



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 10:20 am BST

PDB ID : 8CM4
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

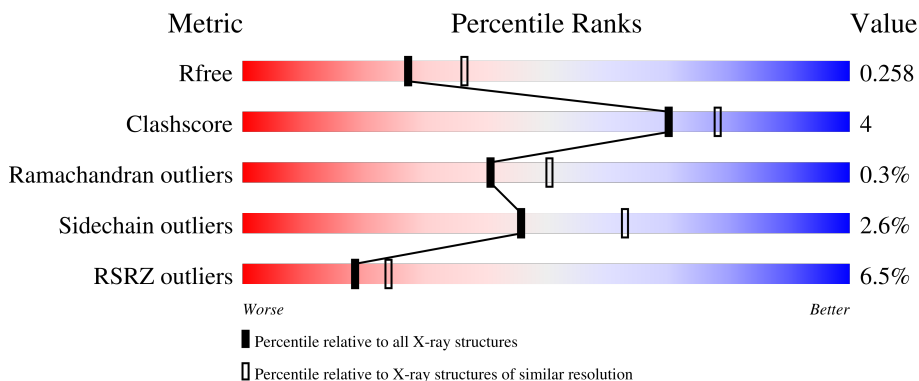
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	 8% 86% 10%
1	C	1013	 7% 85% 10%
2	B	215	 90% 8%
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
			Total	C	N	O	S	Se			
1	A	973	7621	4858	1328	1394	40	1	0	0	0
1	C	970	7591	4838	1322	1390	40	1	0	0	0

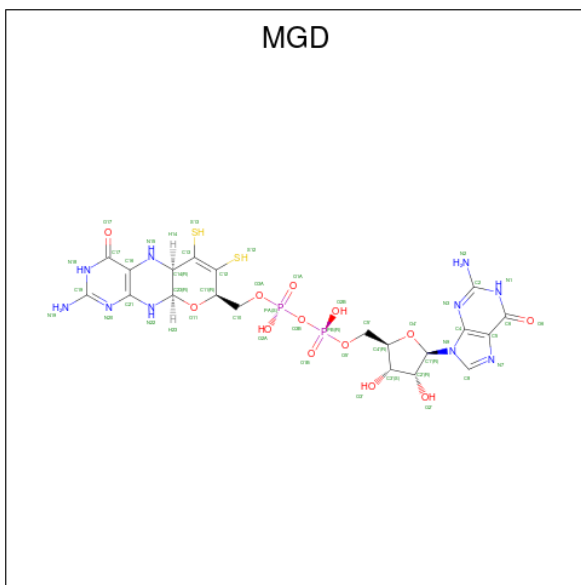
There are 18 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	S			
2	B	214	Total 1664	C 1041	N 291	O 316	S 16	0	0	0
2	D	214	Total 1664	C 1041	N 291	O 316	S 16	0	0	0

- 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 (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

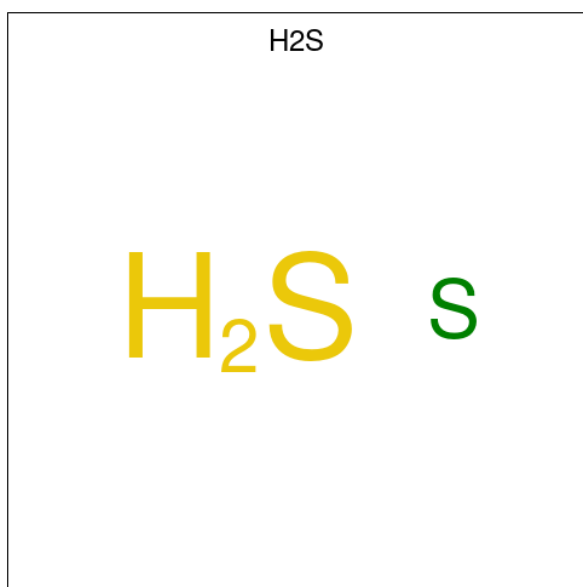


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	A	1	Total	C O	0	0
			6	3 3		
5	C	1	Total	C O	0	0
			6	3 3		

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

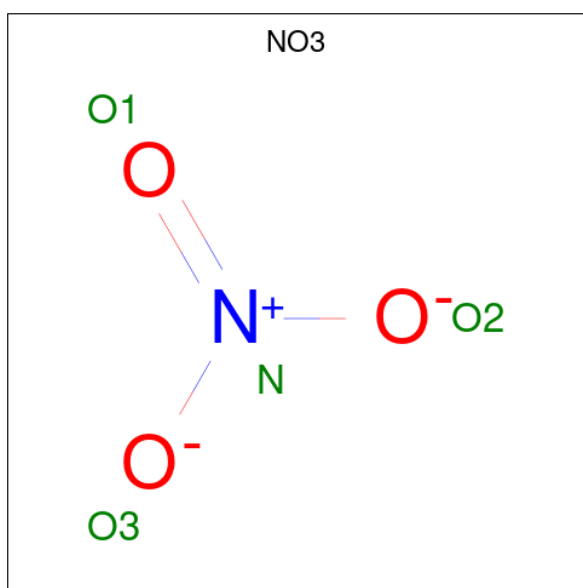
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	W	0	0
			1	1		
6	C	1	Total	W	0	0
			1	1		

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



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

- Molecule 8 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

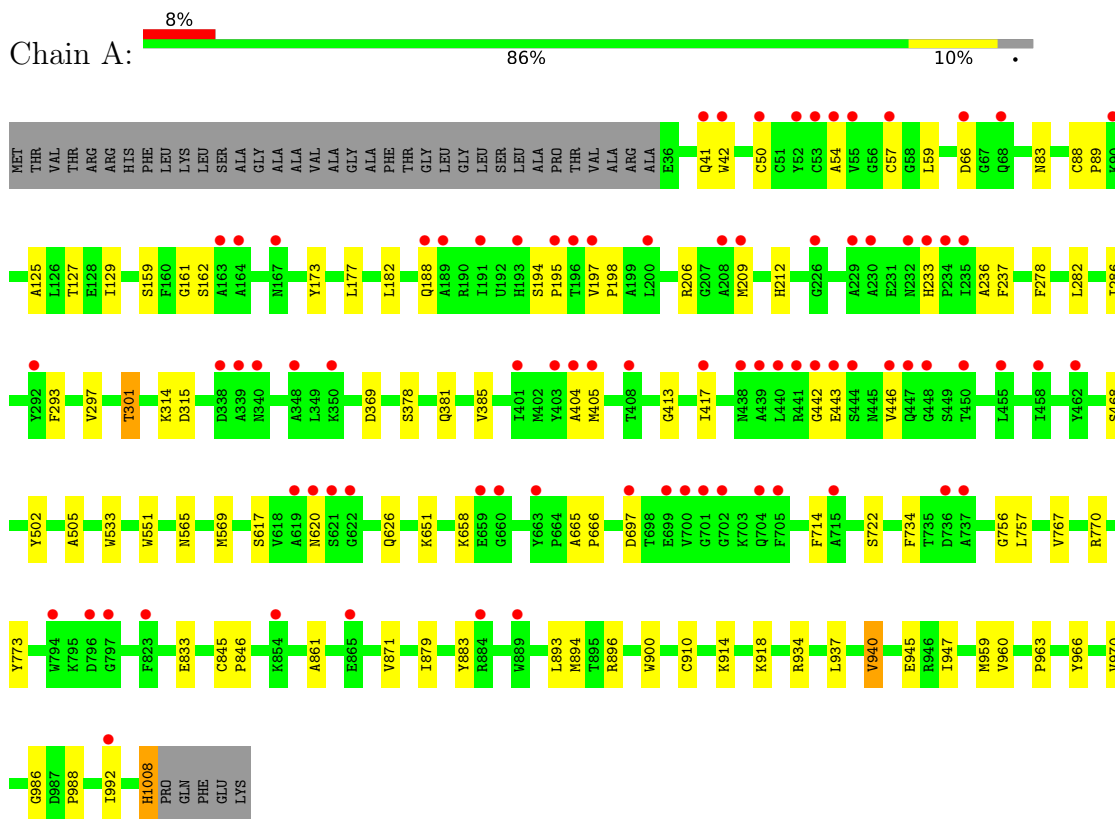
- Molecule 10 is water.

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

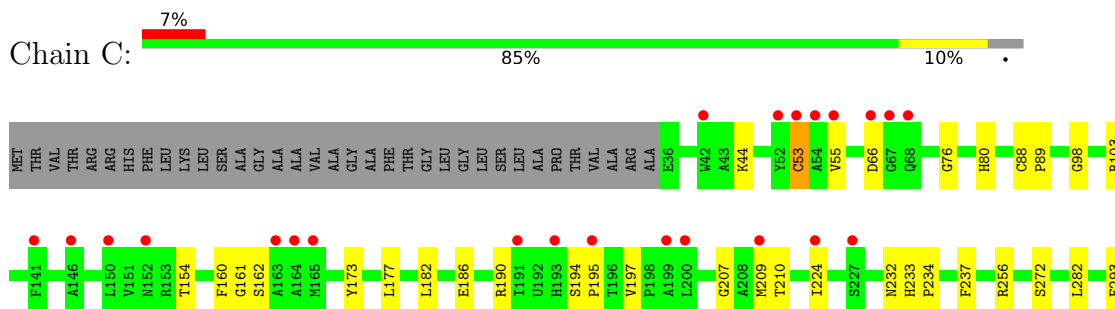
3 Residue-property plots

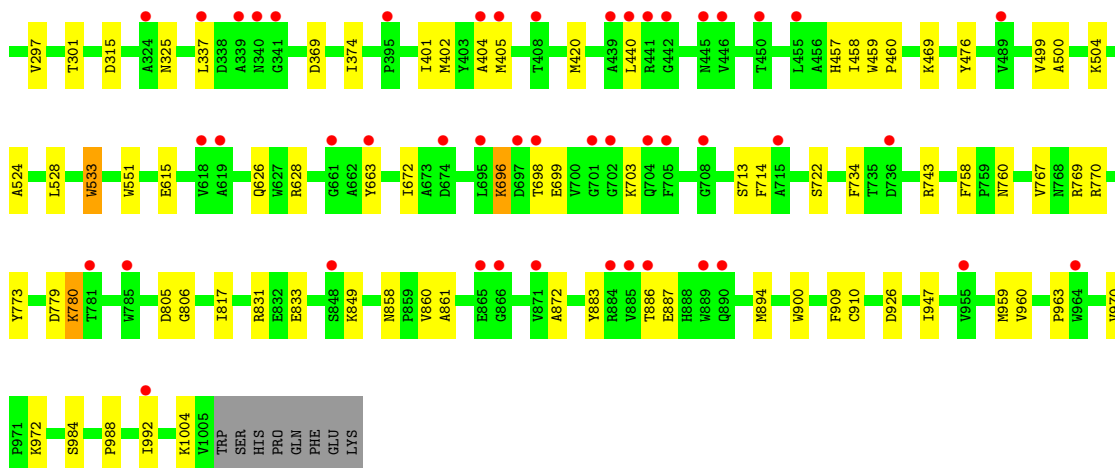
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

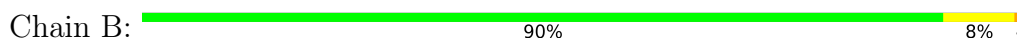


- Molecule 1: Formate dehydrogenase, alpha subunit, selenocysteine-containing

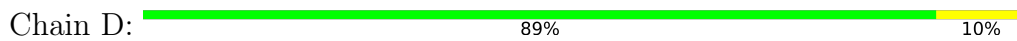




● Molecule 2: Formate dehydrogenase, beta subunit, putative



● Molecule 2: Formate dehydrogenase, beta subunit, putative



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 48.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.31-2.30) 99.8 (48.27-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.29Å)	Xtrriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.572	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: GOL, MGD, W, SEC, H2S, SF4, PEG, NO3

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	0.64	0/7826	0.78	0/10617
1	C	0.65	0/7793	0.77	0/10571
2	B	0.62	0/1699	0.81	0/2302
2	D	0.63	0/1699	0.79	0/2302
All	All	0.64	0/19017	0.78	0/25792

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	7621	0	7447	53	0
1	C	7591	0	7425	59	0
2	B	1664	0	1633	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	133	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 (133) 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:HE2	1.67	0.76
2:B:7:VAL:HG13	2:B:162:MET:CE	2.20	0.70
1:C:88:CYS:HB2	1:C:89:PRO:HD2	1.74	0.70
1:C:887:GLU:OE2	2:D:16:ARG:NH2	2.26	0.67
1:C:224:ILE:HG12	1:C:402:MET:HE3	1.78	0.66
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
1:A:947:ILE:HG23	1:A:959:MET:HE3	1.80	0.63
1:A:1008:HIS:ND1	1:A:1008:HIS:C	2.52	0.63
1:A:378:SER:OG	1:A:381:GLN:HG3	2.00	0.62
2:D:139:ASP:HB3	9:D:304:PEG:H42	1.82	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:LEU:HD12	1:C:337:LEU:N	2.24	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
1:C:209:MET:HE2	1:C:440:LEU:HD23	1.92	0.51
1:A:918:LYS:HE3	2:D:193:PRO:HD2	1.91	0.51
1:A:947:ILE:CG2	1:A:959:MET:HE3	2.40	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
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.47	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
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:224:ILE:HG12	1:C:402:MET:CE	2.42	0.48
1:C:404:ALA:HB3	3:C:1101:MGD:O2A	2.13	0.48
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.54	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
2:B:162:MET:HE3	4:B:301:SF4:S3	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:PHE:CE2	1:C:963:PRO:HG3	2.50	0.47
2:D:41:ASN:HA	2:D:42:PRO:C	2.34	0.47
1:A:845:CYS:SG	1:A:871:VAL:HG13	2.55	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: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
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.98	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
1:A:297:VAL:HA	1:A:301:THR:HG23	2.00	0.44
1:C:297:VAL:O	1:C:301:THR:OG1	2.25	0.44
1:A:282:LEU:O	1:A:286:ILE:HG13	2.17	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:HG	1:A:173:TYR:HH	1.62	0.42
1:C:947:ILE:HD12	1:C:959:MET:CE	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
1:C:947:ILE:HD12	1:C:959:MET:HE1	2.01	0.41
2:D:188:ALA:HA	2:D:202:PHE:O	2.20	0.41
1:A:209:MET:CE	1:A:212:HIS:HA	2.50	0.41
1:C:457:HIS:CD2	1:C:458:ILE:HG23	2.56	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:194:SER:O	1:A:198:PRO:HD2	2.21	0.41
1:A:937:LEU:HD12	1:A:937:LEU:C	2.41	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: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
2:B:41:ASN:HA	2:B:42:PRO:C	2.41	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: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

