLY	3.8
1	A	637	GLU	3.8
2	B	131	VAL	3.8
1	A	681	PHE	3.8
1	A	548	LEU	3.8
1	A	142	THR	3.8
1	A	130	ALA	3.8
1	A	593	GLY	3.7
1	A	575	LEU	3.7
1	A	638	THR	3.7
1	A	572	LEU	3.7
1	A	657	ALA	3.7
1	A	549	PHE	3.7
1	A	602	GLU	3.6
1	A	630	ARG	3.6
1	A	125	ALA	3.6
1	A	323	ALA	3.5
1	A	919	LEU	3.5
1	A	664	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	121	THR	3.5
1	A	600	GLY	3.5
1	A	933	LEU	3.5
1	A	798	LYS	3.4
1	A	577	ASN	3.4
1	A	590	LYS	3.4
1	A	570	GLY	3.4
1	A	695	LEU	3.4
1	A	119	PRO	3.4
1	A	658	LYS	3.3
1	A	71	ALA	3.3
1	A	645	MET	3.3
1	A	136	THR	3.3
1	A	738	GLY	3.3
1	A	578	VAL	3.3
1	A	176	ILE	3.2
1	A	700	VAL	3.2
1	A	937	LEU	3.2
1	A	124	PHE	3.2
1	A	680	GLU	3.2
1	A	631	GLY	3.2
1	A	667	ILE	3.1
1	A	783	LYS	3.1
1	A	126	LEU	3.1
1	A	655	LEU	3.1
1	A	649	PHE	3.1
1	A	668	ALA	3.1
1	A	180	LEU	3.1
1	A	588	PHE	3.1
1	A	565	ASN	3.0
1	A	870	ALA	3.0
1	A	659	GLU	3.0
1	A	141	PHE	3.0
1	A	705	PHE	3.0
1	A	609	CYS	3.0
1	A	64	ALA	3.0
1	A	140	SER	3.0
1	A	154	THR	3.0
1	A	797	GLY	3.0
1	A	874	PRO	3.0
2	B	134	ARG	3.0
1	A	111	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	598	GLU	3.0
1	A	922	ILE	3.0
1	A	594	MET	2.9
1	A	663	TYR	2.9
1	A	63	THR	2.9
1	A	954	GLY	2.9
1	A	970	VAL	2.9
1	A	683	PRO	2.9
1	A	146	ALA	2.9
1	A	704	GLN	2.9
1	A	133	ILE	2.9
1	A	670	LEU	2.9
1	A	576	VAL	2.8
1	A	949	PRO	2.8
1	A	849	LYS	2.8
1	A	647	ASP	2.8
1	A	701	GLY	2.8
1	A	633	LYS	2.8
1	A	138	ASP	2.8
1	A	669	LYS	2.8
1	A	684	THR	2.8
1	A	134	LYS	2.8
1	A	546	LYS	2.8
1	A	795	LYS	2.8
1	A	315	ASP	2.8
1	A	665	ALA	2.7
1	A	694	PHE	2.7
1	A	711	VAL	2.7
1	A	847	VAL	2.7
2	B	61	LYS	2.7
1	A	642	GLY	2.7
1	A	708	GLY	2.7
1	A	135	LYS	2.7
1	A	918	LYS	2.7
1	A	951	LYS	2.7
2	B	93	ALA	2.7
1	A	587	SER	2.7
1	A	678	HIS	2.7
1	A	651	LYS	2.6
1	A	735	THR	2.6
1	A	537	PHE	2.6
1	A	916	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	2.6
1	A	541	ASP	2.6
1	A	967	GLY	2.6
1	A	348	ALA	2.6
1	A	722	SER	2.6
1	A	70	ARG	2.6
1	A	65	LYS	2.5
1	A	601	THR	2.5
1	A	538	GLU	2.5
1	A	608	CYS	2.5
2	B	143	ASP	2.5
1	A	685	LYS	2.5
1	A	936	ALA	2.5
1	A	610	VAL	2.5
1	A	677	GLU	2.5
1	A	368	LEU	2.5
1	A	503	LEU	2.5
1	A	856	LEU	2.5
1	A	794	TRP	2.5
1	A	44	LYS	2.5
1	A	736	ASP	2.5
1	A	873	ASP	2.5
1	A	132	ARG	2.4
1	A	580	LEU	2.4
1	A	131	LYS	2.4
1	A	525	GLY	2.4
1	A	595	ASN	2.4
1	A	699	GLU	2.4
1	A	674	ASP	2.4
1	A	47	THR	2.4
1	A	172	ALA	2.4
2	B	63	PRO	2.4
1	A	865	GLU	2.4
1	A	702	GLY	2.4
1	A	910	CYS	2.4
1	A	518	TYR	2.4
1	A	545	PHE	2.4
1	A	676	GLU	2.4
1	A	361	LYS	2.4
1	A	928	VAL	2.3
1	A	627	TRP	2.3
1	A	510	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	953	GLU	2.3
1	A	709	GLN	2.3
1	A	864	ILE	2.3
1	A	666	PRO	2.3
1	A	114	SER	2.3
1	A	643	ASP	2.3
1	A	585	THR	2.3
2	B	171	LEU	2.3
1	A	147	ALA	2.2
1	A	629	TYR	2.2
1	A	60	ILE	2.2
1	A	115	ASP	2.2
1	A	550	ALA	2.2
1	A	742	ALA	2.2
1	A	246	LYS	2.2
1	A	123	ASP	2.2
1	A	581	PHE	2.2
2	B	96	LYS	2.2
1	A	474	GLU	2.2
2	B	112	VAL	2.2
1	A	893	LEU	2.2
1	A	750	PRO	2.2
1	A	875	ARG	2.2
1	A	635	TYR	2.1
1	A	799	TRP	2.1
1	A	686	VAL	2.1
1	A	591	GLY	2.1
1	A	872	CYS	2.1
1	A	128	GLU	2.1
1	A	556	ALA	2.1
1	A	956	ASP	2.1
1	A	566	ARG	2.1
1	A	754	ARG	2.1
1	A	871	VAL	2.1
1	A	370	LYS	2.1
1	A	36	GLU	2.1
1	A	573	GLU	2.1
1	A	352	PRO	2.1
1	A	100	ASN	2.1
1	A	679	ASN	2.1
2	B	89	ASP	2.1
2	B	128	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLU	2.1
1	A	1002	VAL	2.1
1	A	790	ALA	2.1
1	A	137	ARG	2.1
1	A	921	GLY	2.0
1	A	183	VAL	2.0
1	A	118	LYS	2.0
1	A	789	LYS	2.0
1	A	579	ASN	2.0
1	A	693	TYR	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
4	EDO	A	1202	4/4	0.67	0.19	41,49,57,62	0
4	EDO	A	1208	4/4	0.70	0.19	33,41,62,93	0
4	EDO	A	1207	4/4	0.72	0.15	30,37,45,48	0
5	PEG	A	1206	7/7	0.75	0.20	29,49,66,78	0
3	GOL	A	1203	6/6	0.76	0.19	31,58,59,64	0
3	GOL	A	1201	6/6	0.82	0.20	31,49,61,63	0
6	SO2	A	1209	3/3	0.83	0.18	21,21,30,36	3
4	EDO	A	1205	4/4	0.88	0.13	32,38,54,61	0
4	EDO	A	1204	4/4	0.92	0.09	23,23,23,39	0
9	MGD	A	1212	47/47	0.96	0.06	10,16,22,29	0
9	MGD	A	1213	47/47	0.96	0.07	13,22,36,47	0
7	H2S	A	1210	1/1	0.98	0.12	27,27,27,27	0
10	SF4	A	1214	8/8	0.99	0.03	15,17,19,20	0

