



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2026 – 04:23 pm BST

PDB ID : 30GK / pdb_000030gk
Title : W-formate dehydrogenase from Nitratidesulfovibrio vulgaris (Desulfovibrio vulgaris) - Same Batch SSX 2025/04/01
Authors : Vilela-Alves, G.; Martins, G.; von Stetten, D.; Mehrabi, P.; Pereira, I.C.; Romao, M.J.; Pearson, A.R.; Mota, C.
Deposited on : 2026-04-23
Resolution : 1.95 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	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

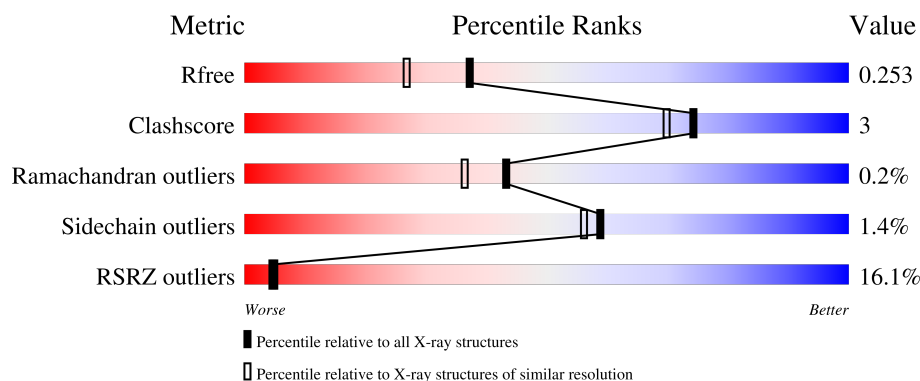
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	16% 89% 6% 5%
2	B	215	15% 92% 7%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9954 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	Se	0	1	0
			7578	4830	1323	1383	41	1			

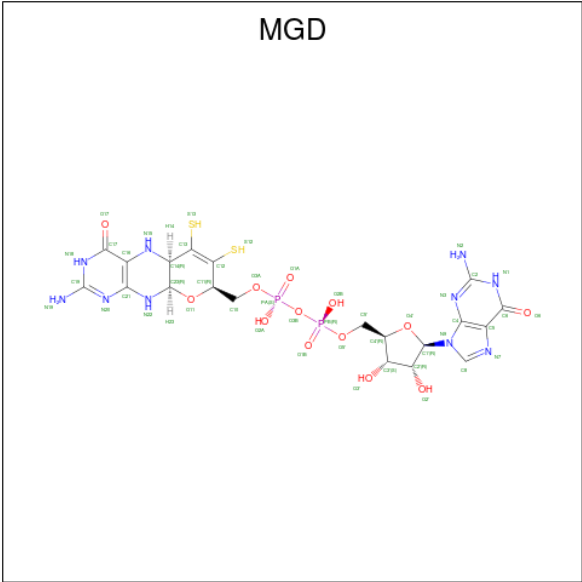
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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.

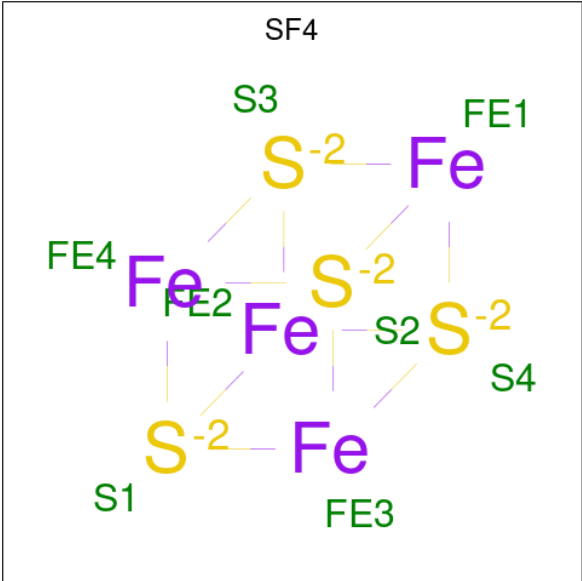
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S		0	0	0
			1664	1041	291	316	16				

- Molecule 3 is 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		

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



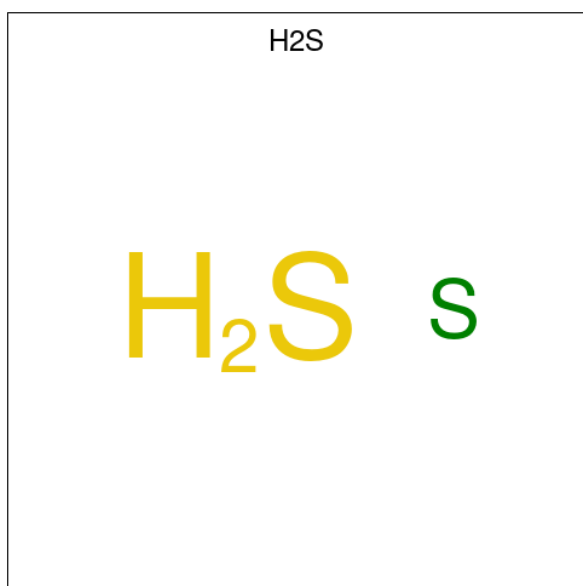
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



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

- 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		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

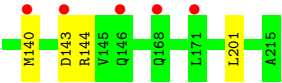
- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	417	Total	O	0	0
			417	417		
10	B	74	Total	O	0	0
			74	74		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.90Å 127.88Å 149.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.52 – 1.95 59.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (59.52-1.95) 98.7 (59.52-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.251 0.217 , 0.253	Depositor DCC
R_{free} test set	4482 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9954	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, W, H2S, MGD, GOL, EDO, PEG, 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	0/7785	1.36	2/10562 (0.0%)
2	B	0.99	0/1699	1.38	0/2302
All	All	0.98	0/9484	1.36	2/12864 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	THR	CA-C-N	5.77	123.87	120.24
1	A	196	THR	C-N-CA	5.77	123.87	120.24

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	7578	0	7408	44	0
2	B	1664	0	1633	14	0
3	A	94	0	44	2	0
4	A	8	0	0	0	0
4	B	24	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	16	3	0
8	A	56	0	84	7	0
8	B	4	0	6	0	0
9	A	14	0	20	0	0
9	B	7	0	10	0	0
10	A	417	0	0	0	0
10	B	74	0	0	0	0
All	All	9954	0	9221	57	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 3.

All (57) 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:132:THR:HG23	2:B:134:ARG:HG3	1.47	0.93
1:A:457:HIS:NE2	7:A:1106:GOL:H12	2.06	0.70
2:B:132:THR:CG2	2:B:134:ARG:HG3	2.21	0.69
1:A:197:VAL:HG11	7:A:1106:GOL:H2	1.78	0.66
1:A:129:ILE:HG21	1:A:648:MET:HE2	1.80	0.62
1:A:172:ALA:HB3	1:A:645:MET:CE	2.29	0.61
1:A:336:GLU:OE1	1:A:353:ARG:NH2	2.33	0.60
1:A:209:MET:CE	1:A:440:LEU:HD23	2.36	0.56
1:A:209:MET:HE1	1:A:440:LEU:HD23	1.89	0.55
1:A:457:HIS:NE2	7:A:1106:GOL:C1	2.68	0.55
1:A:197:VAL:HG13	1:A:207:GLY:HA3	1.88	0.55
2:B:109:THR:HG21	2:B:135:LEU:H	1.72	0.55
2:B:41:ASN:HA	2:B:42:PRO:C	2.32	0.54
2:B:132:THR:HG23	2:B:134:ARG:CG	2.29	0.54
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.88	0.53
1:A:405:MET:HE1	1:A:884:ARG:HH12	1.73	0.53
1:A:172:ALA:HB3	1:A:645:MET:HE1	1.92	0.51
1:A:789:LYS:HE2	8:A:1116:EDO:H12	1.91	0.51
1:A:992:ILE:HG23	1:A:993:PRO:HD2	1.93	0.51
1:A:698:THR:HG21	1:A:722:SER:CB	2.42	0.50
1:A:937:LEU:C	1:A:937:LEU:HD12	2.37	0.49
2:B:143:ASP:OD1	2:B:144:ARG:N	2.43	0.49
2:B:5:PHE:HE1	2:B:140:MET:HG3	1.77	0.49
1:A:472:THR:HA	8:A:1117:EDO:C1	2.43	0.49
1:A:206:ARG:HH21	8:A:1111:EDO:H12	1.78	0.48
1:A:128:GLU:O	1:A:132:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:HE1	1:A:884:ARG:NH1	2.29	0.48
1:A:195:PRO:HG3	1:A:992:ILE:HD13	1.96	0.48
1:A:194:SER:N	1:A:195:PRO:CD	2.77	0.47
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.55	0.47
1:A:753:ALA:HB3	8:A:1113:EDO:H21	1.96	0.47
1:A:162:SER:HB2	1:A:551:TRP:O	2.15	0.46
1:A:577:ASN:OD1	1:A:586:SER:HB3	2.17	0.44
1:A:698:THR:HG21	1:A:722:SER:HB3	1.99	0.44
1:A:169:GLU:O	1:A:645:MET:HE1	2.18	0.44
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.52	0.44
2:B:201:LEU:C	2:B:201:LEU:HD23	2.43	0.44
1:A:110:ARG:NH1	1:A:601:THR:O	2.50	0.43
1:A:196:THR:HB	1:A:417:ILE:HG13	2.00	0.43
2:B:5:PHE:CE1	2:B:140:MET:HG3	2.53	0.43
2:B:129:ASP:HB3	2:B:132:THR:HG22	2.00	0.43
2:B:109:THR:CG2	2:B:135:LEU:H	2.30	0.43
1:A:130:ALA:HB2	1:A:651:LYS:HB3	2.00	0.43
1:A:806:GLY:HA3	1:A:817:ILE:HG21	2.01	0.43
1:A:206:ARG:HB2	1:A:773:TYR:OH	2.18	0.42
1:A:172:ALA:HB3	1:A:645:MET:HE3	2.00	0.42
1:A:882:THR:HA	1:A:962:LEU:O	2.20	0.41
1:A:472:THR:HA	8:A:1117:EDO:H12	2.01	0.41
2:B:131:VAL:HG13	2:B:132:THR:N	2.35	0.41
1:A:355:VAL:HG13	1:A:827:TYR:HB2	2.02	0.41
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.55	0.41
1:A:232:ASN:HA	3:A:1101:MGD:N20	2.36	0.41
1:A:472:THR:HA	8:A:1117:EDO:H11	2.03	0.41
1:A:909:PHE:CE2	1:A:963:PRO:HG3	2.56	0.41
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.55	0.40
1:A:491:TRP:CD1	8:A:1111:EDO:C2	3.04	0.40
1:A:282:LEU:HD23	1:A:423:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	963/1013 (95%)	933 (97%)	28 (3%)	2 (0%)	43	36
2	B	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	1175/1228 (96%)	1138 (97%)	35 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	GLU
1	A	985	ALA