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	970/1013 (96%)	936 (96%)	31 (3%)	3 (0%)	41	50
1	C	967/1013 (96%)	918 (95%)	45 (5%)	4 (0%)	34	42
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%)	41	50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	TRP
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 [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	790/818 (97%)	773 (98%)	17 (2%)	52	69
1	C	787/818 (96%)	765 (97%)	22 (3%)	43	60
2	B	185/186 (100%)	182 (98%)	3 (2%)	62	78
2	D	185/186 (100%)	177 (96%)	8 (4%)	29	40
All	All	1947/2008 (97%)	1897 (97%)	50 (3%)	46	63

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP

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Mol	Chain	Res	Type
1	A	237	PHE
1	A	293	PHE
1	A	301	THR
1	A	314	LYS
1	A	315	ASP
1	A	369	ASP
1	A	468	SER
1	A	658	LYS
1	A	697	ASP
1	A	722	SER
1	A	734	PHE
1	A	833	GLU
1	A	934	ARG
1	A	940	VAL
1	A	970	VAL
1	A	1008	HIS
2	B	24	GLN
2	B	132	THR
2	B	156	THR
1	C	44	LYS
1	C	53	CYS
1	C	66	ASP
1	C	154	THR
1	C	237	PHE
1	C	282	LEU
1	C	293	PHE
1	C	315	ASP
1	C	369	ASP
1	C	528	LEU
1	C	672	ILE
1	C	696	LYS
1	C	713	SER
1	C	734	PHE
1	C	780	LYS
1	C	831	ARG
1	C	833	GLU
1	C	849	LYS
1	C	886	THR
1	C	970	VAL
1	C	972	LYS
1	C	984	SER
2	D	10	SER

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Mol	Chain	Res	Type
2	D	24	GLN
2	D	116	SER
2	D	119	SER
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	863	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	302	2	0,12,12	-	-	-		
4	SF4	D	302	2	0,12,12	-	-	-		
4	SF4	A	1103	1	0,12,12	-	-	-		
5	GOL	A	1107	-	5,5,5	0.12	0	5,5,5	0.28	0
3	MGD	C	1102	6	41,52,52	1.08	2 (4%)	40,81,81	1.31	6 (15%)
4	SF4	D	303	2	0,12,12	-	-	-		
4	SF4	C	1103	1	0,12,12	-	-	-		
5	GOL	A	1104	-	5,5,5	0.10	0	5,5,5	0.28	0
8	NO3	B	304	-	1,3,3	0.12	0	0,3,3	-	-
4	SF4	B	303	2	0,12,12	-	-	-		
9	PEG	D	304	-	6,6,6	0.49	0	5,5,5	0.33	0
4	SF4	B	301	2	0,12,12	-	-	-		
4	SF4	D	301	2	0,12,12	-	-	-		
5	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.27	0
5	GOL	C	1104	-	5,5,5	0.09	0	5,5,5	0.32	0
3	MGD	A	1101	6	41,52,52	0.86	3 (7%)	40,81,81	1.07	2 (5%)
3	MGD	A	1102	6	41,52,52	1.01	2 (4%)	40,81,81	1.07	3 (7%)
3	MGD	C	1101	6	41,52,52	0.87	3 (7%)	40,81,81	1.05	3 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	302	2	-	-	0/6/5/5
4	SF4	D	302	2	-	-	0/6/5/5
4	SF4	A	1103	1	-	-	0/6/5/5
5	GOL	A	1107	-	-	2/4/4/4	-
3	MGD	C	1102	6	-	7/18/66/66	0/6/6/6
4	SF4	D	303	2	-	-	0/6/5/5
4	SF4	C	1103	1	-	-	0/6/5/5
5	GOL	A	1104	-	-	2/4/4/4	-
4	SF4	B	303	2	-	-	0/6/5/5
9	PEG	D	304	-	-	4/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
4	SF4	D	301	2	-	-	0/6/5/5
5	GOL	A	1106	-	-	2/4/4/4	-
5	GOL	C	1104	-	-	2/4/4/4	-
3	MGD	A	1101	6	-	2/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MGD	A	1102	6	-	5/18/66/66	0/6/6/6
3	MGD	C	1101	6	-	2/18/66/66	0/6/6/6

All (10) 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	A	1101	MGD	C5-C6	-2.90	1.41	1.47
3	C	1101	MGD	C5-C6	-2.62	1.42	1.47
3	C	1102	MGD	C5-C6	-2.59	1.42	1.47
3	A	1102	MGD	C5-C6	-2.52	1.42	1.47
3	C	1101	MGD	C23-C14	2.30	1.55	1.53
3	A	1101	MGD	C5-C4	-2.21	1.37	1.43
3	A	1101	MGD	C8-N7	-2.20	1.31	1.35
3	C	1101	MGD	C8-N7	-2.01	1.31	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1102	MGD	O4'-C1'-C2'	-3.44	101.90	106.93
3	C	1102	MGD	O11-C23-C14	2.93	110.92	108.96
3	C	1102	MGD	C19-N20-C21	2.78	118.45	113.43
3	A	1101	MGD	C19-N20-C21	2.75	118.39	113.43
3	C	1101	MGD	C19-N20-C21	2.74	118.38	113.43
3	A	1102	MGD	C19-N20-C21	2.49	117.92	113.43
3	A	1102	MGD	O11-C23-C14	2.42	110.58	108.96
3	C	1101	MGD	O4'-C1'-C2'	-2.31	103.55	106.93
3	A	1102	MGD	O6-C6-C5	2.31	128.87	124.37
3	A	1101	MGD	O4'-C1'-C2'	-2.29	103.58	106.93
3	C	1102	MGD	O6-C6-C5	2.21	128.69	124.37
3	C	1101	MGD	O6-C6-C5	2.17	128.61	124.37
3	C	1102	MGD	O3'-C3'-C4'	-2.13	104.89	111.05
3	C	1102	MGD	PA-O3B-PB	-2.07	125.73	132.83

There are no chirality outliers.

All (28) 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

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Mol	Chain	Res	Type	Atoms
5	A	1104	GOL	O1-C1-C2-C3
5	A	1107	GOL	C1-C2-C3-O3
5	C	1104	GOL	C1-C2-C3-O3
3	A	1102	MGD	O4'-C4'-C5'-O5'
3	C	1102	MGD	O4'-C4'-C5'-O5'
5	A	1104	GOL	O1-C1-C2-O2
9	D	304	PEG	O2-C3-C4-O4
5	A	1106	GOL	O1-C1-C2-C3
9	D	304	PEG	O1-C1-C2-O2
5	A	1107	GOL	O2-C2-C3-O3
5	C	1104	GOL	O2-C2-C3-O3
3	C	1102	MGD	PA-O3B-PB-O1B
3	A	1102	MGD	C3'-C4'-C5'-O5'
3	C	1102	MGD	C3'-C4'-C5'-O5'
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
3	A	1102	MGD	PA-O3B-PB-O1B
5	A	1106	GOL	O1-C1-C2-O2
9	D	304	PEG	C1-C2-O2-C3
3	A	1101	MGD	C10-O3A-PA-O3B
3	C	1102	MGD	C5'-O5'-PB-O3B
3	A	1102	MGD	PA-O3B-PB-O2B
3	C	1101	MGD	PA-O3B-PB-O2B
3	C	1102	MGD	C5'-O5'-PB-O1B

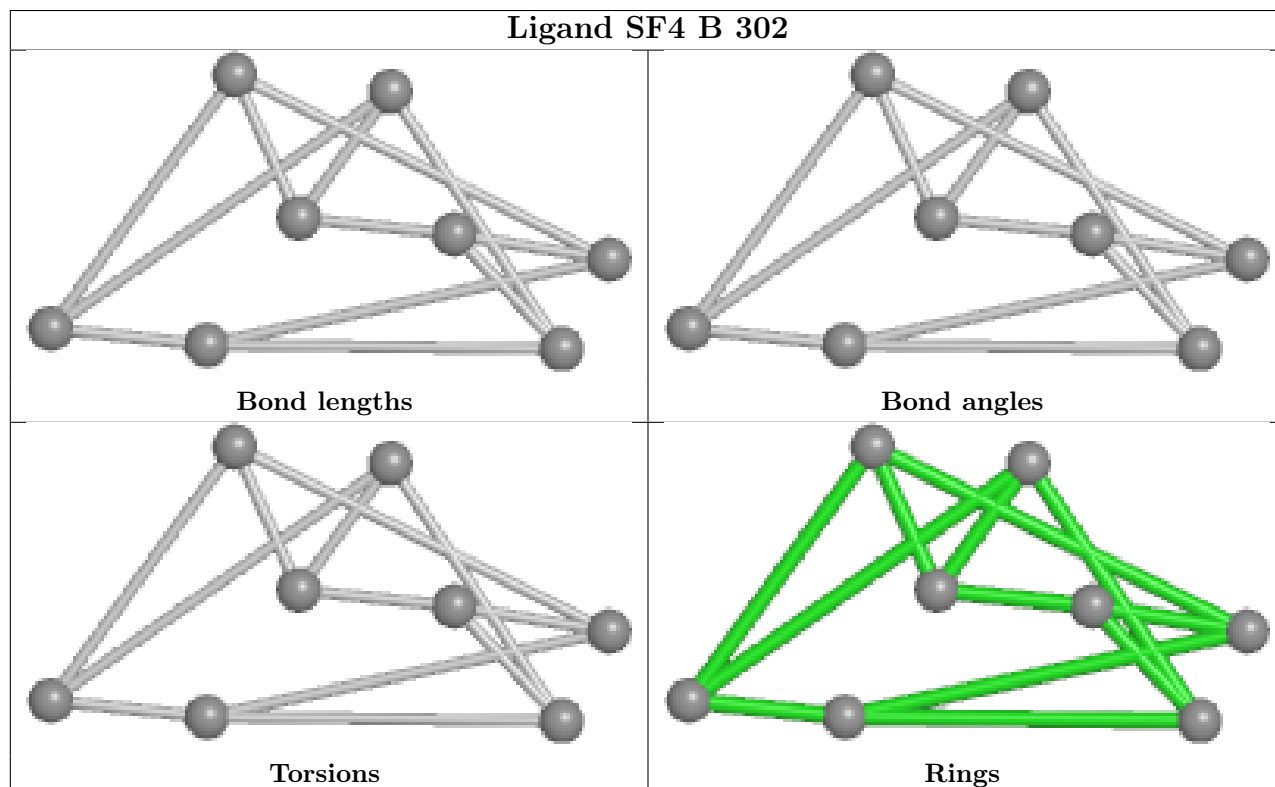
There are no ring outliers.