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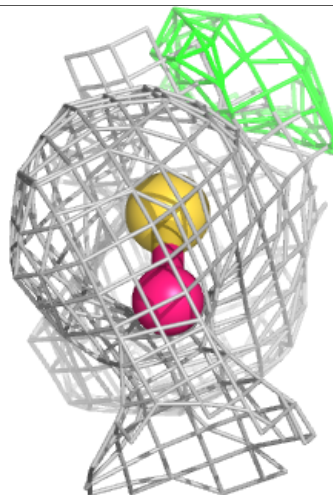
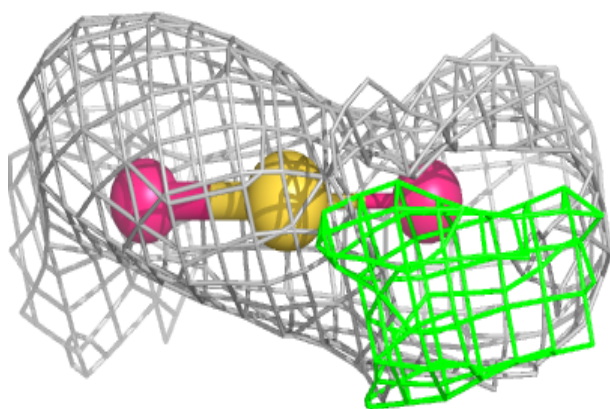
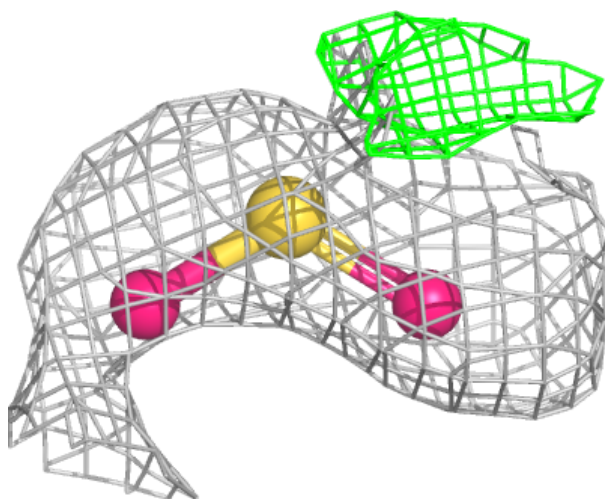
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	SF4	B	301	8/8	0.99	0.03	13,15,17,17	0
10	SF4	B	302	8/8	0.99	0.04	18,19,21,23	0
10	SF4	B	303	8/8	0.99	0.03	21,21,22,24	0
8	W	A	1211	1/1	1.00	0.02	18,18,18,18	0