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	787/819 (96%)	775 (98%)	12 (2%)	57	54
2	B	185/186 (100%)	183 (99%)	2 (1%)	65	64
All	All	972/1005 (97%)	958 (99%)	14 (1%)	59	56

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	A	271	ARG
1	A	484	LYS
1	A	633	LYS
1	A	651	LYS
1	A	698	THR
1	A	703	LYS
1	A	854	LYS
1	A	959	MET
1	A	969	MET
1	A	984	SER

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Mol	Chain	Res	Type
1	A	987	ASP
2	B	61	LYS
2	B	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	41	GLN
1	A	45	GLN
1	A	383	GLN
1	A	409	GLN
1	A	710	GLN
1	A	989	ASN
1	A	1008	HIS
2	B	24	GLN
2	B	147	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 26 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
8	EDO	A	1110	-	3,3,3	0.06	0	2,2,2	0.20	0
4	SF4	B	301	2	0,12,12	-	-	-	-	-
8	EDO	A	1112	-	3,3,3	0.08	0	2,2,2	0.14	0
8	EDO	A	1113	-	3,3,3	0.05	0	2,2,2	0.30	0
7	GOL	A	1107	-	5,5,5	0.09	0	5,5,5	0.27	0
8	EDO	A	1115	-	3,3,3	0.04	0	2,2,2	0.19	0
8	EDO	A	1118	-	3,3,3	0.06	0	2,2,2	0.19	0
8	EDO	B	305	-	3,3,3	0.05	0	2,2,2	0.30	0
8	EDO	A	1123	-	3,3,3	0.07	0	2,2,2	0.21	0
4	SF4	B	303	2	0,12,12	-	-	-	-	-
7	GOL	A	1106	-	5,5,5	0.10	0	5,5,5	0.31	0
8	EDO	A	1120	-	3,3,3	0.09	0	2,2,2	0.22	0
8	EDO	A	1122	-	3,3,3	0.06	0	2,2,2	0.21	0
9	PEG	A	1114	-	6,6,6	0.15	0	5,5,5	0.13	0
8	EDO	A	1119	-	3,3,3	0.09	0	2,2,2	0.10	0
3	MGD	A	1102	6	45,52,52	0.61	1 (2%)	54,81,81	0.88	3 (5%)
9	PEG	A	1109	-	6,6,6	0.14	0	5,5,5	0.10	0
3	MGD	A	1101	6	45,52,52	0.48	0	54,81,81	0.90	2 (3%)
8	EDO	A	1108	-	3,3,3	0.10	0	2,2,2	0.18	0
8	EDO	A	1121	-	3,3,3	0.07	0	2,2,2	0.24	0
4	SF4	A	1103	1	0,12,12	-	-	-	-	-
8	EDO	A	1116	-	3,3,3	0.15	0	2,2,2	0.19	0
8	EDO	A	1111	-	3,3,3	0.03	0	2,2,2	0.28	0
8	EDO	A	1117	-	3,3,3	0.09	0	2,2,2	0.36	0
9	PEG	B	304	-	6,6,6	0.15	0	5,5,5	0.07	0
4	SF4	B	302	2	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	1110	-	-	0/1/1/1	-
8	EDO	A	1112	-	-	0/1/1/1	-
4	SF4	B	301	2	-	-	0/6/5/5
8	EDO	A	1113	-	-	0/1/1/1	-
7	GOL	A	1107	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	1115	-	-	0/1/1/1	-
8	EDO	A	1118	-	-	0/1/1/1	-
8	EDO	B	305	-	-	0/1/1/1	-
8	EDO	A	1123	-	-	0/1/1/1	-
4	SF4	B	303	2	-	-	0/6/5/5
7	GOL	A	1106	-	-	2/4/4/4	-
8	EDO	A	1120	-	-	0/1/1/1	-
8	EDO	A	1122	-	-	0/1/1/1	-
9	PEG	A	1114	-	-	3/4/4/4	-
8	EDO	A	1119	-	-	1/1/1/1	-
3	MGD	A	1102	6	-	6/22/66/66	0/6/6/6
9	PEG	A	1109	-	-	0/4/4/4	-
3	MGD	A	1101	6	-	1/22/66/66	0/6/6/6
8	EDO	A	1108	-	-	1/1/1/1	-
8	EDO	A	1121	-	-	0/1/1/1	-
4	SF4	A	1103	1	-	-	0/6/5/5
8	EDO	A	1116	-	-	1/1/1/1	-
8	EDO	A	1111	-	-	1/1/1/1	-
8	EDO	A	1117	-	-	0/1/1/1	-
9	PEG	B	304	-	-	2/4/4/4	-
4	SF4	B	302	2	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	MGD	C23-C14	2.82	1.55	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	C19-N20-C21	2.93	118.72	113.43
3	A	1102	MGD	C19-N20-C21	2.89	118.65	113.43
3	A	1101	MGD	O11-C23-N22	2.20	110.82	108.57
3	A	1102	MGD	O11-C23-C14	2.16	110.41	108.96
3	A	1102	MGD	C17-C16-N15	2.15	122.52	116.76

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C4'-C5'-O5'-PB
7	A	1106	GOL	O1-C1-C2-O2
7	A	1106	GOL	O1-C1-C2-C3
7	A	1107	GOL	C1-C2-C3-O3
3	A	1102	MGD	O4'-C4'-C5'-O5'
7	A	1107	GOL	O2-C2-C3-O3
9	A	1114	PEG	O1-C1-C2-O2
8	A	1108	EDO	O1-C1-C2-O2
8	A	1116	EDO	O1-C1-C2-O2
8	A	1119	EDO	O1-C1-C2-O2
9	A	1114	PEG	O2-C3-C4-O4
9	B	304	PEG	O1-C1-C2-O2
3	A	1101	MGD	PA-O3B-PB-O5'
3	A	1102	MGD	C3'-C4'-C5'-O5'
9	A	1114	PEG	C4-C3-O2-C2
3	A	1102	MGD	C5'-O5'-PB-O3B
9	B	304	PEG	O2-C3-C4-O4
8	A	1111	EDO	O1-C1-C2-O2
3	A	1102	MGD	C5'-O5'-PB-O1B
3	A	1102	MGD	C5'-O5'-PB-O2B