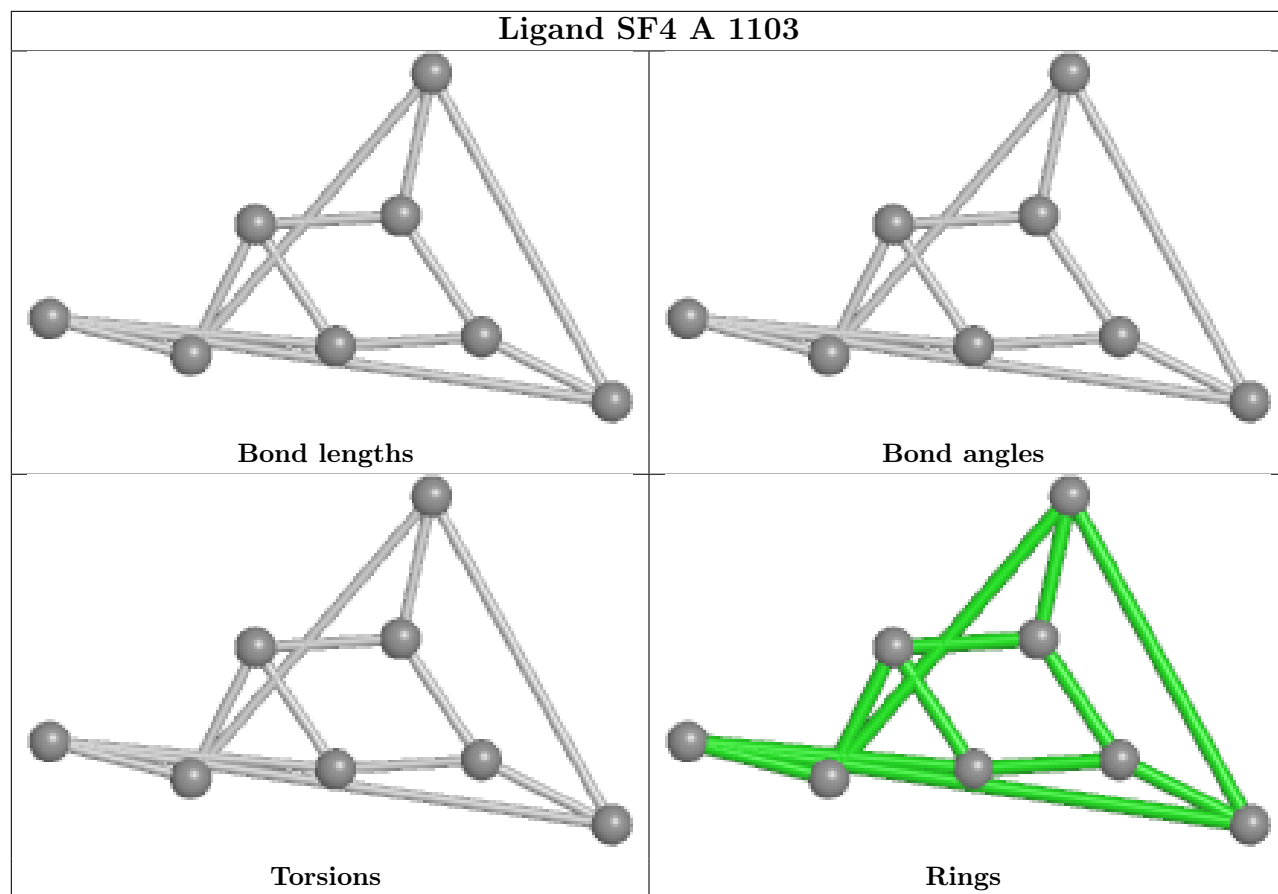
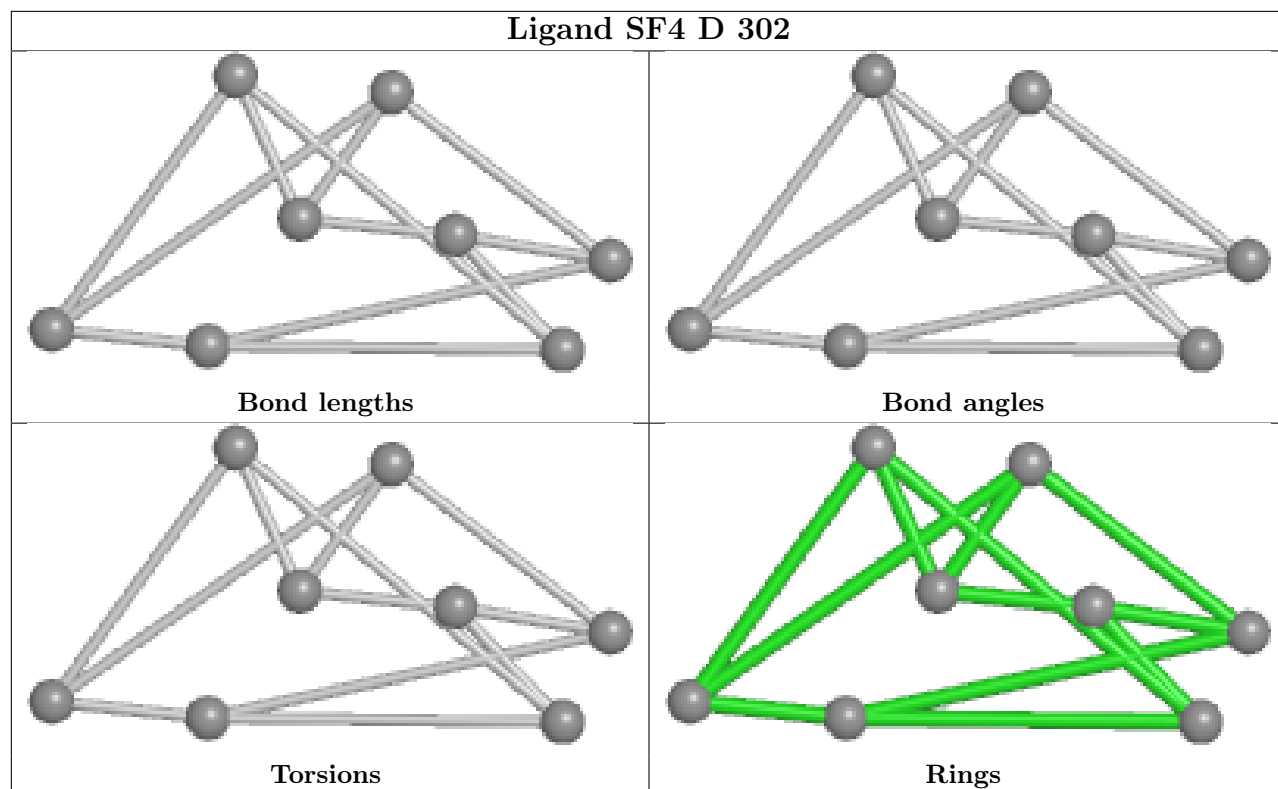
7 monomers are involved in 16 short contacts:

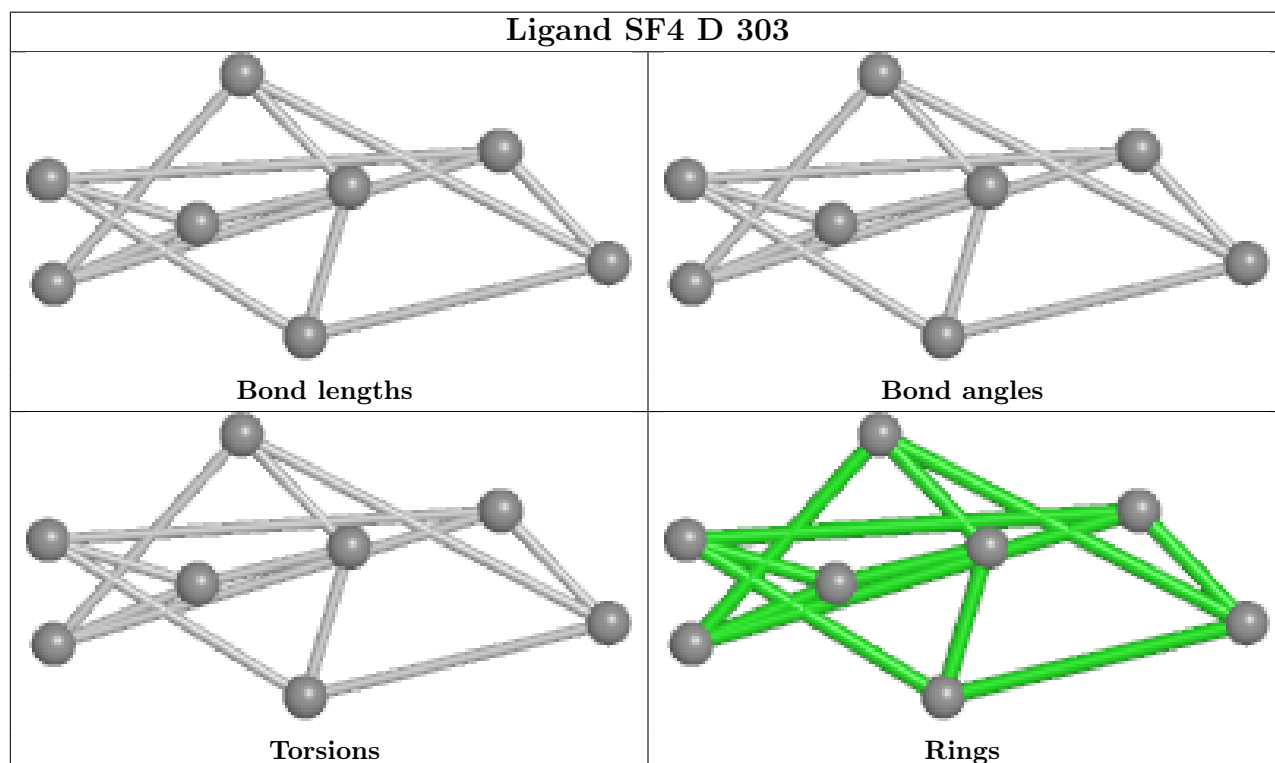
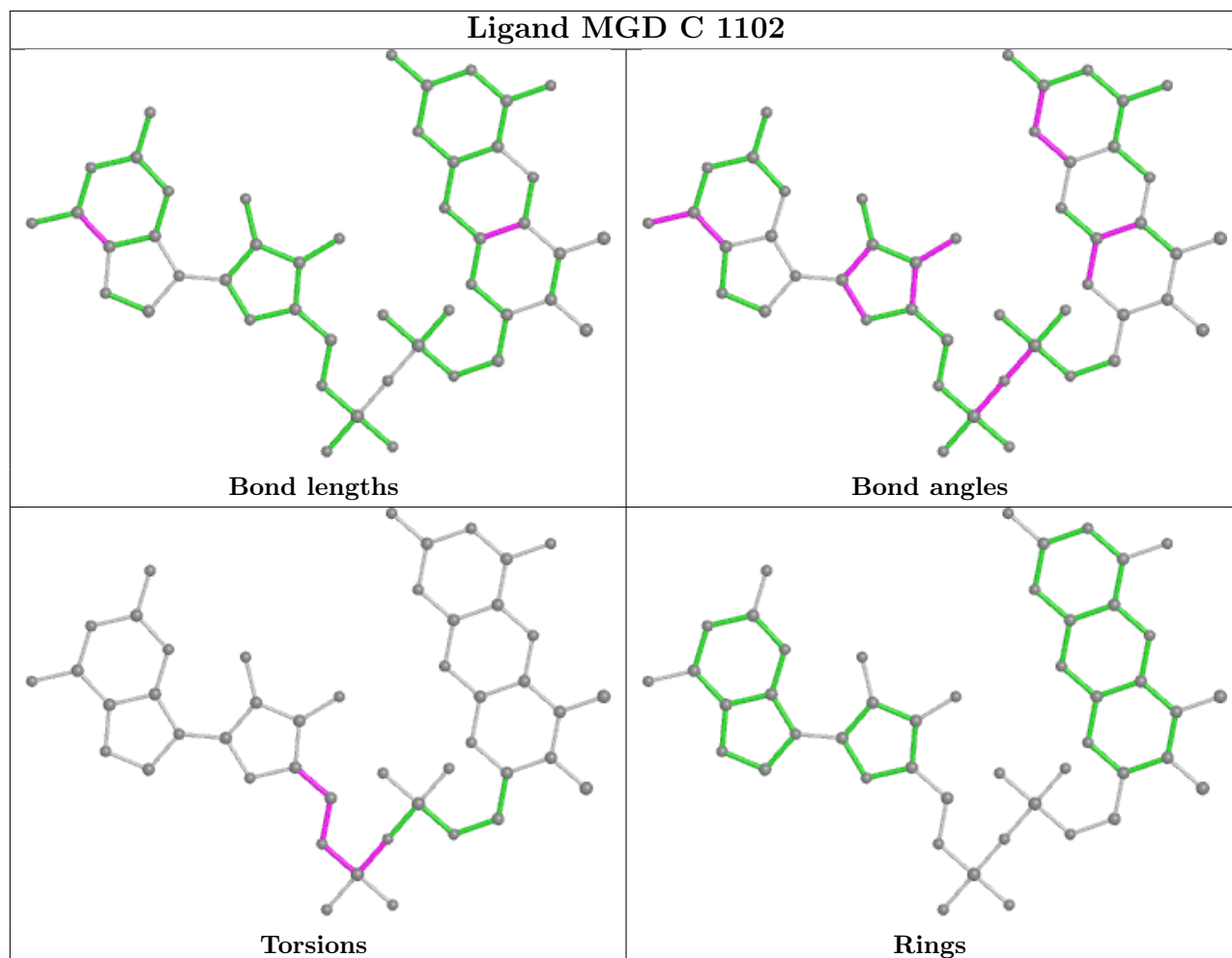
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1102	MGD	1	0
4	C	1103	SF4	1	0
9	D	304	PEG	4	0
4	B	301	SF4	1	0
3	A	1101	MGD	2	0
3	A	1102	MGD	3	0
3	C	1101	MGD	4	0

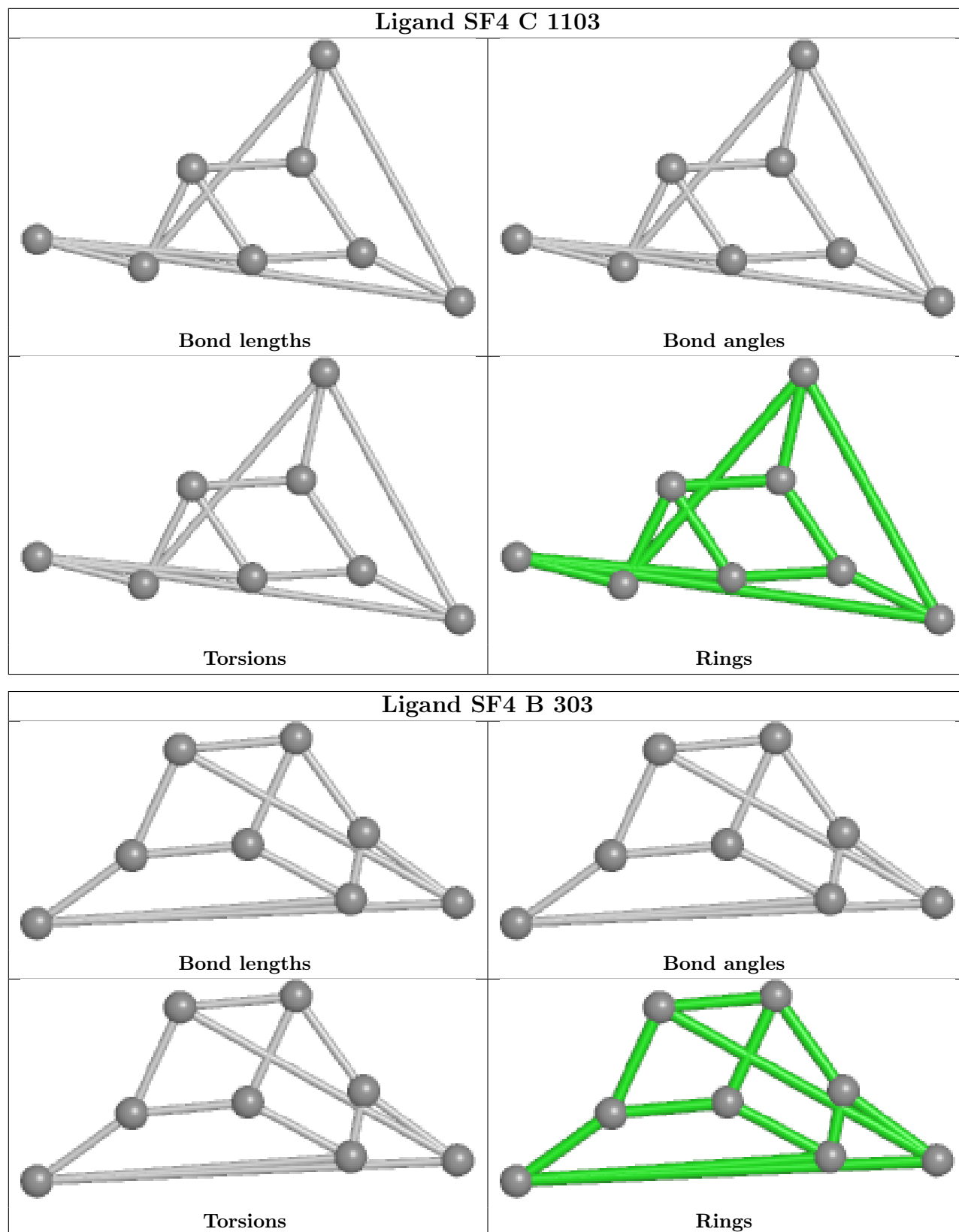
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