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.

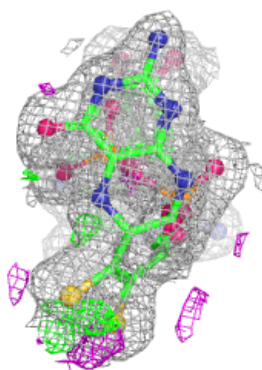
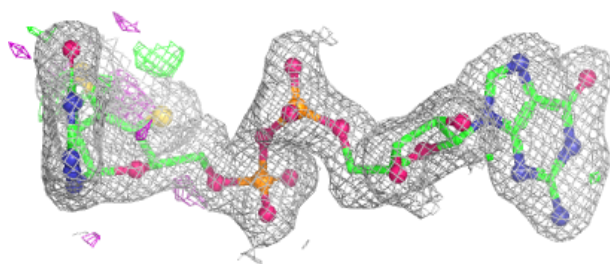
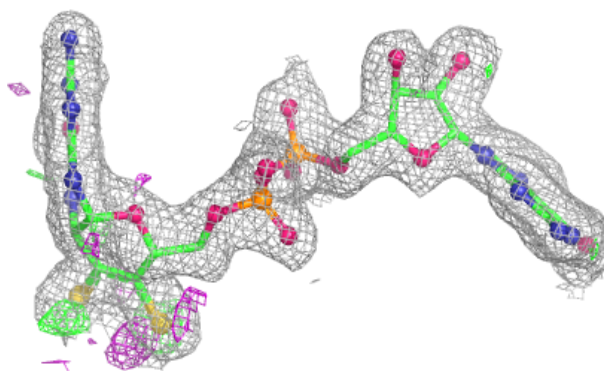
Electron density around SO2 A 1209:

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

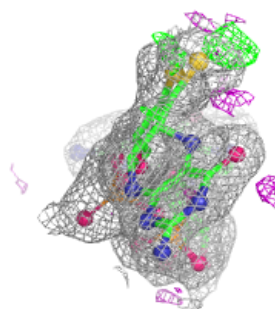
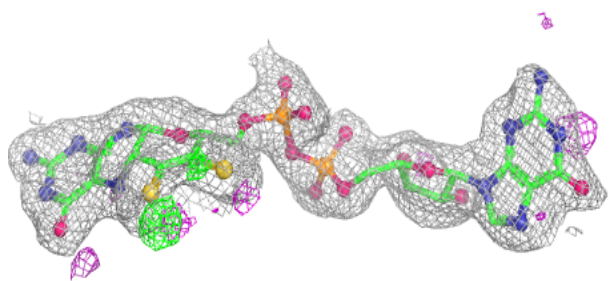
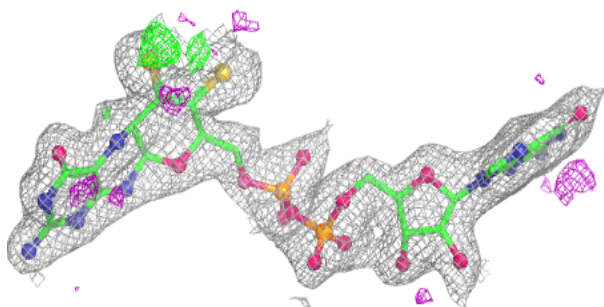