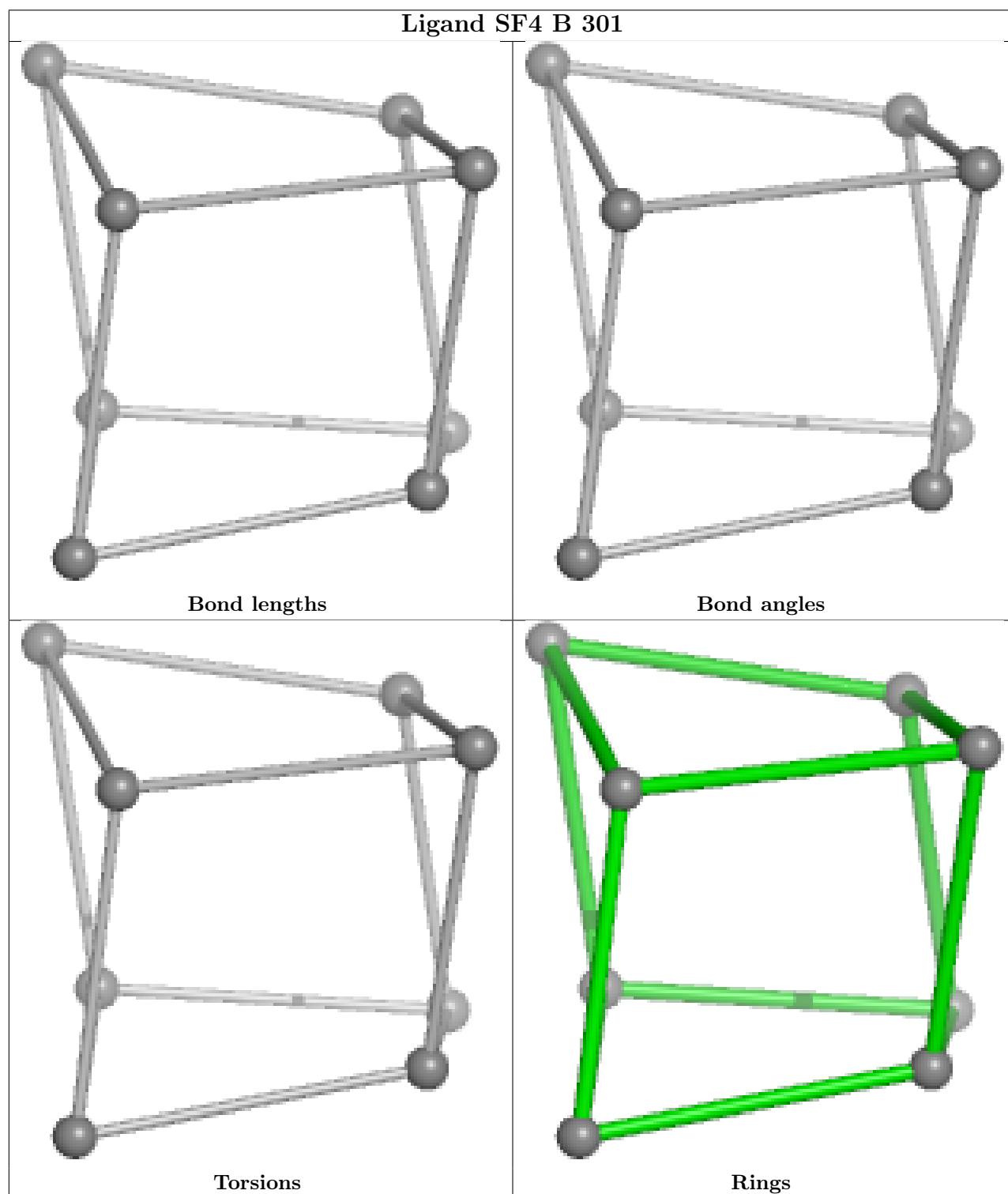
There are no ring outliers.

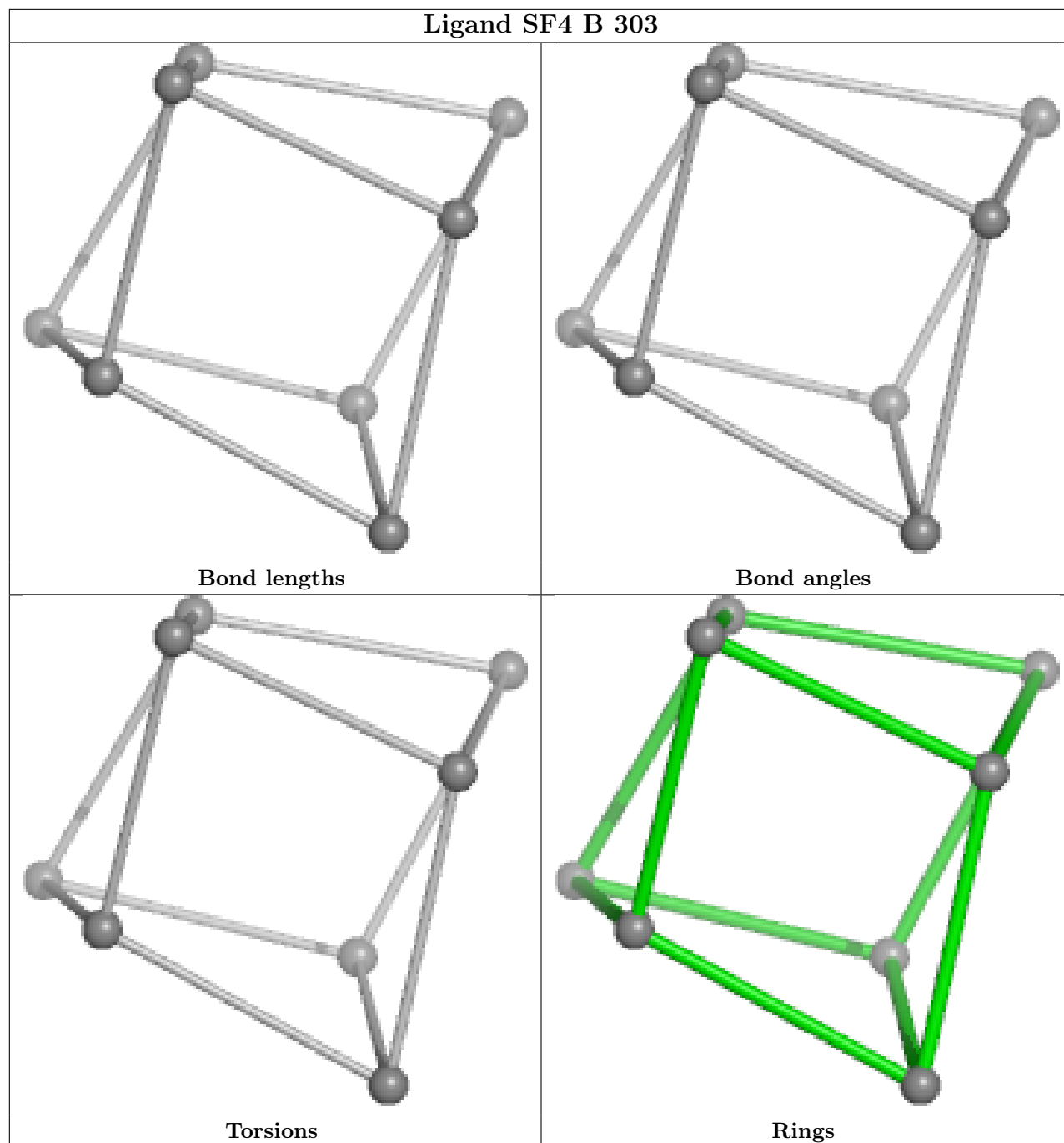
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1113	EDO	1	0
7	A	1106	GOL	3	0
3	A	1102	MGD	1	0
3	A	1101	MGD	1	0
8	A	1116	EDO	1	0
8	A	1111	EDO	2	0
8	A	1117	EDO	3	0

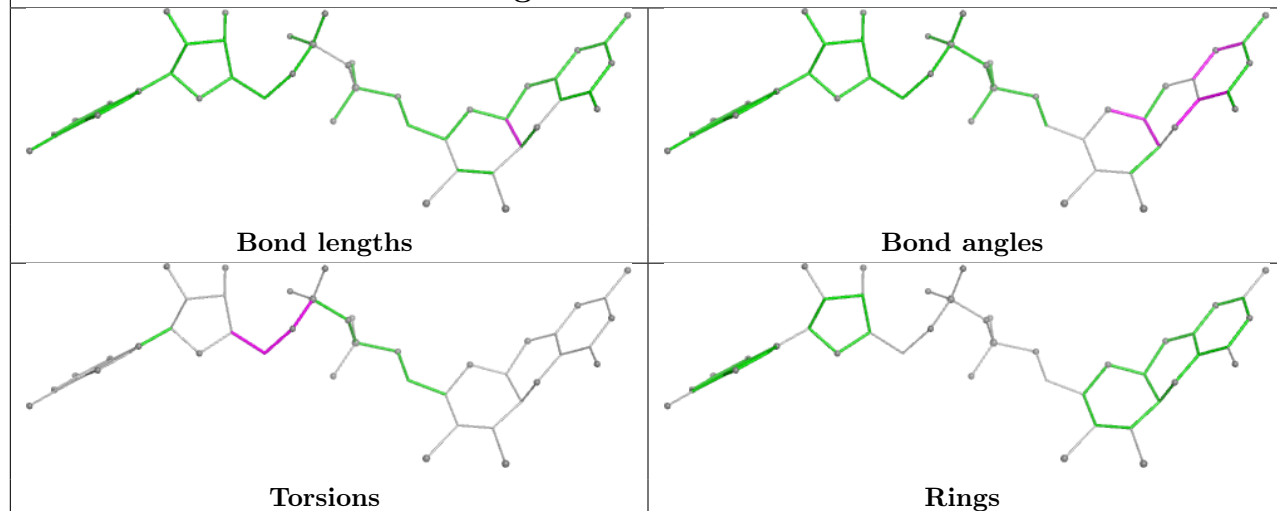
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