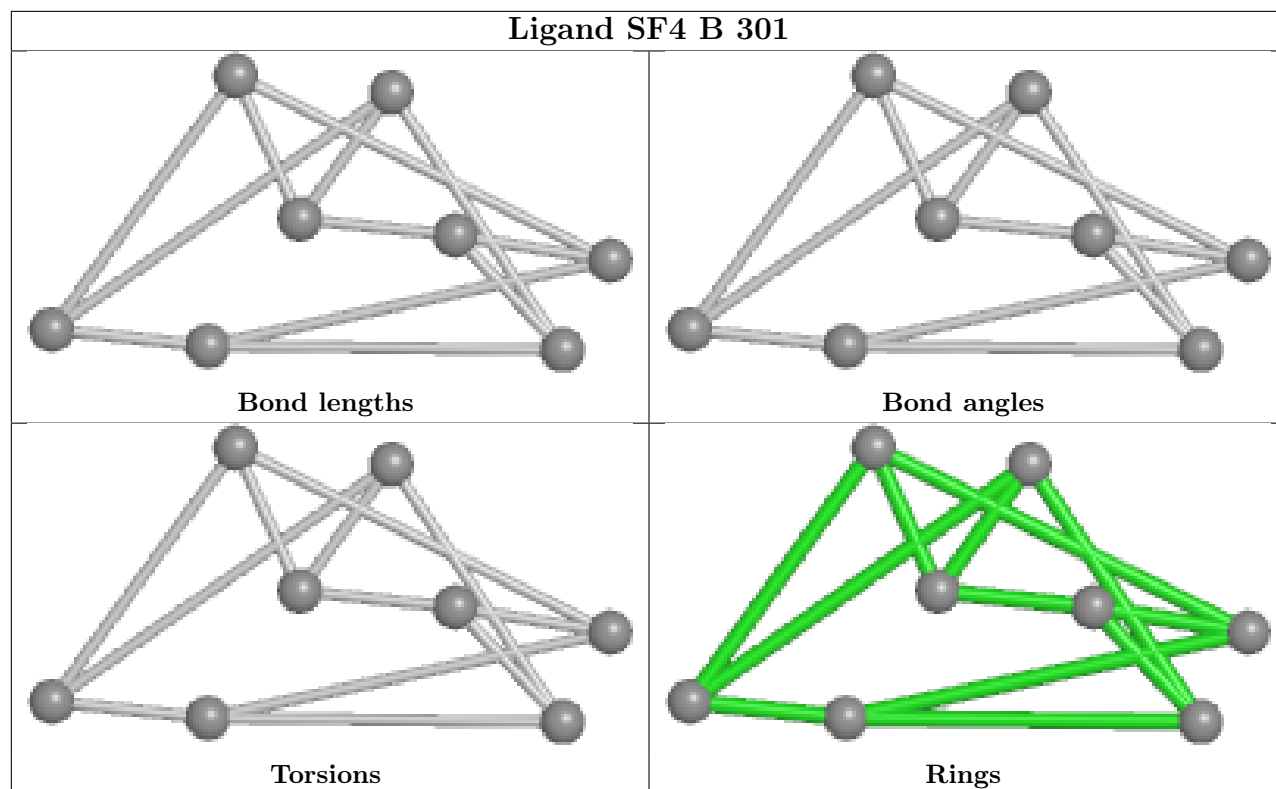
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