Electron density around MGD A 1212:

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

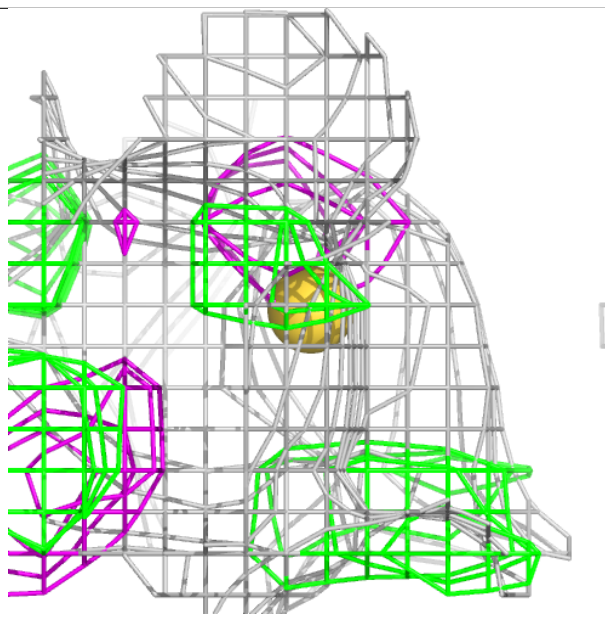
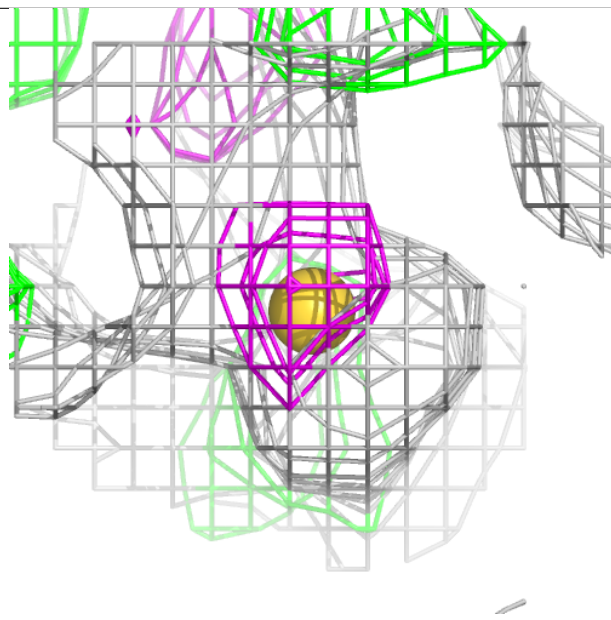
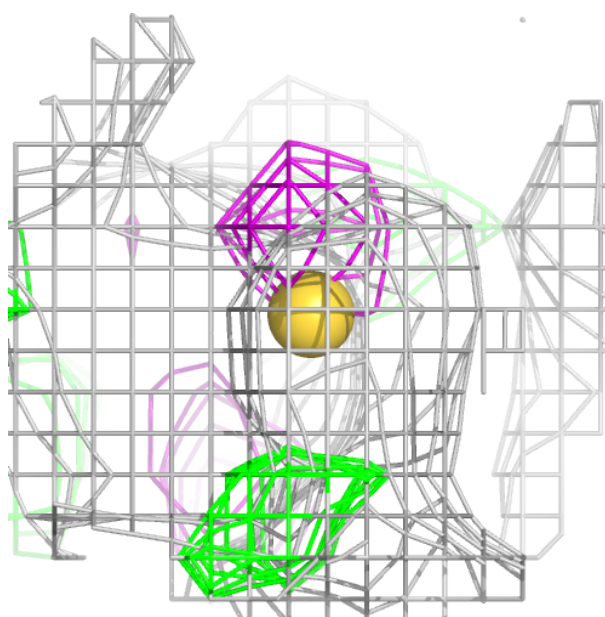
**Electron density around MGD A 1213:**