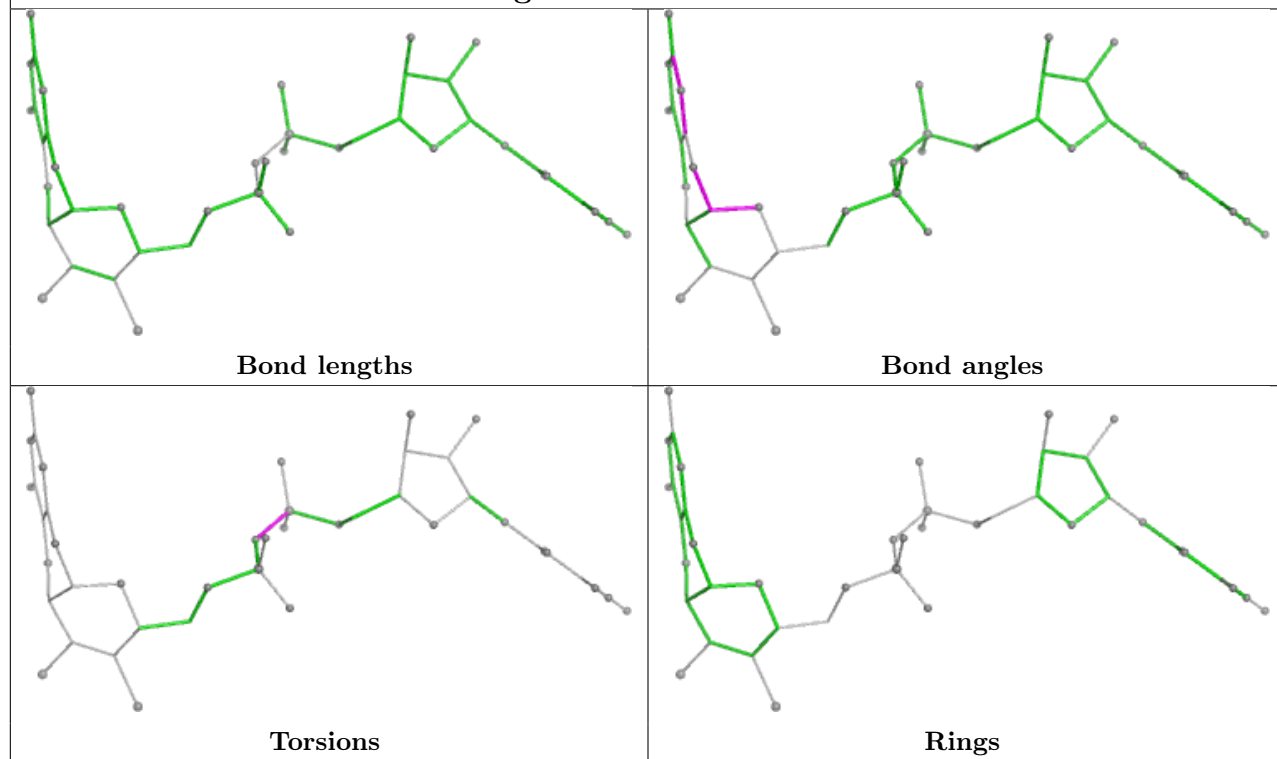


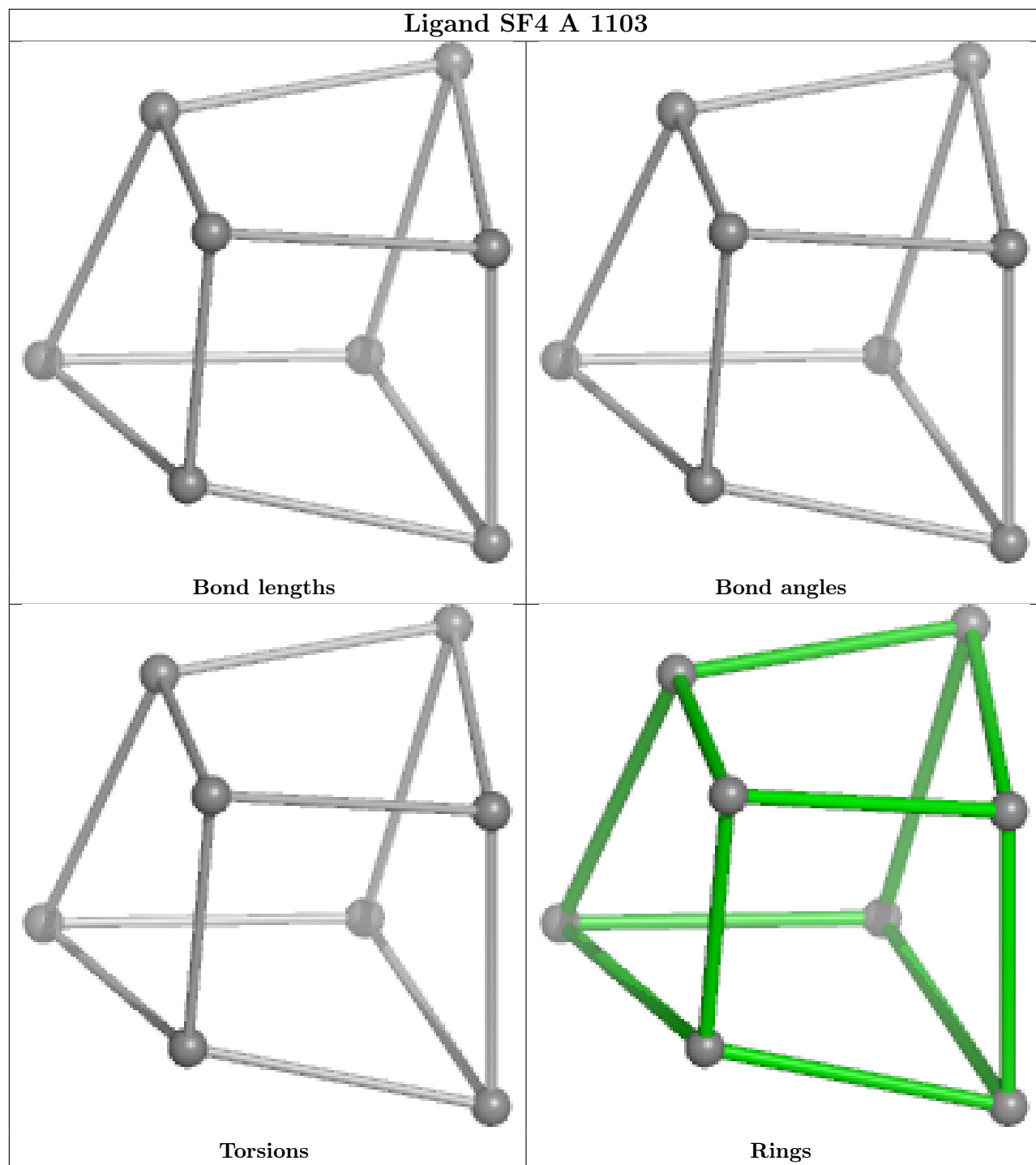


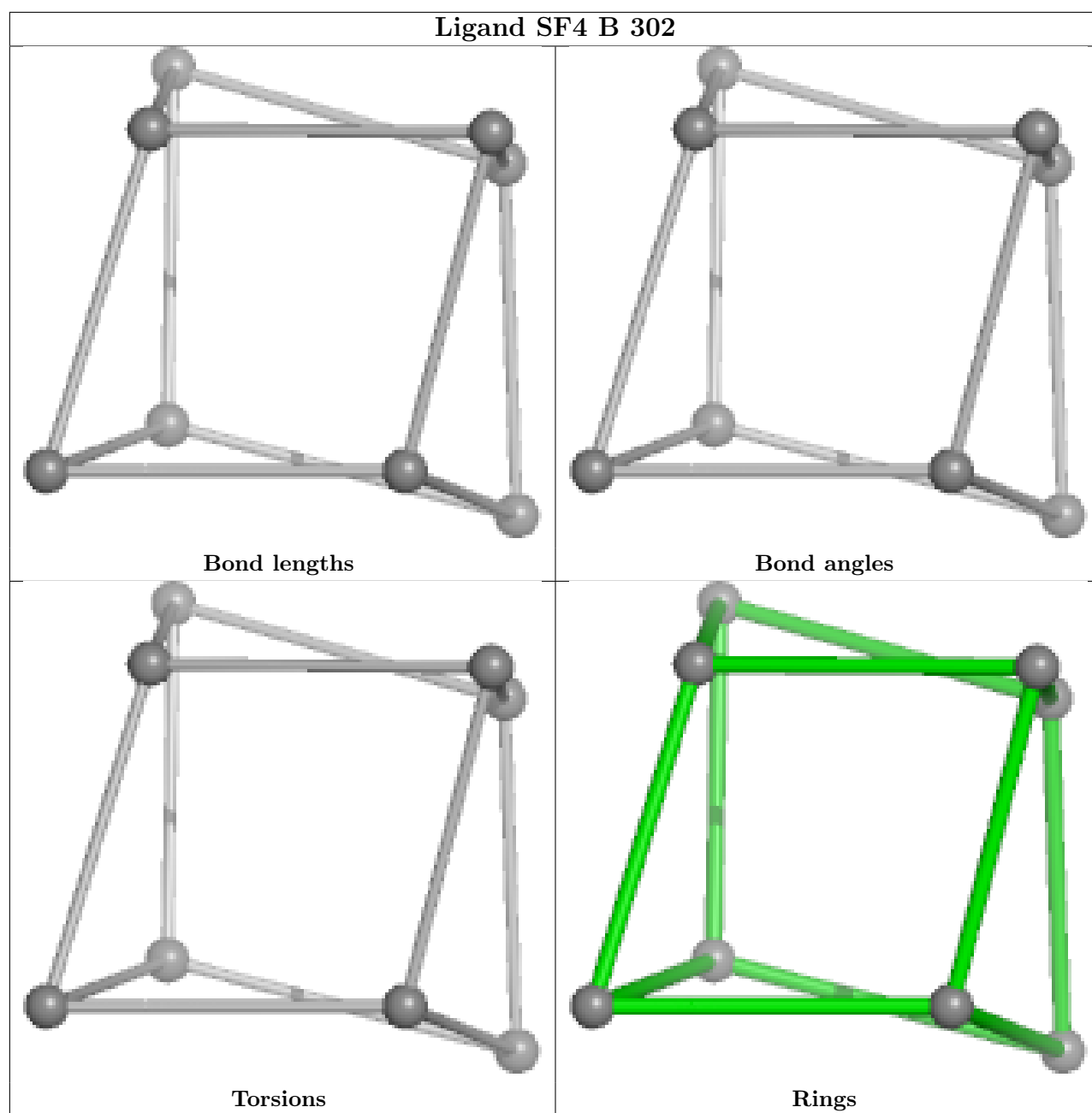
Ligand MGD A 1102



Ligand MGD A 1101







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	966/1013 (95%)	1.01	158 (16%) 4 5	21, 40, 65, 103	1 (0%)
2	B	214/215 (99%)	1.05	32 (14%) 5 6	26, 44, 72, 77	0
All	All	1180/1228 (96%)	1.01	190 (16%) 4 5	21, 41, 67, 103	1 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1006	TRP	6.9
1	A	1009	PRO	5.7
1	A	661	GLY	5.6
1	A	985	ALA	5.2
1	A	988	PRO	5.1
1	A	129	ILE	4.9
1	A	125	ALA	4.5
1	A	993	PRO	4.5
1	A	108	LEU	4.4
1	A	599	ILE	4.4
1	A	109	TYR	4.4
1	A	986	GLY	4.3
1	A	604	PHE	4.3
1	A	113	PHE	4.0
1	A	990	THR	4.0
1	A	597	ALA	3.9
1	A	1005	VAL	3.9
1	A	1008	HIS	3.7
1	A	992	ILE	3.7
1	A	989	ASN	3.7
2	B	117	VAL	3.7
2	B	131	VAL	3.7
1	A	122	TRP	3.6
1	A	991	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	88	VAL	3.6
1	A	124	PHE	3.6
1	A	141	PHE	3.6
2	B	135	LEU	3.6
1	A	652	VAL	3.5
1	A	605	PHE	3.5
1	A	660	GLY	3.5
2	B	108	LEU	3.4
1	A	537	PHE	3.4
1	A	603	VAL	3.4
1	A	354	CYS	3.3
1	A	593	GLY	3.3
1	A	133	ILE	3.3
1	A	146	ALA	3.3
1	A	665	ALA	3.3
1	A	700	VAL	3.3
2	B	86	ALA	3.3
1	A	130	ALA	3.3
2	B	110	ALA	3.3
1	A	117	TRP	3.2
1	A	861	ALA	3.2
1	A	997	ALA	3.2
1	A	151	VAL	3.2
1	A	126	LEU	3.2
1	A	545	PHE	3.2
1	A	596	PRO	3.1
1	A	673	ALA	3.1
1	A	705	PHE	3.1
1	A	128	GLU	3.1
1	A	114	SER	3.1
1	A	664	PRO	3.1
1	A	559	GLY	3.1
1	A	930	VAL	3.0
1	A	576	VAL	3.0
1	A	591	GLY	3.0
1	A	644	ILE	3.0
1	A	672	ILE	3.0
1	A	919	LEU	3.0
1	A	656	TYR	3.0
2	B	112	VAL	3.0
1	A	570	GLY	3.0
1	A	595	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	663	TYR	2.9
2	B	132	THR	2.9
1	A	589	TRP	2.9
1	A	987	ASP	2.9
2	B	95	VAL	2.9
1	A	600	GLY	2.9
1	A	721	GLY	2.9
2	B	94	VAL	2.9
1	A	657	ALA	2.9
1	A	686	VAL	2.8
2	B	143	ASP	2.8
1	A	518	TYR	2.8
1	A	111	ALA	2.8
1	A	667	ILE	2.8
1	A	316	GLY	2.8
1	A	954	GLY	2.8