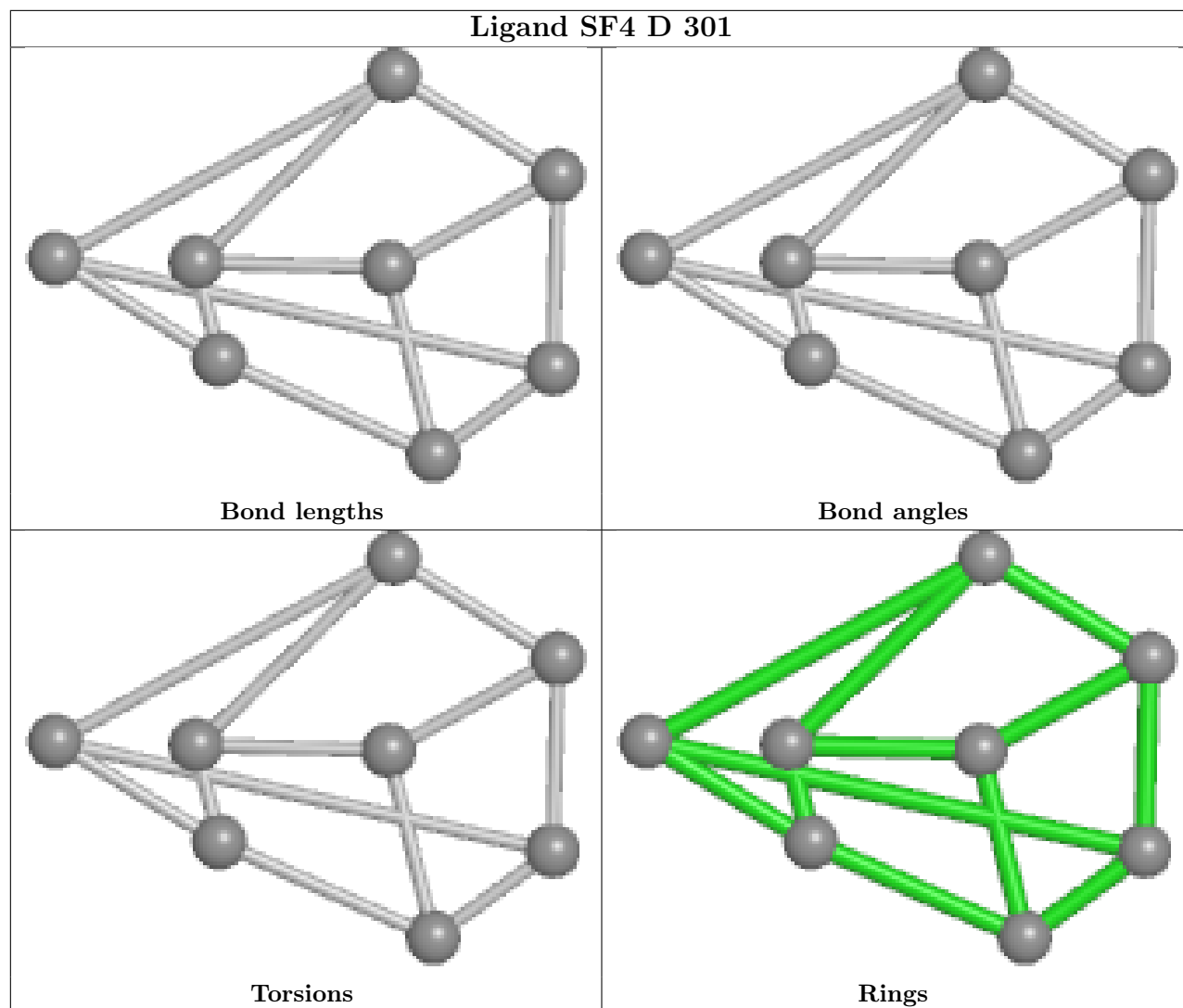


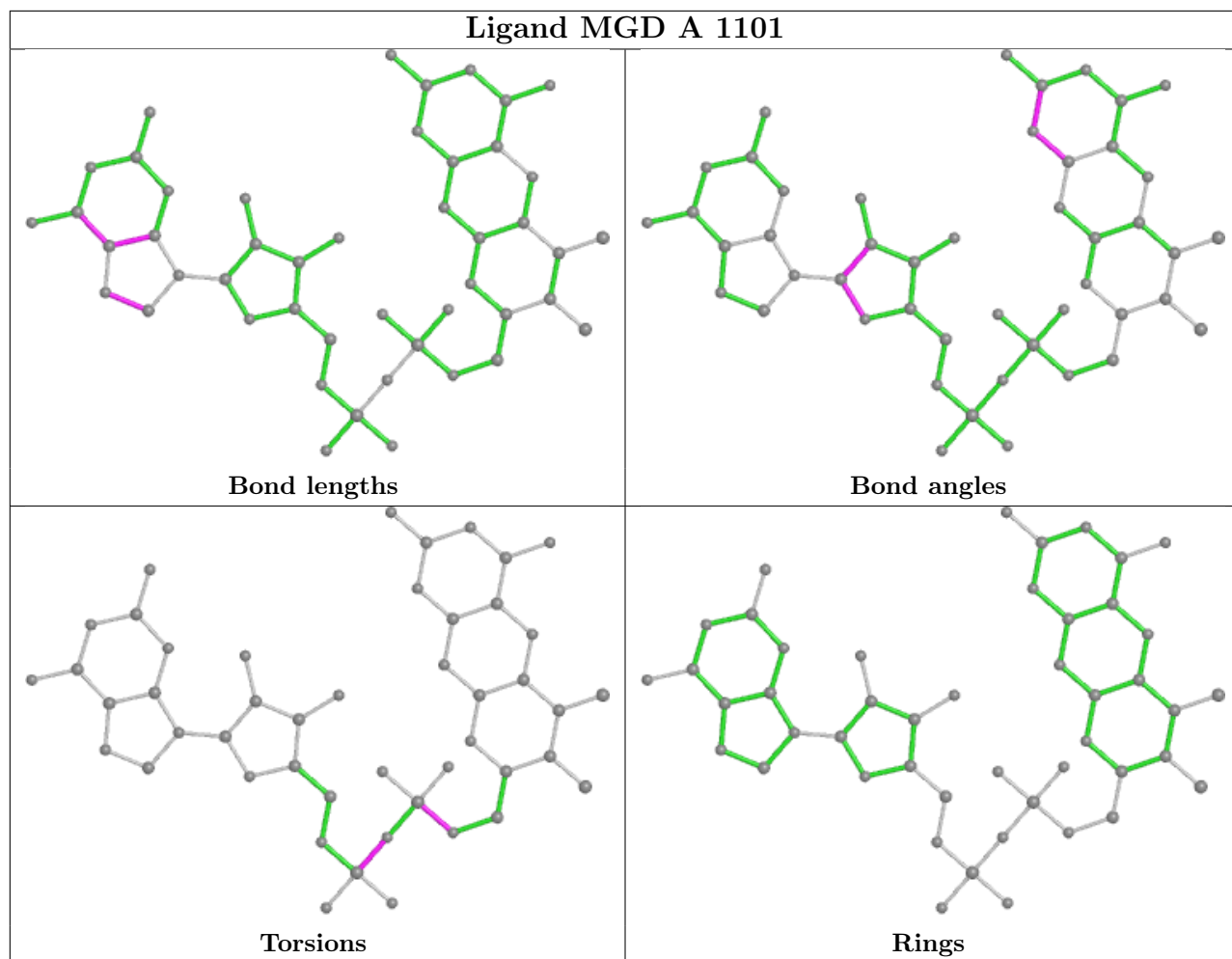


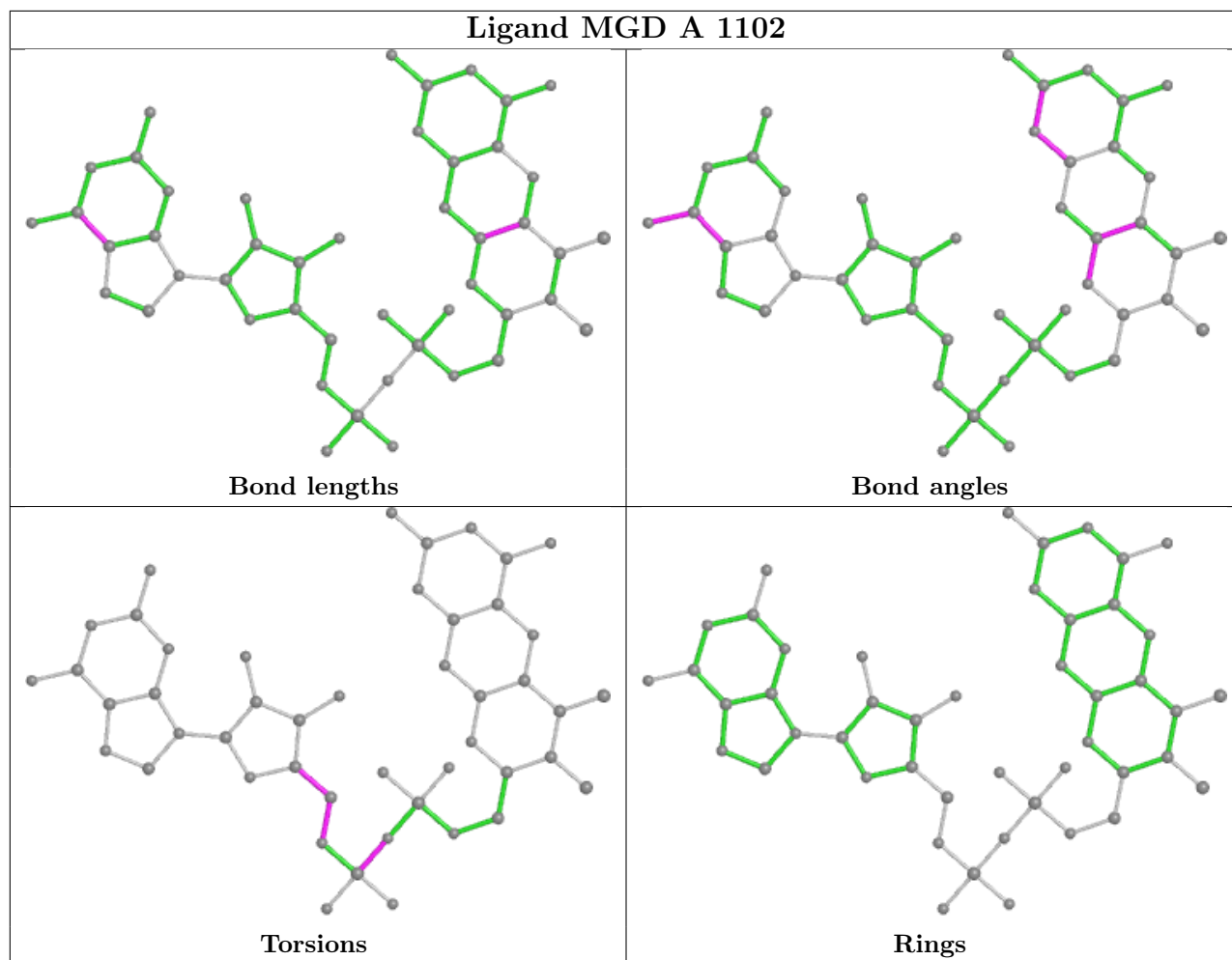


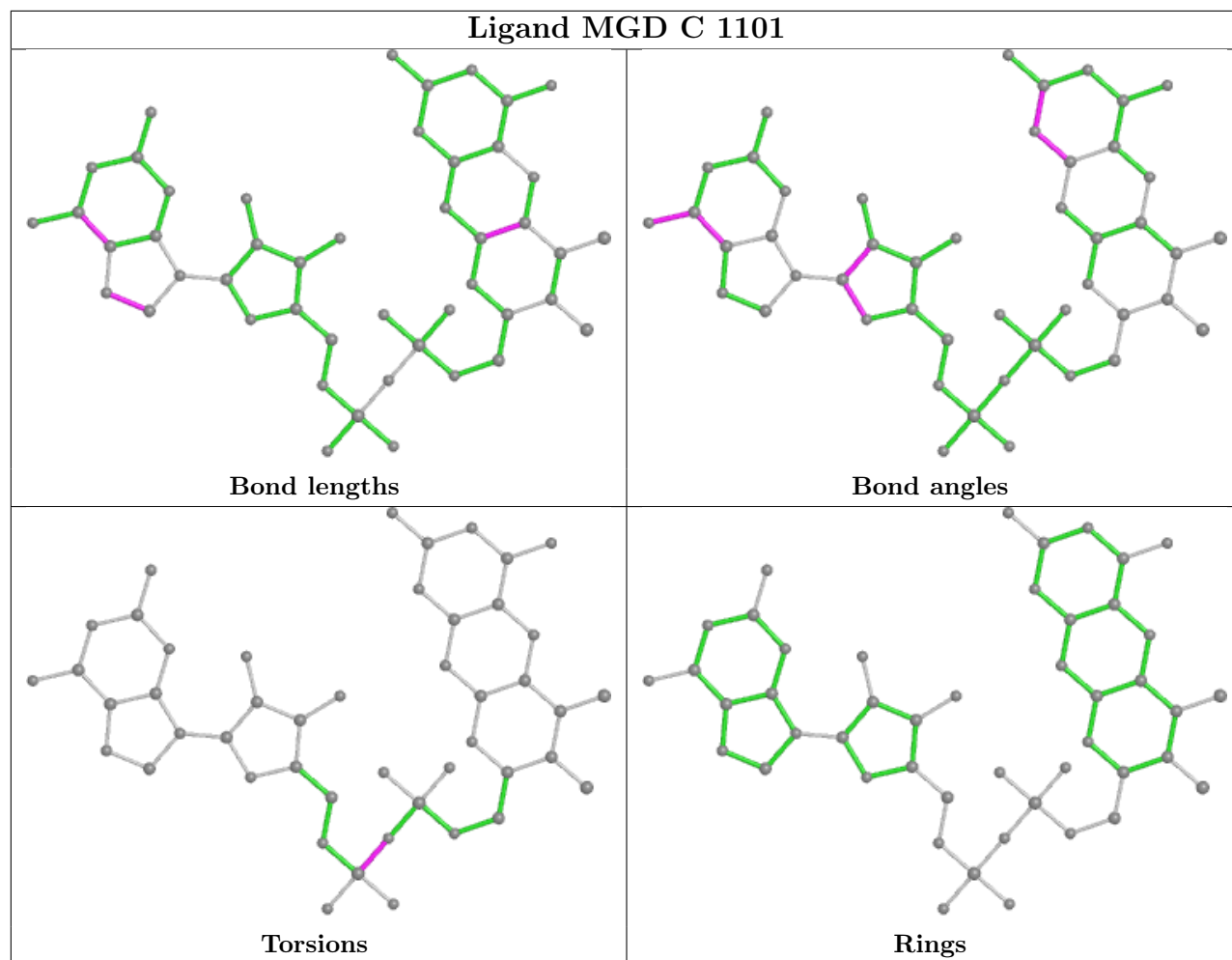












5.7 Other polymers [i](#)

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%)	0.45	83 (8%) 10 14	25, 44, 68, 86	0
1	C	969/1013 (95%)	0.45	70 (7%) 15 20	26, 46, 75, 115	0
2	B	214/215 (99%)	-0.09	0 100 100	25, 34, 52, 65	0
2	D	214/215 (99%)	-0.16	0 100 100	26, 35, 52, 80	0
All	All	2369/2456 (96%)	0.35	153 (6%) 18 24	25, 43, 72, 115	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	446	VAL	4.8
1	A	702	GLY	4.7
1	A	794	TRP	4.6
1	A	446	VAL	4.6
1	A	440	LEU	4.5
1	A	55	VAL	4.5
1	C	68	GLN	4.2
1	C	339	ALA	4.2
1	A	796	ASP	4.2
1	A	196	THR	4.0
1	A	701	GLY	3.9
1	A	797	GLY	3.9
1	C	442	GLY	3.9
1	A	441	ARG	3.8
1	C	708	GLY	3.7
1	C	695	LEU	3.7
1	A	339	ALA	3.7
1	C	42	TRP	3.7
1	A	404	ALA	3.6
1	C	865	GLU	3.6
1	A	193	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	53	CYS	3.6
1	A	442	GLY	3.6
1	C	341	GLY	3.6
1	C	871	VAL	3.5
1	A	68	GLN	3.5
1	A	348	ALA	3.5
1	C	663	TYR	3.4
1	C	163	ALA	3.4
1	C	440	LEU	3.4
1	C	441	ARG	3.4
1	A	444	SER	3.4
1	A	889	TRP	3.3
1	A	197	VAL	3.3
1	C	889	TRP	3.3
1	A	455	LEU	3.3
1	A	458	ILE	3.2
1	C	324	ALA	3.2
1	C	200	LEU	3.2
1	A	408	THR	3.2
1	C	195	PRO	3.1
1	C	191	ILE	3.1
1	C	992	ILE	3.1
1	C	698	THR	3.0
1	A	447	GLN	3.0
1	A	163	ALA	3.0
1	A	208	ALA	3.0
1	A	737	ALA	3.0
1	A	234	PRO	3.0
1	A	189	ALA	2.9
1	C	54	ALA	2.9
1	C	736	ASP	2.9
1	A	200	LEU	2.9
1	C	450	THR	2.9
1	A	52	TYR	2.9
1	C	701	GLY	2.8
1	C	885	VAL	2.8
1	C	884	ARG	2.8
1	C	199	ALA	2.8
1	C	164	ALA	2.8
1	A	229	ALA	2.7
1	A	54	ALA	2.7
1	A	405	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	848	SER	2.7
1	C	405	MET	2.7
1	A	188	GLN	2.7
1	A	235	ILE	2.7
1	C	55	VAL	2.7
1	C	866	GLY	2.7
1	A	403	TYR	2.7
1	A	226	GLY	2.7
1	A	659	GLU	2.6
1	C	53	CYS	2.6
1	A	823	PHE	2.6
1	A	663	TYR	2.6
1	A	700	VAL	2.6
1	C	715	ALA	2.6
1	C	697	ASP	2.6
1	A	42	TRP	2.5
1	A	699	GLU	2.5
1	A	660	GLY	2.5
1	C	705	PHE	2.5
1	C	52	TYR	2.5
1	C	702	GLY	2.5
1	C	890	GLN	2.5
1	C	704	GLN	2.5
1	C	785	TRP	2.5
1	A	439	ALA	2.4
1	A	233	HIS	2.4
1	A	191	ILE	2.4
1	C	227	SER	2.4
1	A	195	PRO	2.4
1	A	417	ILE	2.4
1	C	67	GLY	2.4
1	C	340	ASN	2.4
1	C	455	LEU	2.4
1	C	66	ASP	2.4
1	A	462	TYR	2.4
1	C	150	LEU	2.4
1	C	337	LEU	2.4
1	A	854	LYS	2.4
1	A	621	SER	2.4
1	A	620	ASN	2.4
1	A	705	PHE	2.4
1	A	992	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	GLU	2.3
1	C	489	VAL	2.3
1	A	292	TYR	2.3
1	A	622	GLY	2.3
1	C	404	ALA	2.3
1	C	193	HIS	2.3
1	C	152	ASN	2.3
1	A	715	ALA	2.3
1	A	884	ARG	2.2
1	A	350	LYS	2.2
1	A	340	ASN	2.2
1	A	230	ALA	2.2
1	C	661	GLY	2.2
1	A	232	ASN	2.2
1	A	57	CYS	2.2
1	A	438	ASN	2.2
1	A	41	GLN	2.2
1	A	450	THR	2.2
1	C	209	MET	2.2
1	A	865	GLU	2.2
1	A	448	GLY	2.2
1	C	618	VAL	2.2
1	C	619	ALA	2.2
1	A	704	GLN	2.2
1	A	164	ALA	2.1
1	C	224	ILE	2.1
1	A	90	LYS	2.1
1	A	66	ASP	2.1
1	A	736	ASP	2.1
1	C	781	THR	2.1
1	C	408	THR	2.1
1	C	141	PHE	2.1
1	A	338	ASP	2.1
1	C	146	ALA	2.1
1	C	964	TRP	2.1
1	C	395	PRO	2.1
1	A	401	ILE	2.1
1	A	209	MET	2.1
1	C	445	ASN	2.1
1	C	886	THR	2.1
1	A	619	ALA	2.0
1	C	674	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	955	VAL	2.0
1	A	50	CYS	2.0
1	C	439	ALA	2.0
1	A	167	ASN	2.0
1	C	165	MET	2.0
1	A	697	ASP	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 monosaccharides 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.