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



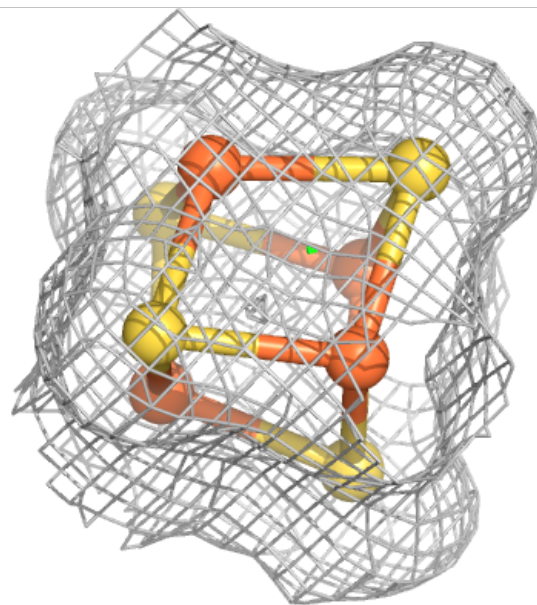
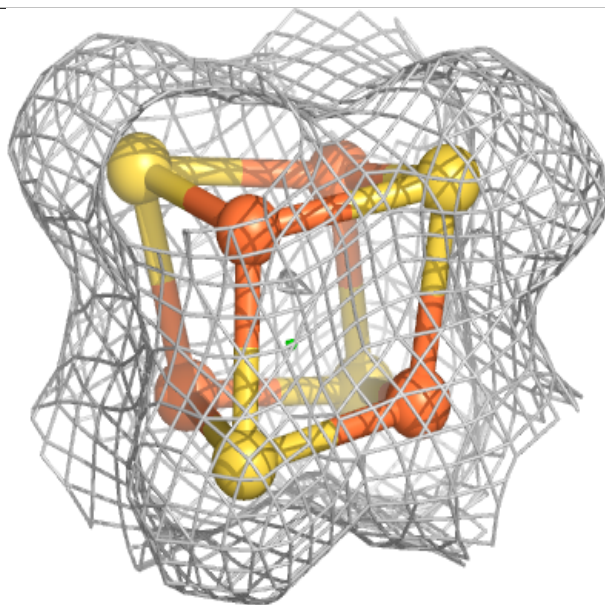
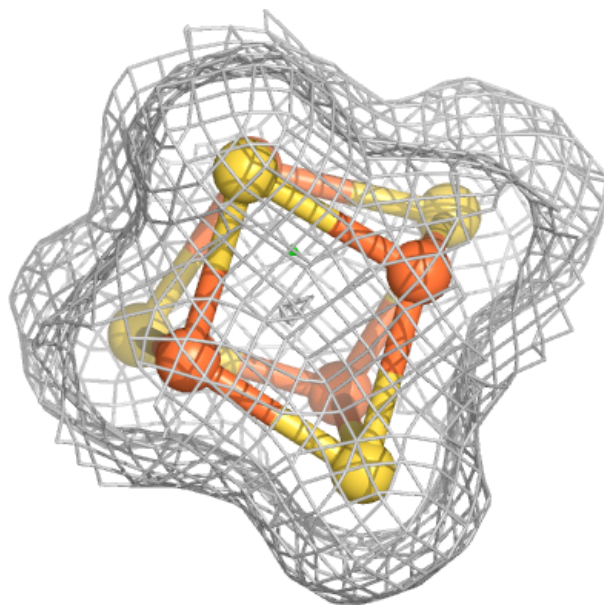
Electron density around H2S A 1210:

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



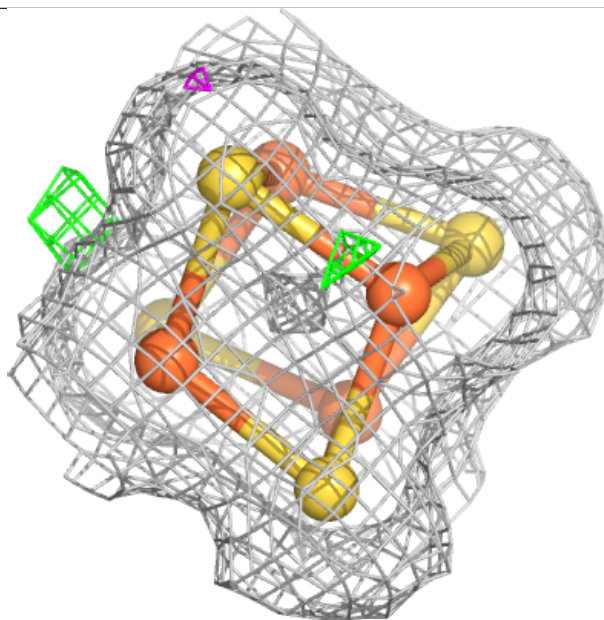
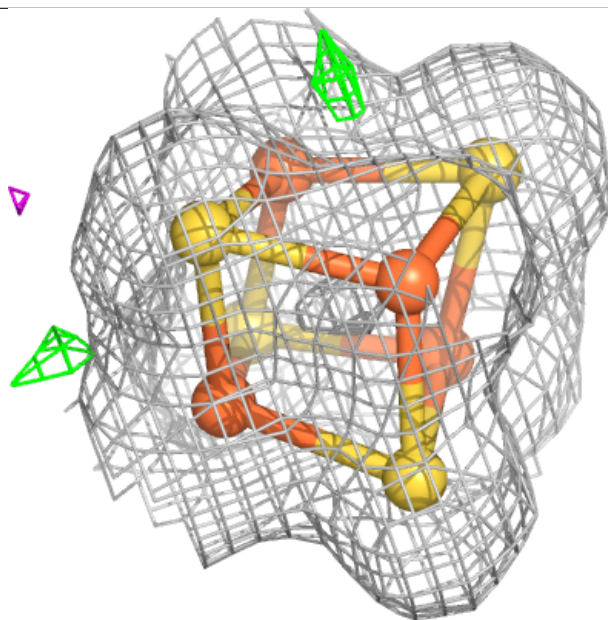
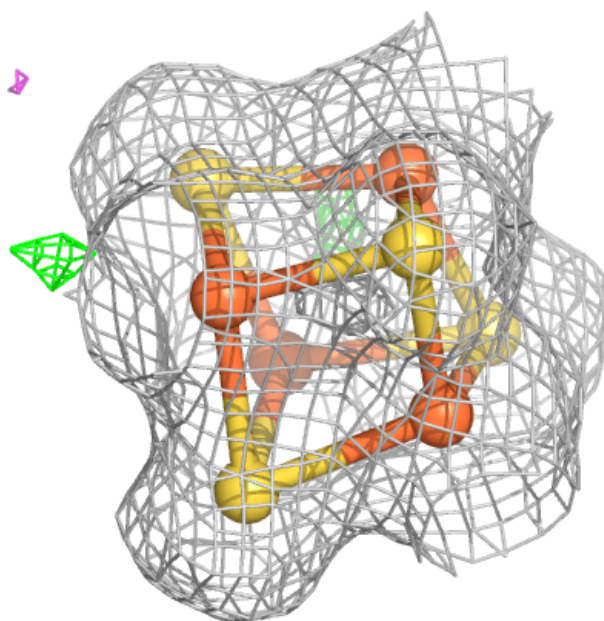
Electron density around SF4 A 1214:

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



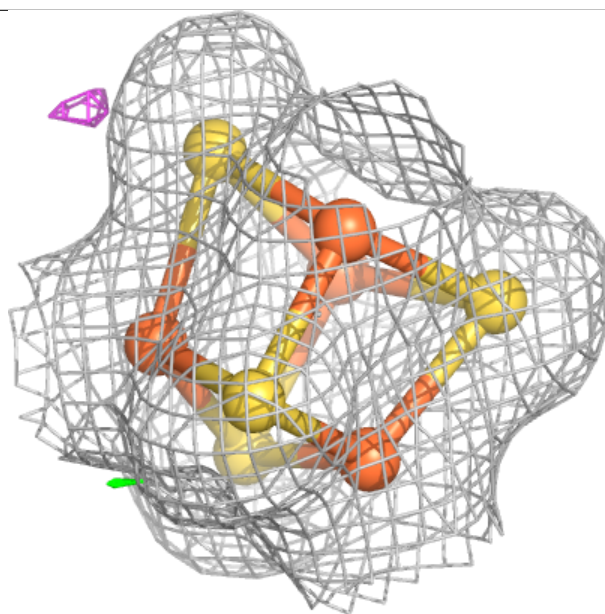
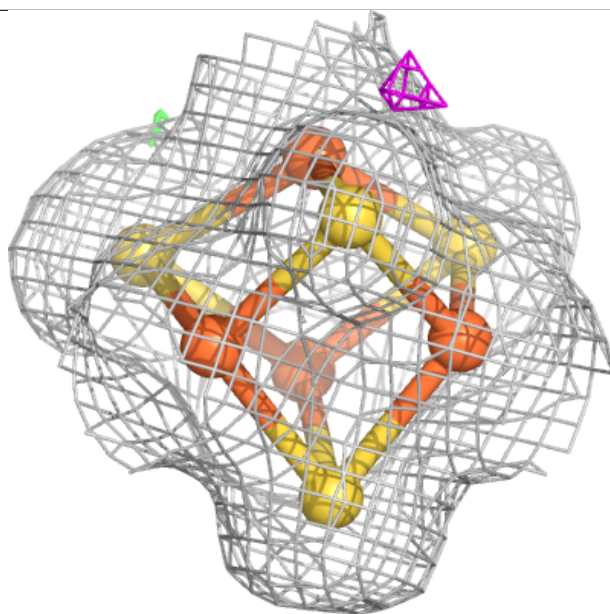
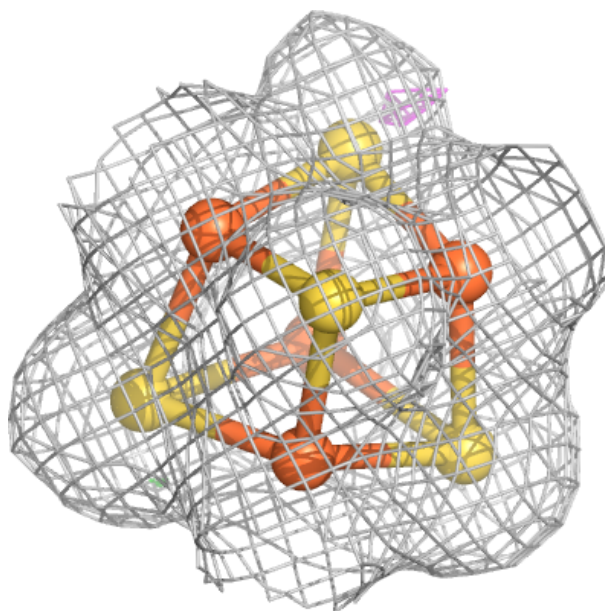
Electron density around SF4 B 301:

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



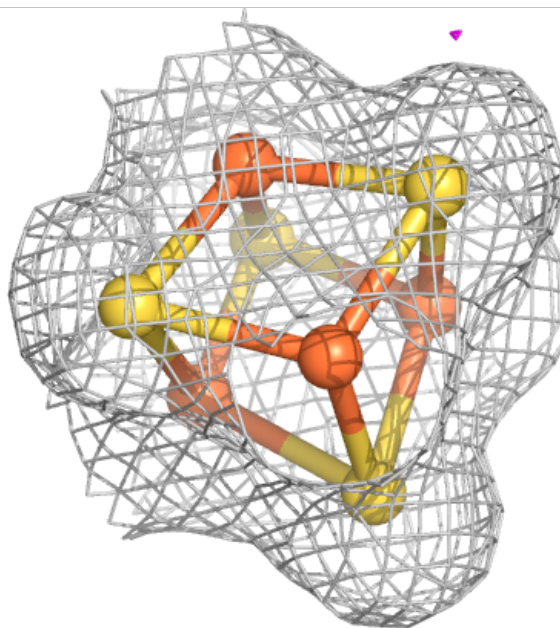
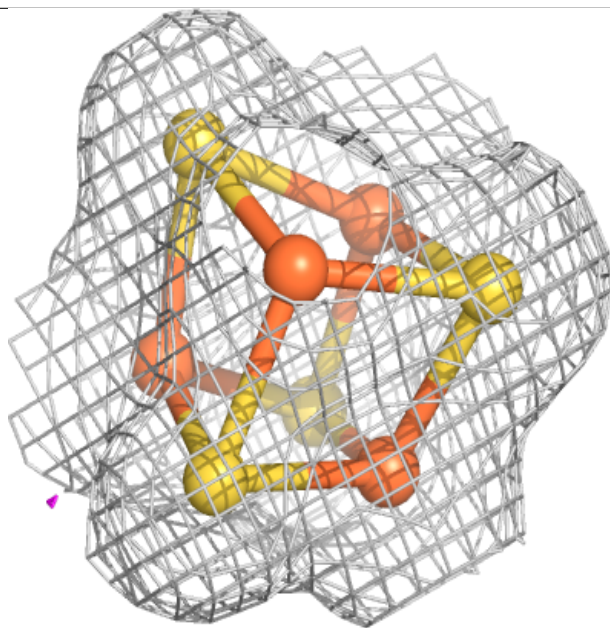
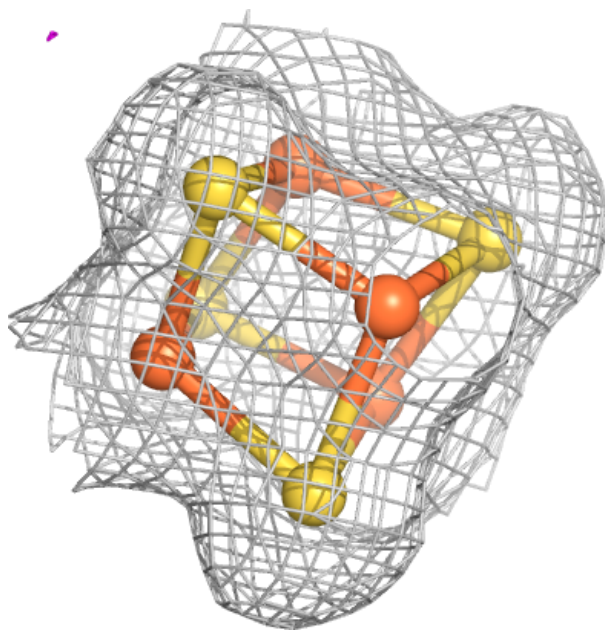
Electron density around SF4 B 302:

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



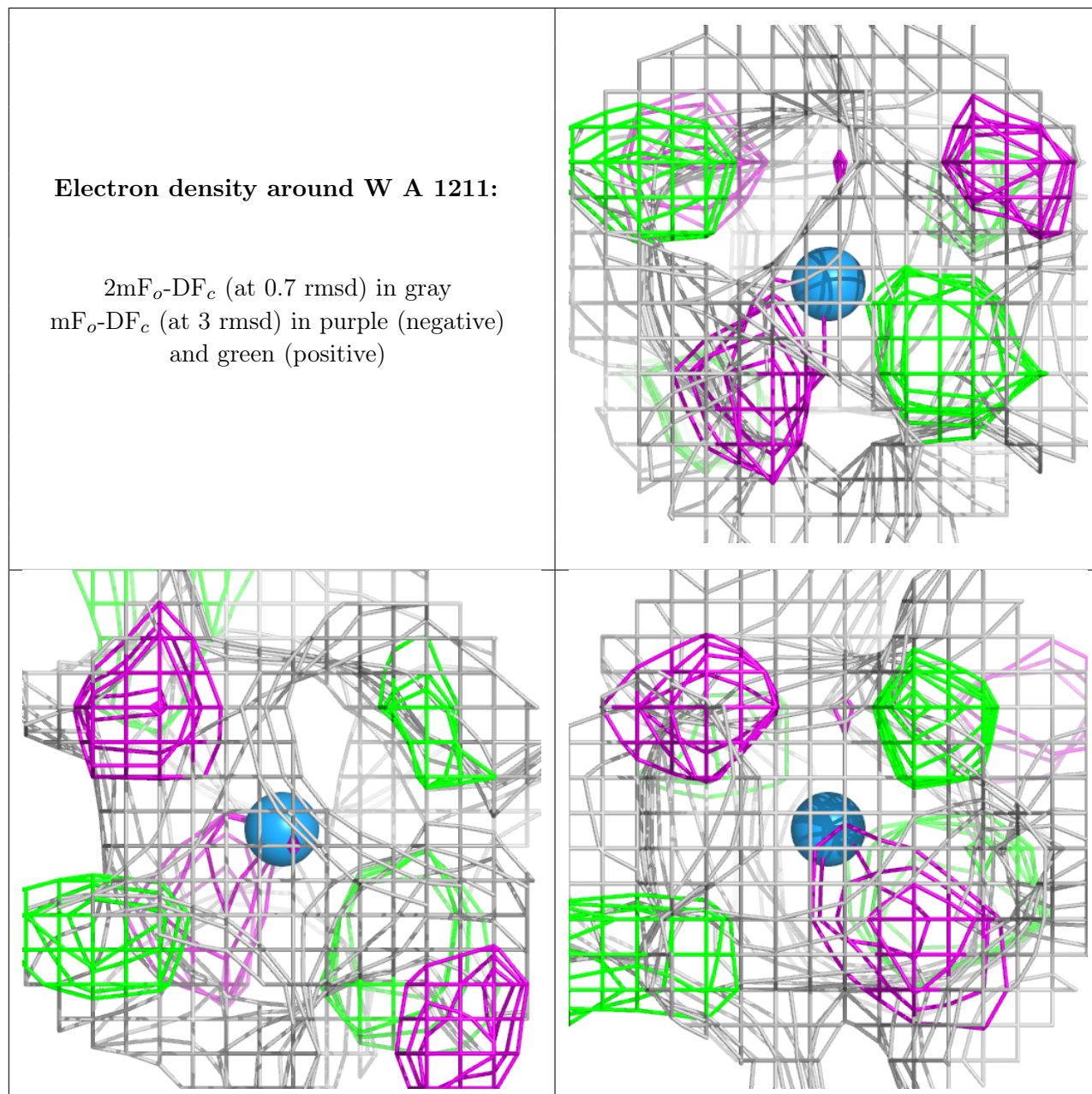
Electron density around SF4 B 303:

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



Electron density around W A 1211:

$2mF_o - DF_c$ (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.