2	B	128	ILE	2.7
1	A	547	GLY	2.7
1	A	950	PHE	2.7
1	A	121	THR	2.7
1	A	601	THR	2.7
1	A	38	GLN	2.7
2	B	146	GLN	2.7
1	A	574	TRP	2.7
1	A	116	THR	2.7
1	A	112	PRO	2.7
1	A	662	ALA	2.6
1	A	968	TRP	2.6
1	A	374	ILE	2.6
1	A	797	GLY	2.6
2	B	82	CYS	2.6
1	A	533	TRP	2.6
1	A	655	LEU	2.6
1	A	737	ALA	2.6
2	B	102	ALA	2.6
1	A	698	THR	2.6
1	A	794	TRP	2.6
1	A	150	LEU	2.5
1	A	140	SER	2.5
1	A	607	PRO	2.5
1	A	796	ASP	2.5
1	A	131	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	2.5
1	A	933	LEU	2.5
1	A	519	LEU	2.4
1	A	606	LEU	2.4
1	A	678	HIS	2.4
2	B	90	LEU	2.4
2	B	93	ALA	2.4
2	B	109	THR	2.4
1	A	969	MET	2.4
2	B	171	LEU	2.4
1	A	694	PHE	2.4
1	A	630	ARG	2.4
1	A	670	LEU	2.4
1	A	706	LYS	2.4
1	A	937	LEU	2.4
1	A	184	TYR	2.4
1	A	295	ASP	2.4
1	A	674	ASP	2.4
2	B	126	PRO	2.4
1	A	955	VAL	2.4
2	B	47	TYR	2.3
1	A	127	THR	2.3
1	A	107	PRO	2.3
1	A	592	PRO	2.3
1	A	142	THR	2.3
1	A	649	PHE	2.3
1	A	681	PHE	2.3
1	A	147	ALA	2.3
1	A	513	ALA	2.3
1	A	568	ALA	2.3
1	A	525	GLY	2.3
1	A	724	CYS	2.3
1	A	154	THR	2.3
1	A	594	MET	2.3
2	B	105	PHE	2.3
1	A	722	SER	2.3
1	A	412	VAL	2.3
2	B	78	VAL	2.2
1	A	869	LYS	2.2
1	A	708	GLY	2.2
1	A	509	ASP	2.2
2	B	106	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	409	GLN	2.2
1	A	572	LEU	2.2
1	A	67	GLY	2.2
1	A	647	ASP	2.2
1	A	844	GLU	2.2
1	A	503	LEU	2.2
1	A	548	LEU	2.2
1	A	646	LEU	2.2
1	A	679	ASN	2.1
2	B	140	MET	2.1
2	B	125	ILE	2.1
1	A	120	VAL	2.1
1	A	342	VAL	2.1
2	B	92	GLY	2.1
1	A	534	LEU	2.1
2	B	130	PRO	2.1
1	A	569	MET	2.1
2	B	168	GLN	2.1
1	A	693	TYR	2.1
1	A	922	ILE	2.1
1	A	179	SER	2.1
1	A	196	THR	2.1
1	A	580	LEU	2.1
2	B	80	PRO	2.1
2	B	104	LEU	2.1
1	A	636	ALA	2.1
1	A	687	ALA	2.1
1	A	1007	SER	2.1
1	A	136	THR	2.1
1	A	171	TRP	2.1
1	A	407	TRP	2.1
1	A	180	LEU	2.1
1	A	980	LEU	2.1
1	A	505	ALA	2.1
1	A	917	ALA	2.1
1	A	540	MET	2.0
1	A	148	GLY	2.0
1	A	340	ASN	2.0
1	A	132	ARG	2.0
1	A	970	VAL	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.

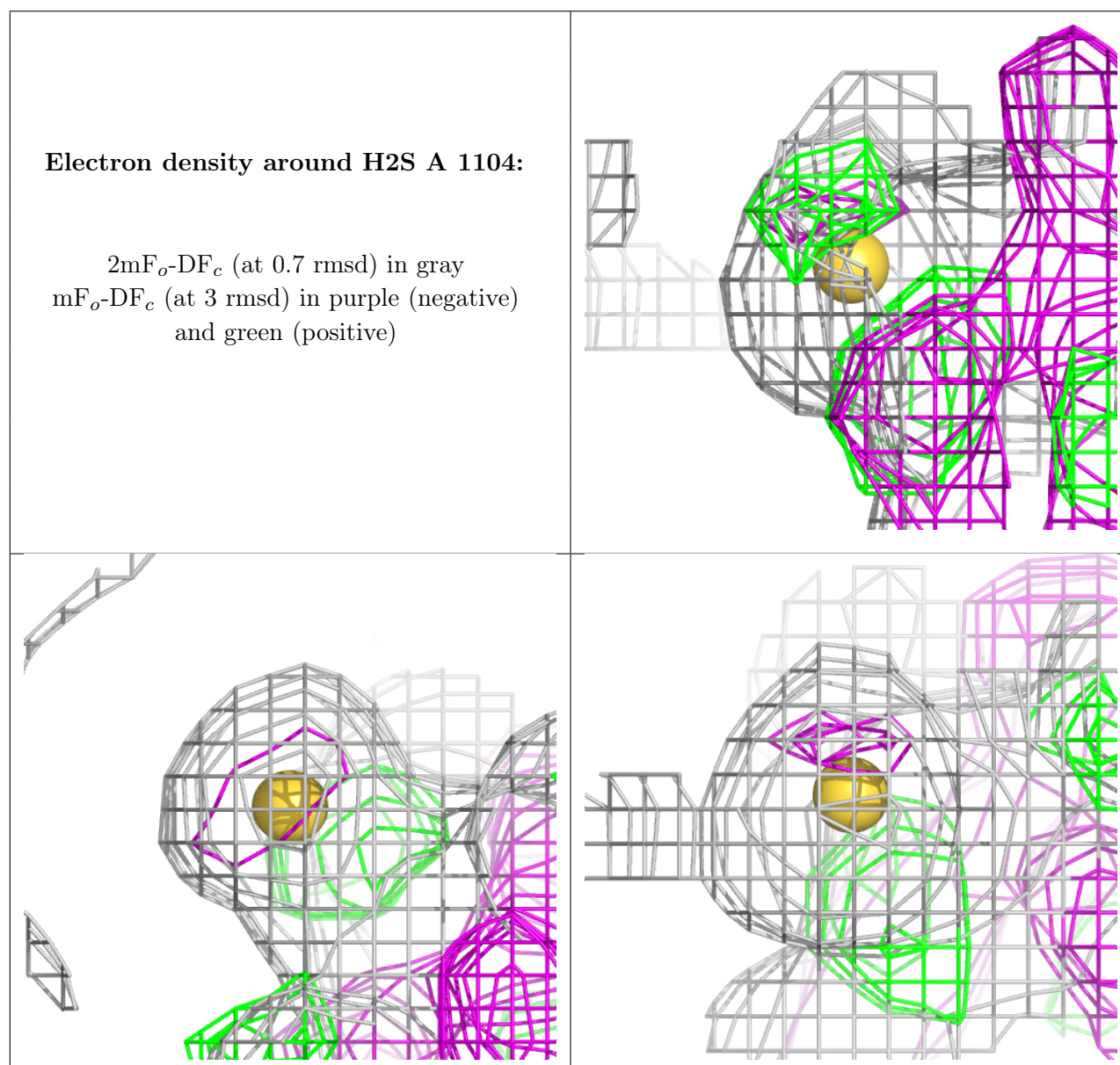
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	A	1108	4/4	0.69	0.21	50,50,50,51	0
9	PEG	A	1114	7/7	0.70	0.17	55,56,59,59	0
9	PEG	B	304	7/7	0.70	0.17	70,72,73,74	0
8	EDO	A	1113	4/4	0.71	0.19	56,58,58,59	0
9	PEG	A	1109	7/7	0.71	0.17	67,67,68,68	0
8	EDO	A	1119	4/4	0.73	0.20	64,64,65,66	0
8	EDO	A	1117	4/4	0.74	0.19	54,54,54,55	0
8	EDO	A	1122	4/4	0.75	0.14	57,57,57,58	0
8	EDO	A	1116	4/4	0.75	0.31	52,53,54,54	0
8	EDO	A	1118	4/4	0.79	0.16	51,51,51,52	0
8	EDO	A	1120	4/4	0.80	0.19	68,68,68,68	0
8	EDO	A	1112	4/4	0.82	0.13	56,56,56,56	0
8	EDO	A	1121	4/4	0.82	0.15	52,52,53,53	0
8	EDO	A	1111	4/4	0.83	0.25	47,48,48,48	0
8	EDO	A	1115	4/4	0.83	0.16	55,55,55,56	0
8	EDO	A	1110	4/4	0.83	0.13	58,59,59,59	0
8	EDO	B	305	4/4	0.84	0.15	55,56,56,57	0
7	GOL	A	1106	6/6	0.84	0.13	37,39,40,41	0
5	H2S	A	1104	1/1	0.89	0.13	32,32,32,32	0
7	GOL	A	1107	6/6	0.90	0.12	37,40,40,41	0
8	EDO	A	1123	4/4	0.91	0.12	37,38,40,42	0
3	MGD	A	1102	47/47	0.97	0.06	24,29,32,33	0
4	SF4	B	302	8/8	0.97	0.06	43,44,47,48	0
4	SF4	B	303	8/8	0.97	0.05	36,36,38,39	0
3	MGD	A	1101	47/47	0.97	0.06	21,23,28,30	0
4	SF4	B	301	8/8	0.98	0.04	25,26,26,26	0
4	SF4	A	1103	8/8	0.99	0.04	21,22,23,23	0

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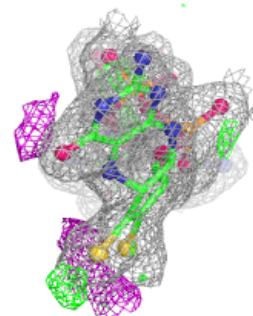
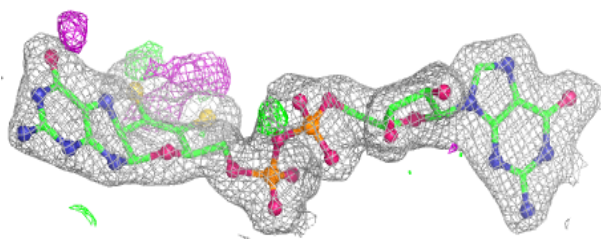
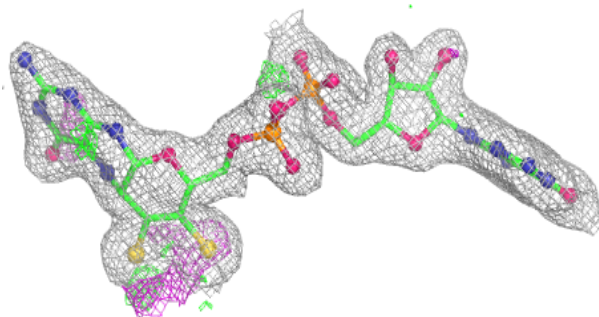
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	W	A	1105	1/1	0.99	0.03	26,26,26,26	0

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.



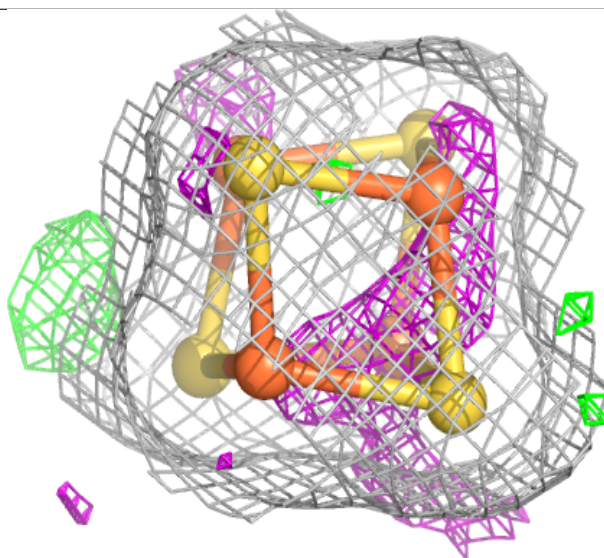
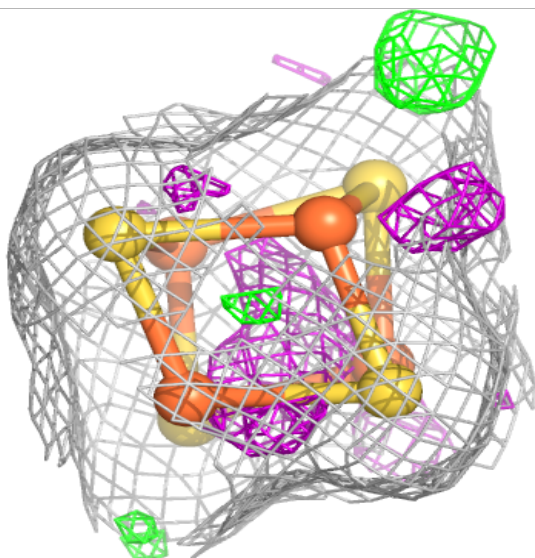
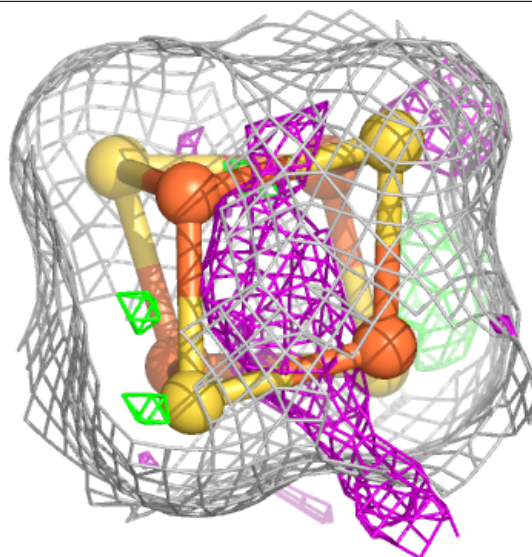
Electron density around MGD A 1102:

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



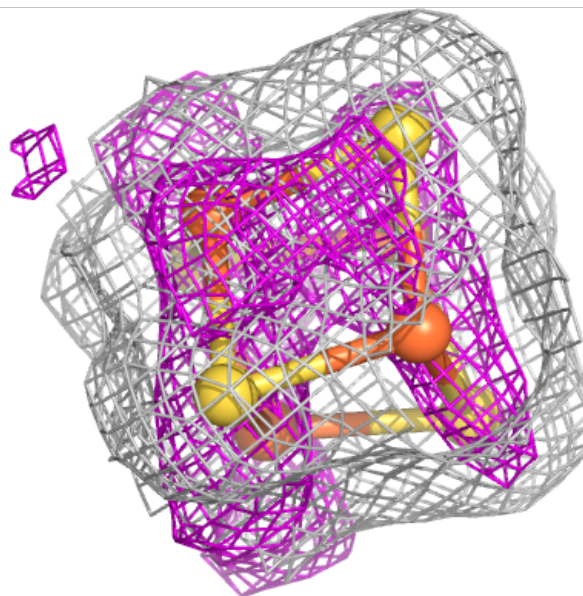
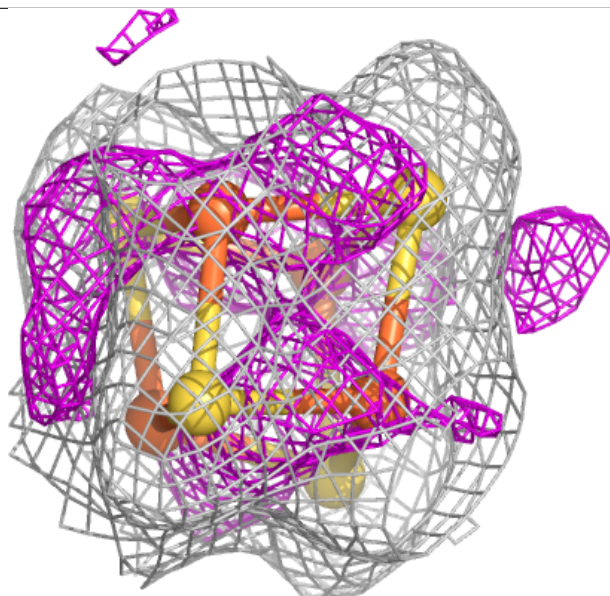
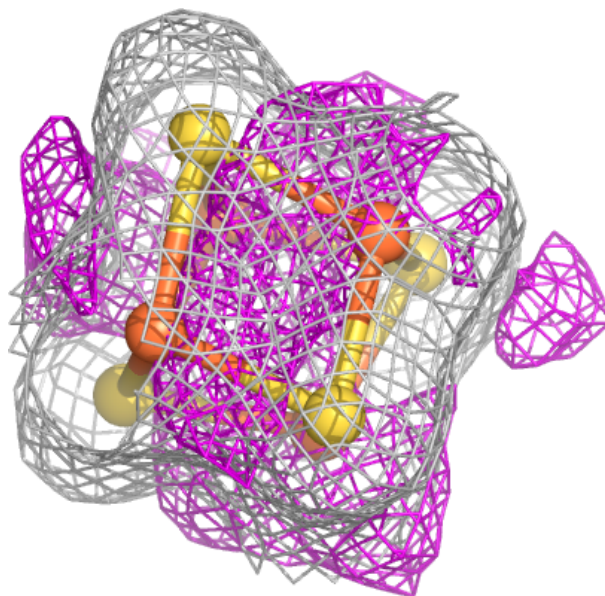
Electron density around SF4 B 302:

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



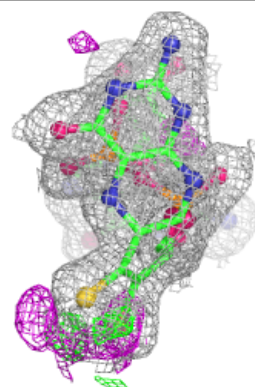
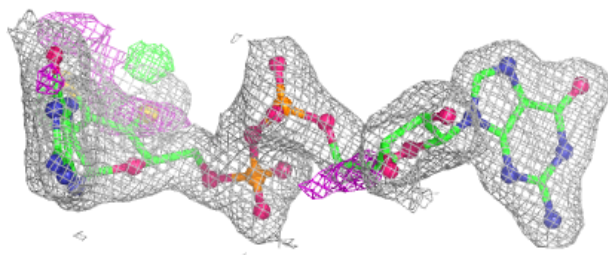
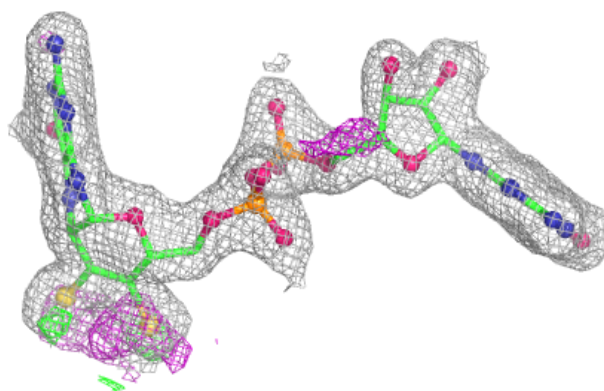
Electron density around SF4 B 303:

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



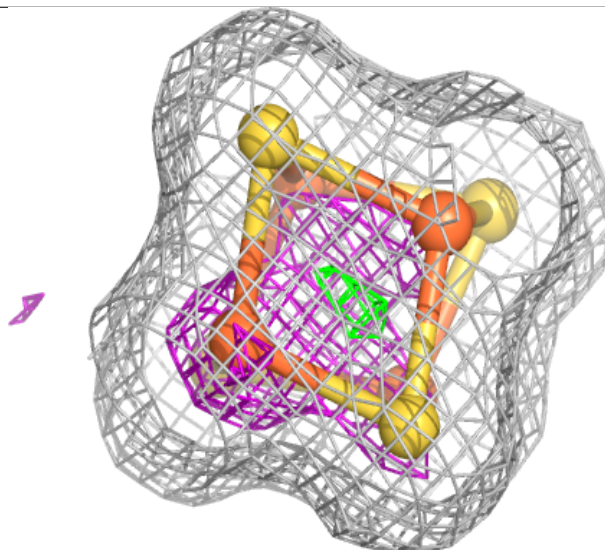
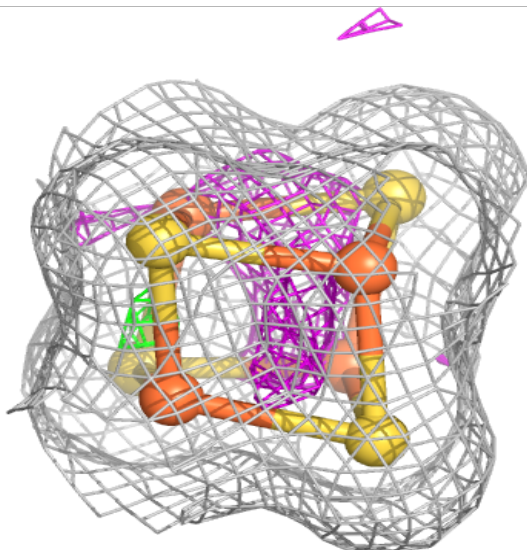
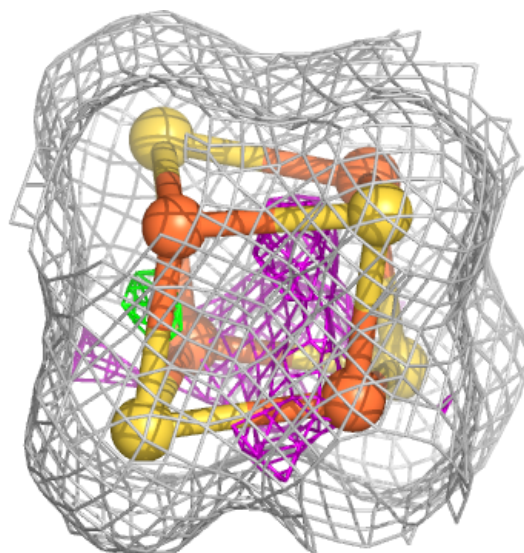
Electron density around MGD A 1101:

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



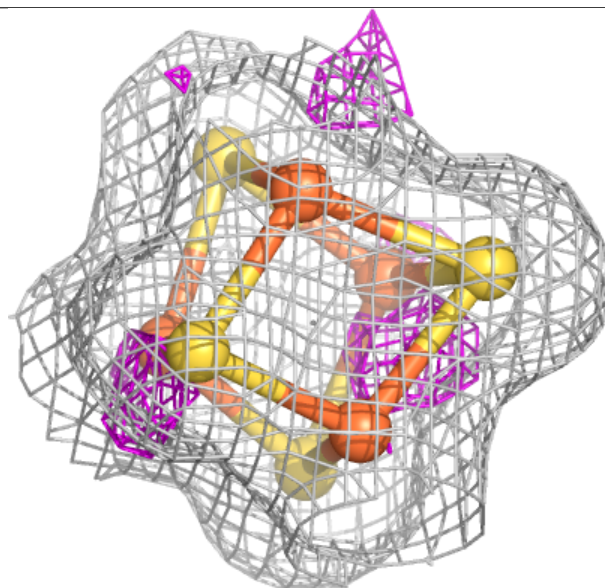
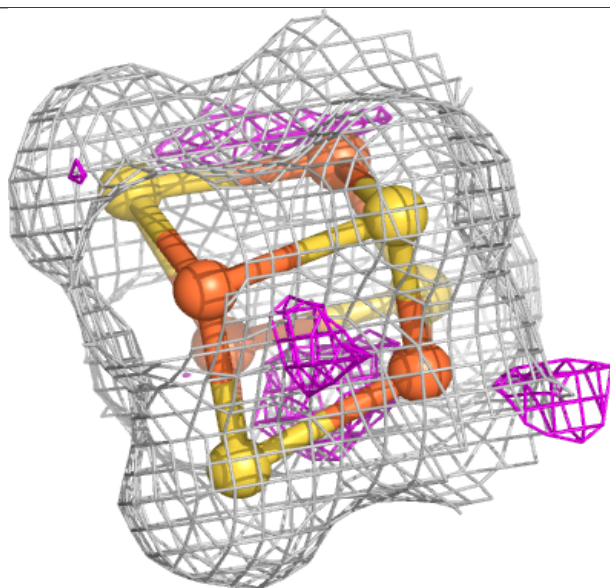
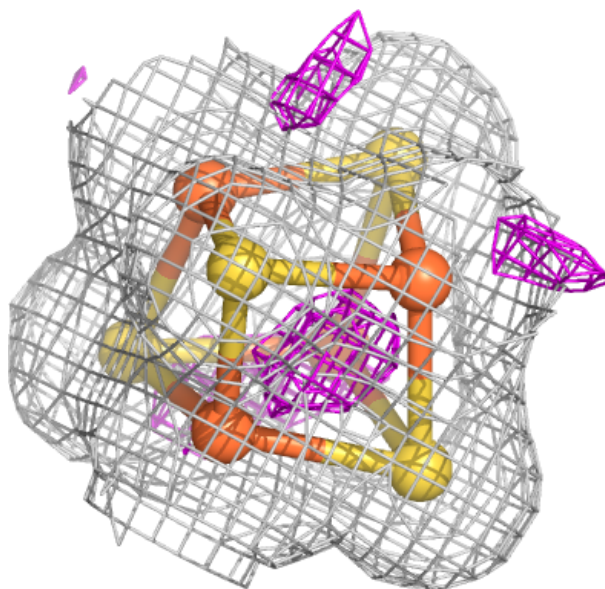
Electron density around SF4 B 301:

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



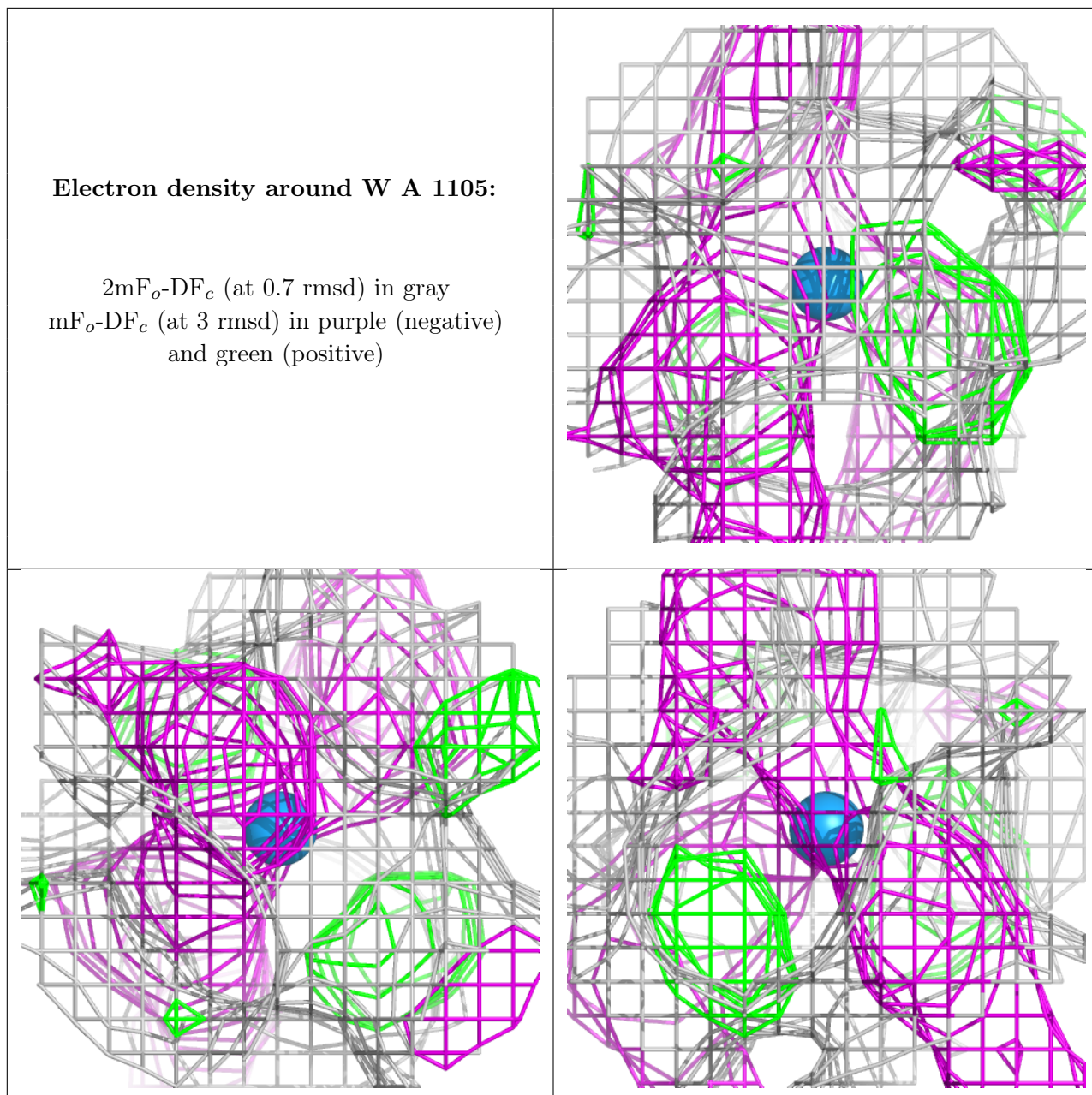
Electron density around SF4 A 1103:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.