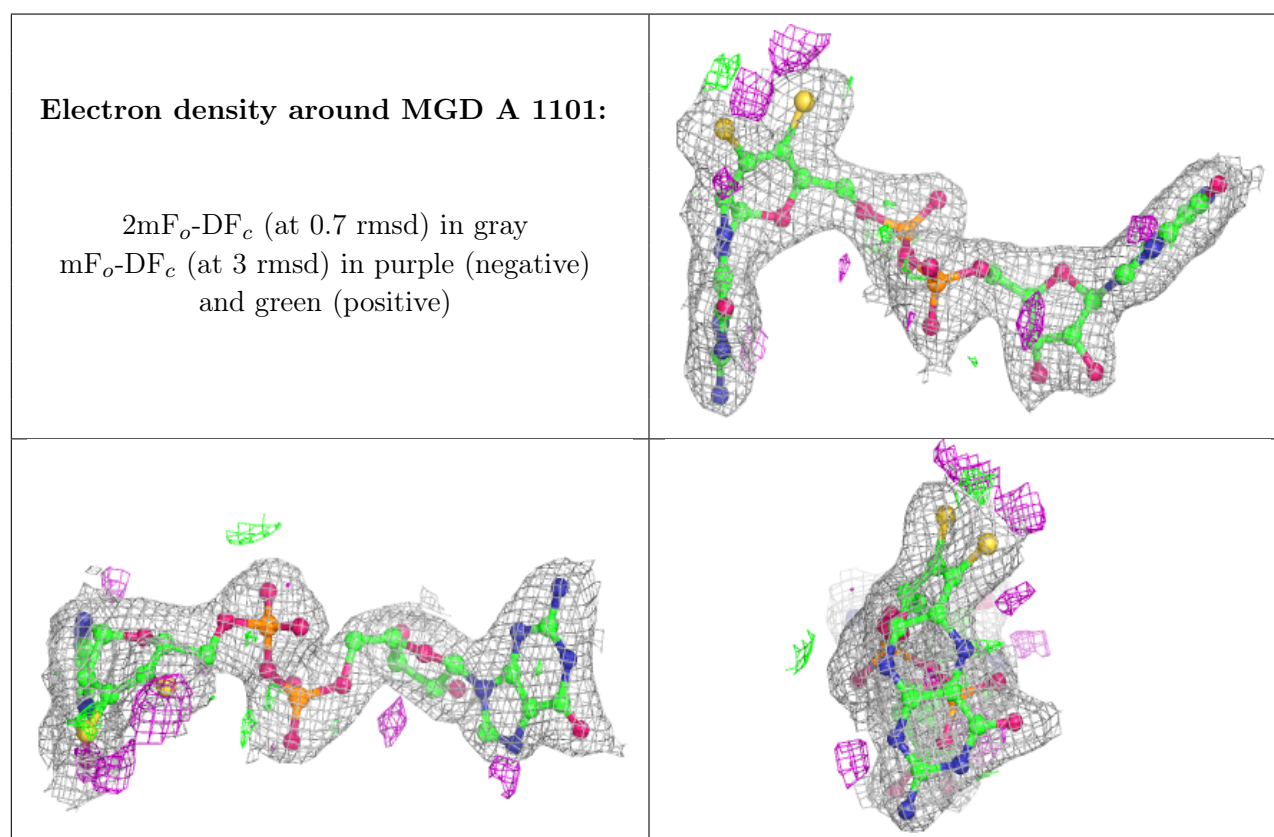
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	1106	6/6	0.81	0.23	64,65,68,69	0
5	GOL	A	1107	6/6	0.89	0.16	57,62,63,64	0
9	PEG	D	304	7/7	0.90	0.28	22,35,46,47	0
8	NO3	B	304	4/4	0.91	0.10	38,45,45,51	0
5	GOL	C	1104	6/6	0.92	0.44	58,60,61,65	0
5	GOL	A	1104	6/6	0.93	0.50	52,57,59,63	0
3	MGD	A	1101	47/47	0.96	0.22	28,31,36,37	0
3	MGD	A	1102	47/47	0.97	0.16	24,35,41,43	0
3	MGD	C	1101	47/47	0.97	0.18	27,32,37,40	0
4	SF4	B	303	8/8	0.98	0.04	27,29,31,32	0
4	SF4	C	1103	8/8	0.98	0.11	28,29,31,34	0
3	MGD	C	1102	47/47	0.98	0.17	22,33,39,43	0
4	SF4	B	302	8/8	0.98	0.05	29,30,31,33	0
4	SF4	A	1103	8/8	0.99	0.10	27,29,31,32	0
4	SF4	D	301	8/8	0.99	0.07	26,27,29,30	0
4	SF4	D	302	8/8	0.99	0.05	27,28,30,30	0
7	H2S	A	1108	1/1	0.99	0.22	29,29,29,29	1

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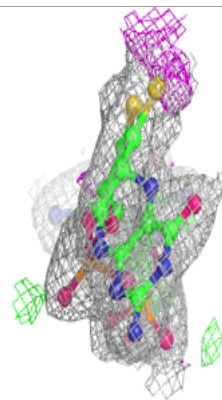
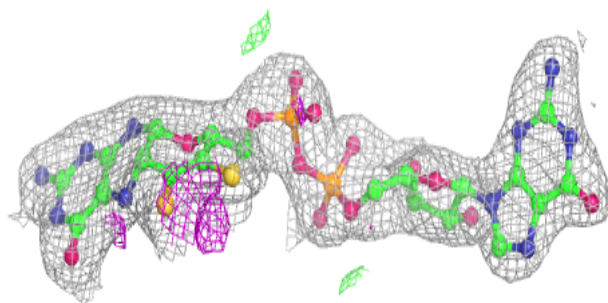
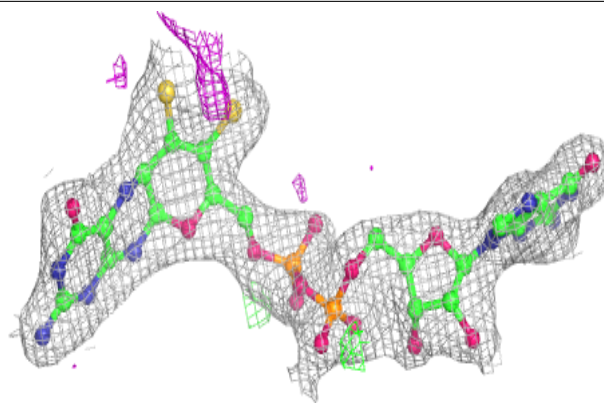
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	H2S	C	1106	1/1	0.99	0.29	30,30,30,30	1
4	SF4	D	303	8/8	0.99	0.06	30,31,34,35	0
4	SF4	B	301	8/8	0.99	0.08	26,26,28,28	0
6	W	A	1105	1/1	1.00	0.07	33,33,33,33	0
6	W	C	1105	1/1	1.00	0.07	34,34,34,34	0

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.

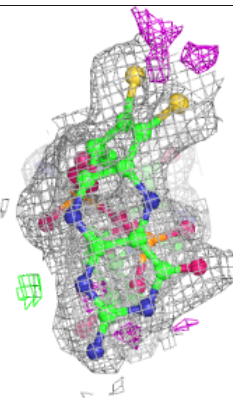
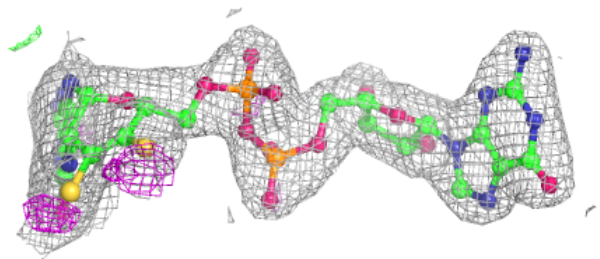
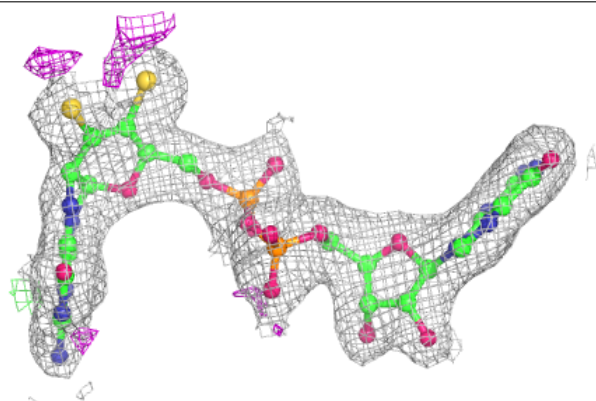


Electron density around MGD A 1102:

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

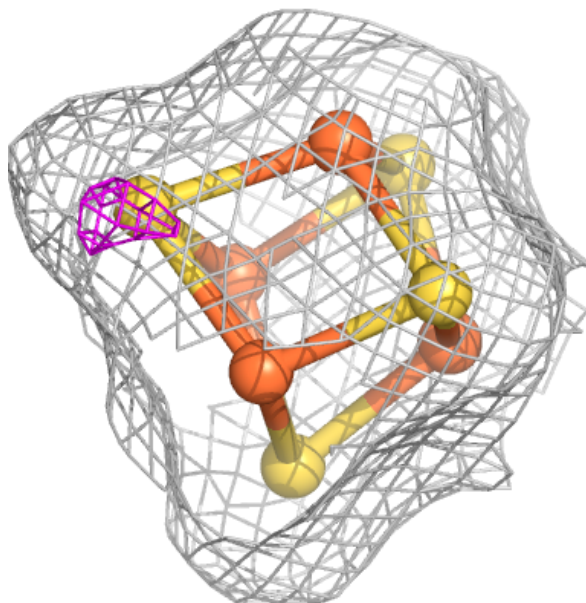
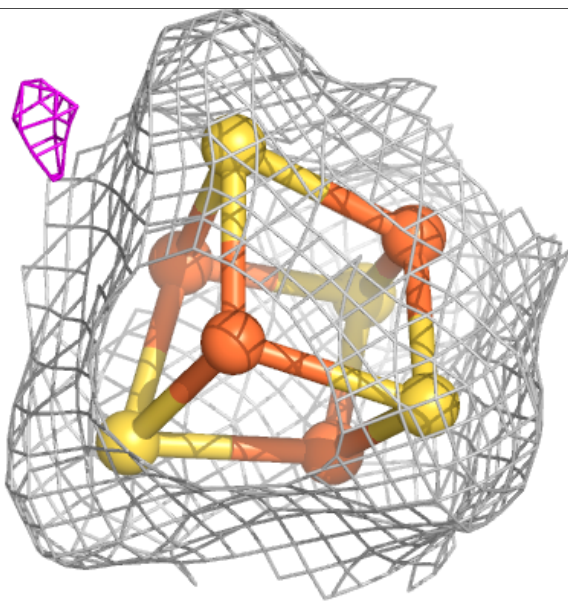
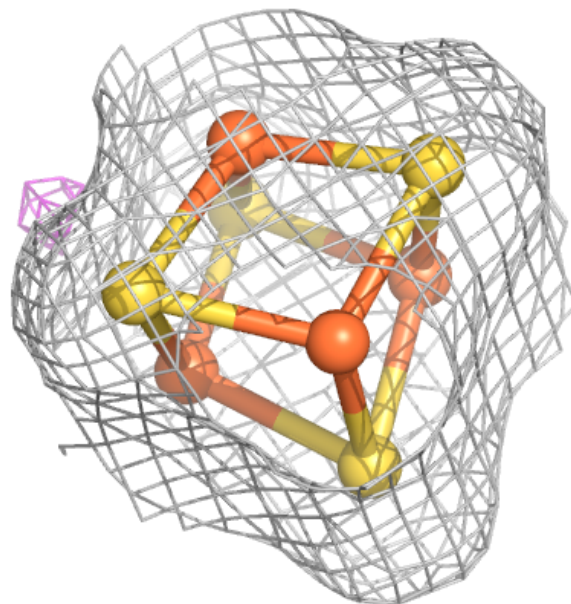
**Electron density around MGD C 1101:**

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



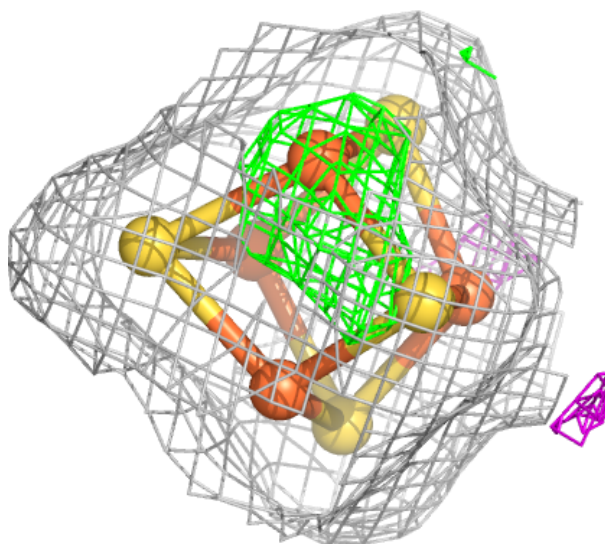
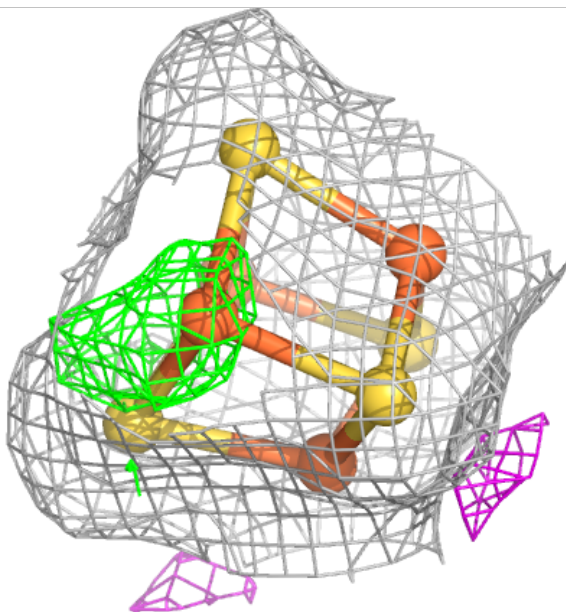
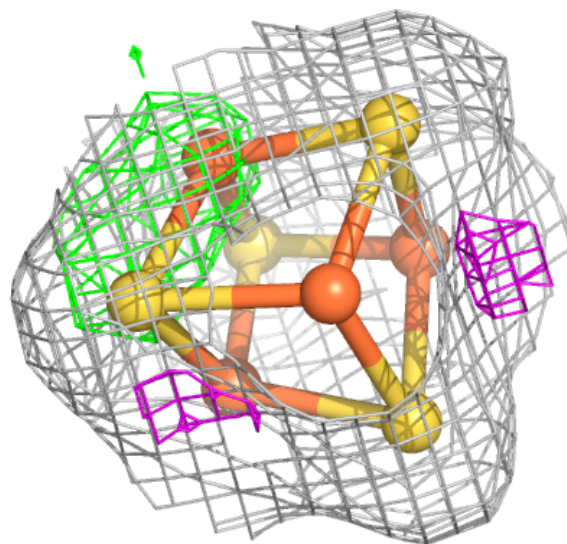
Electron density around SF4 B 303:

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



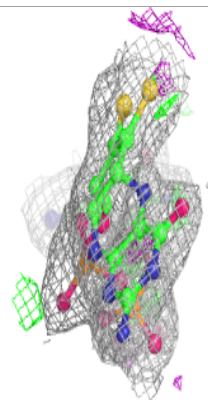
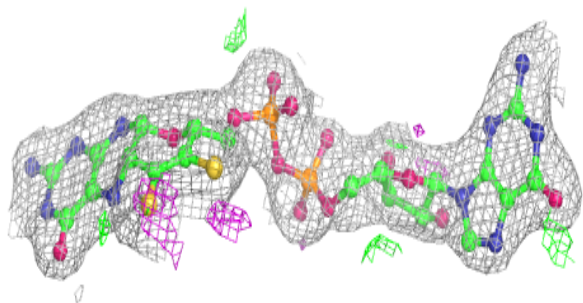
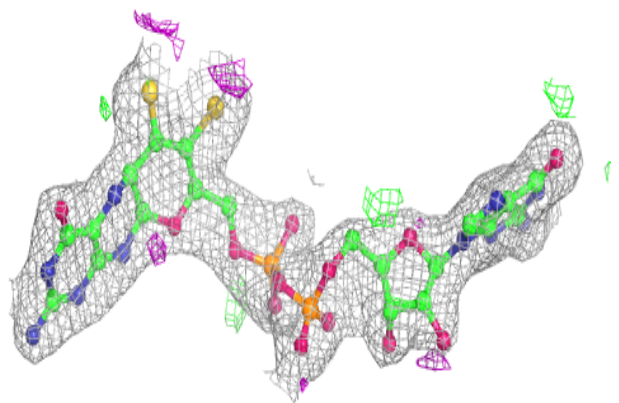
Electron density around SF4 C 1103:

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



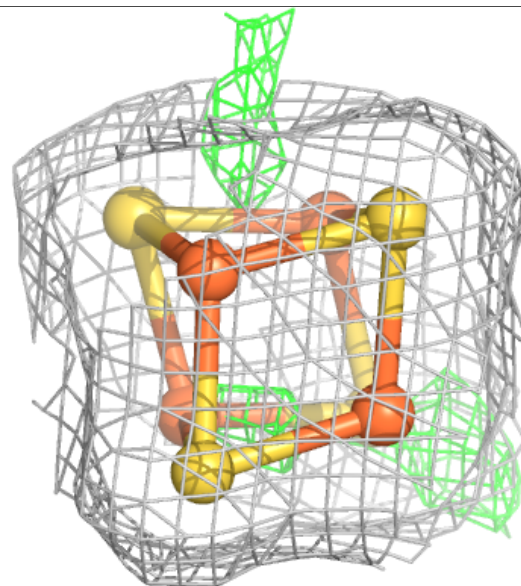
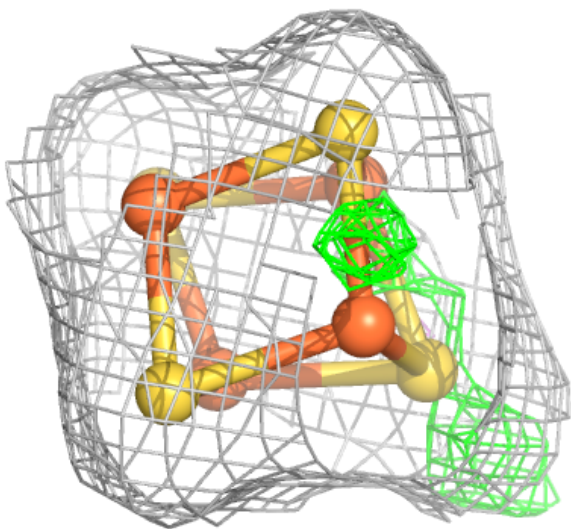
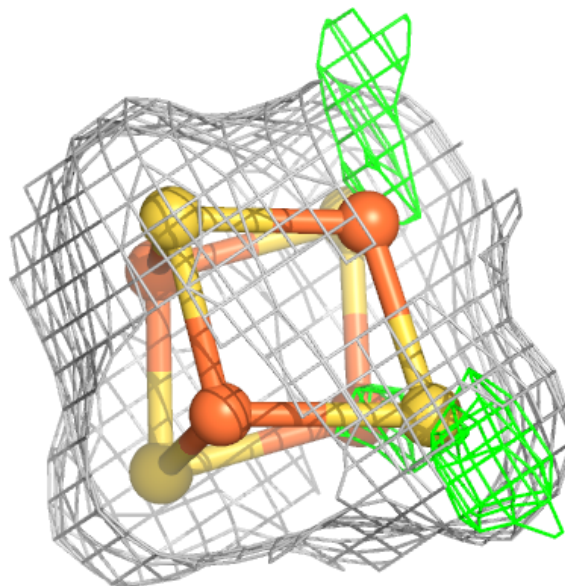
Electron density around MGD C 1102:

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



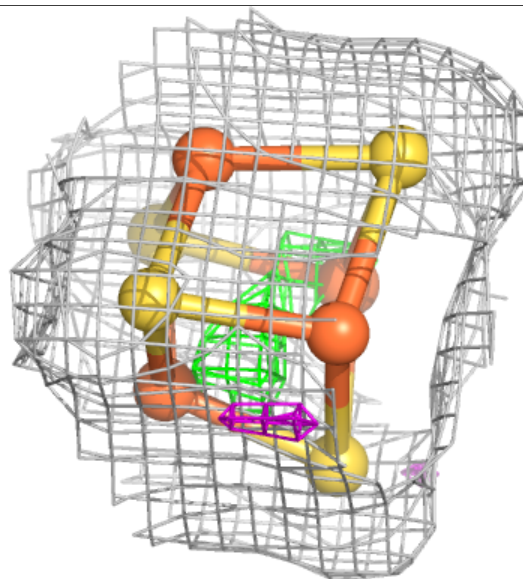
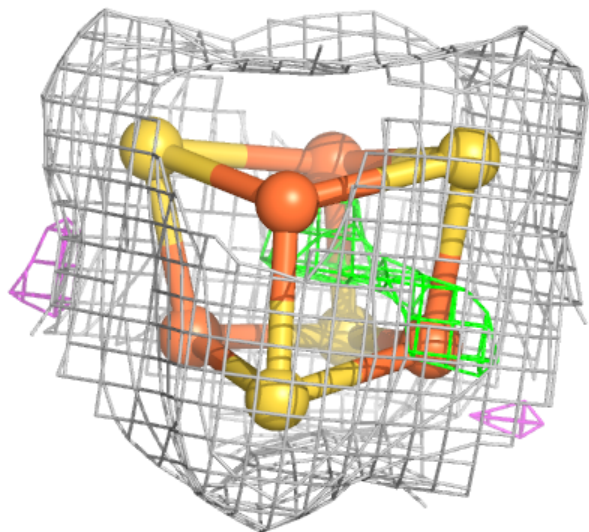
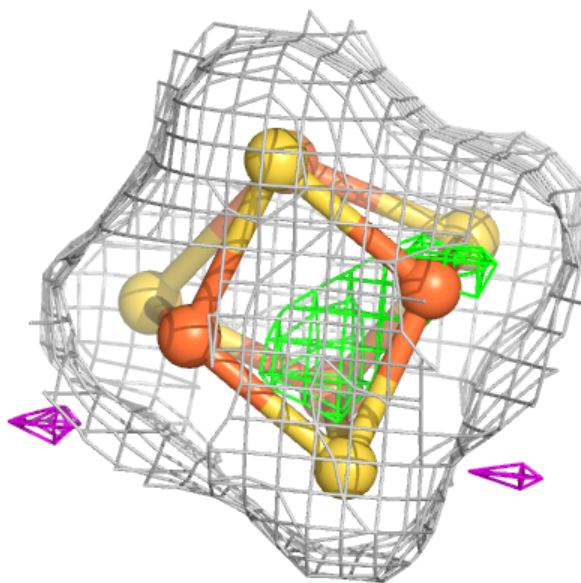
Electron density around SF4 B 302:

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



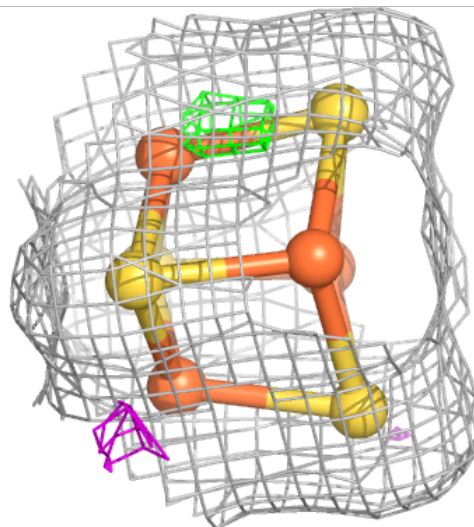
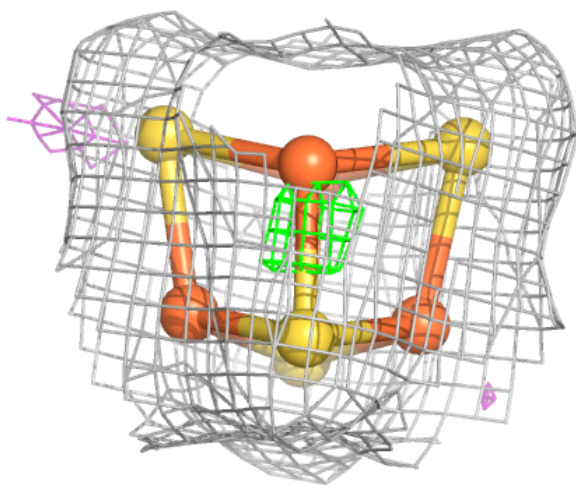
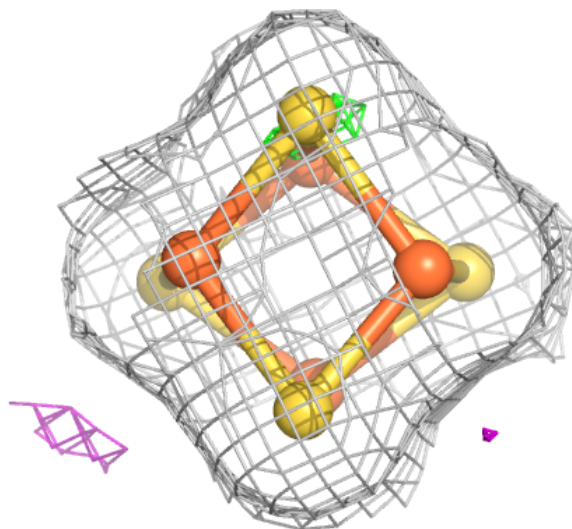
Electron density around SF4 A 1103:

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



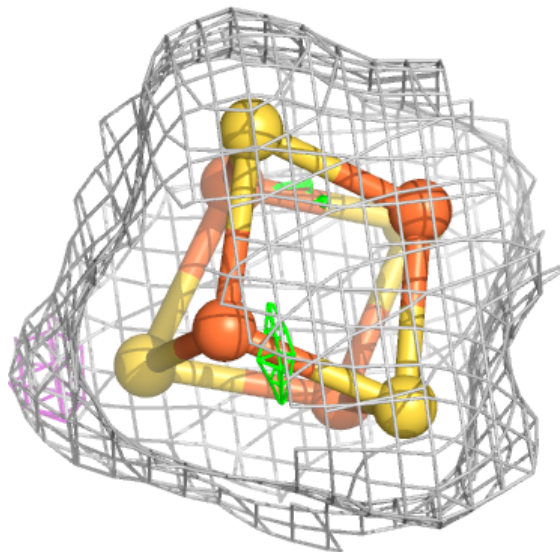
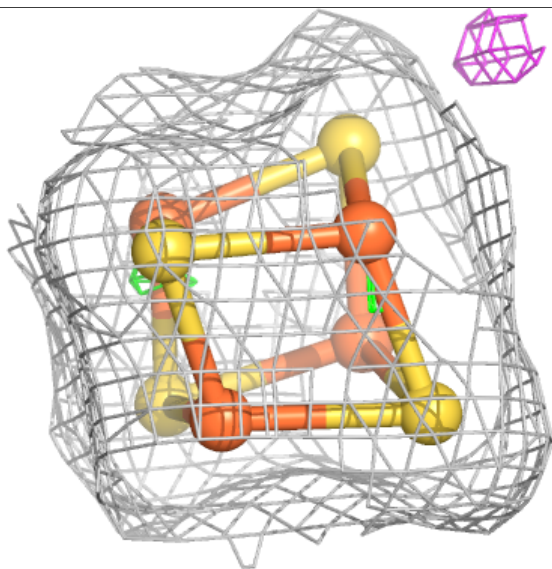
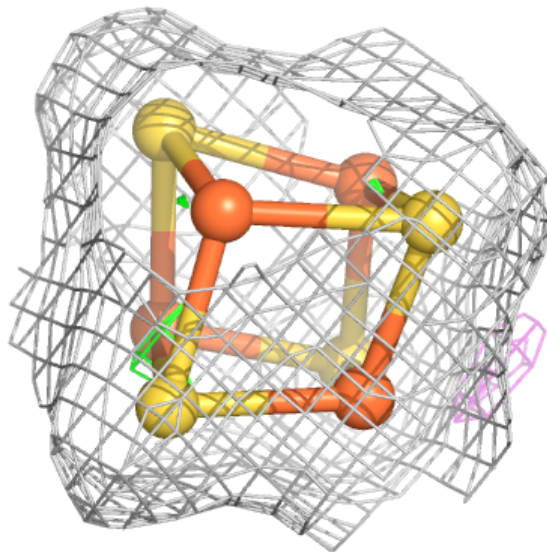
Electron density around SF4 D 301:

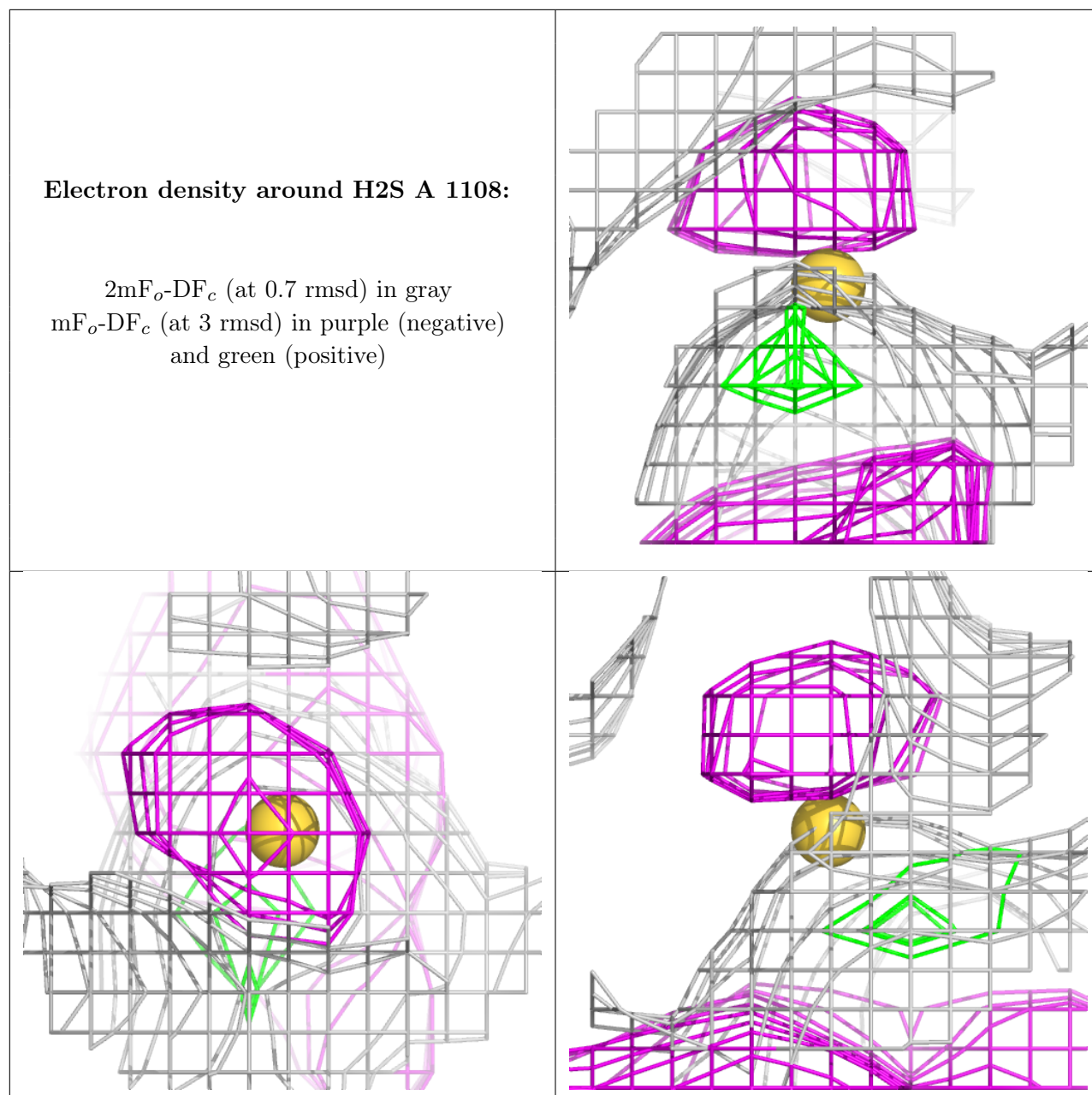
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

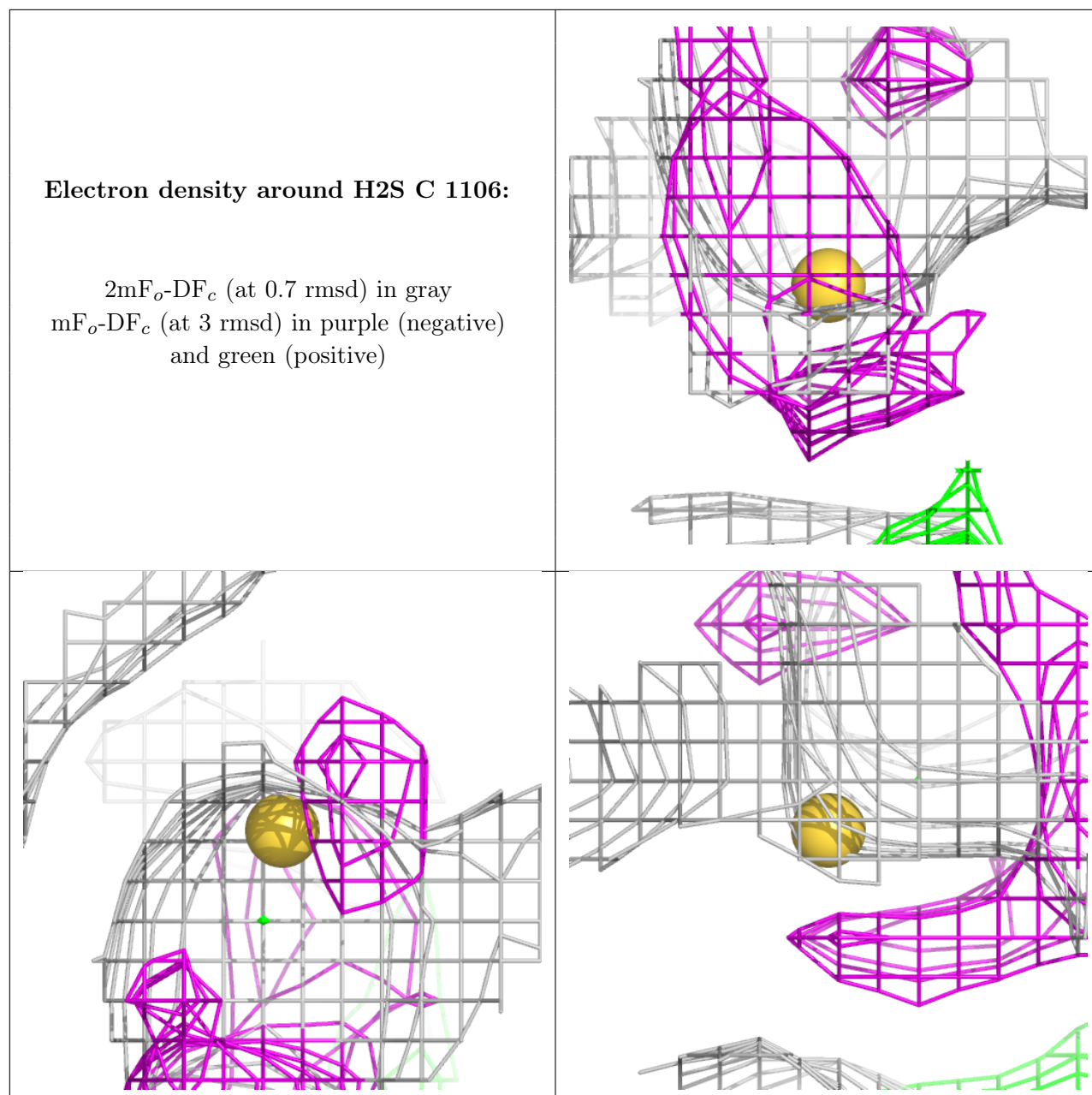


Electron density around SF4 D 302:

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

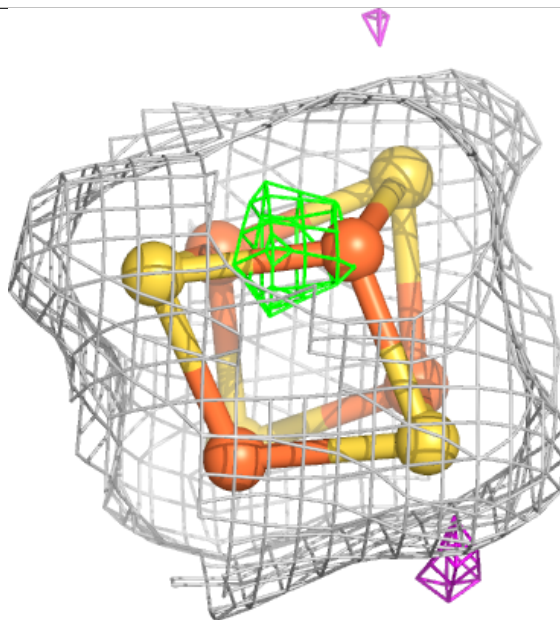
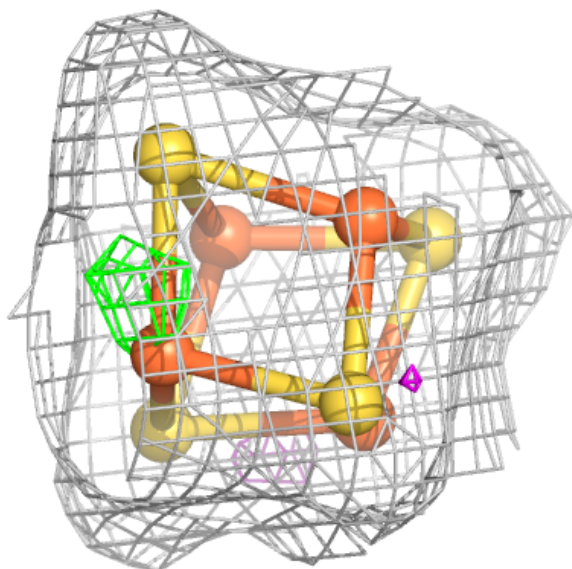
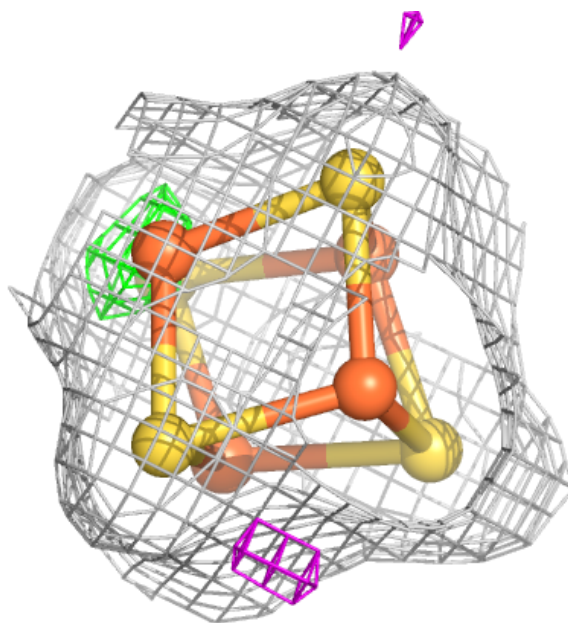






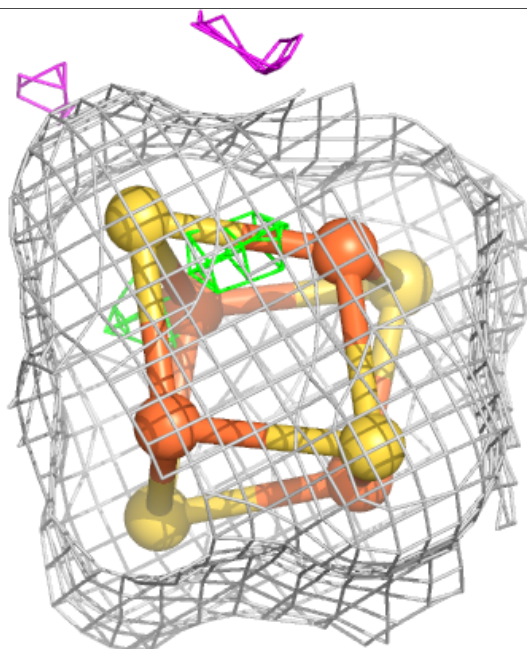
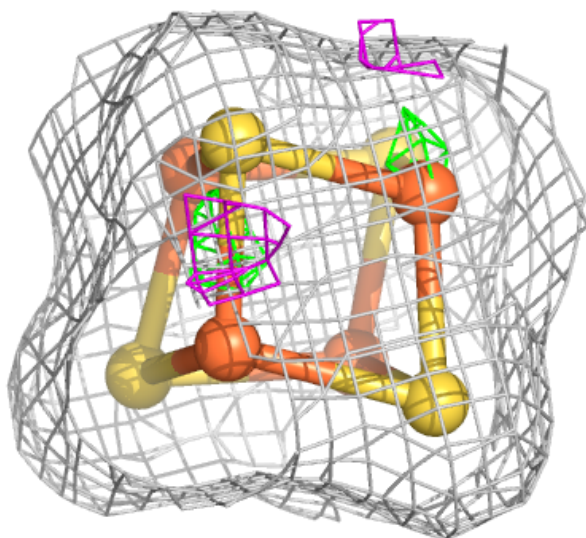
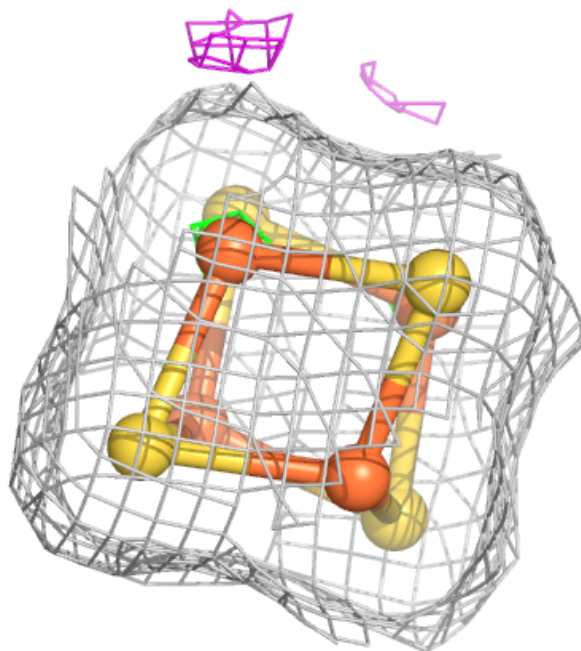
Electron density around SF4 D 303:

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



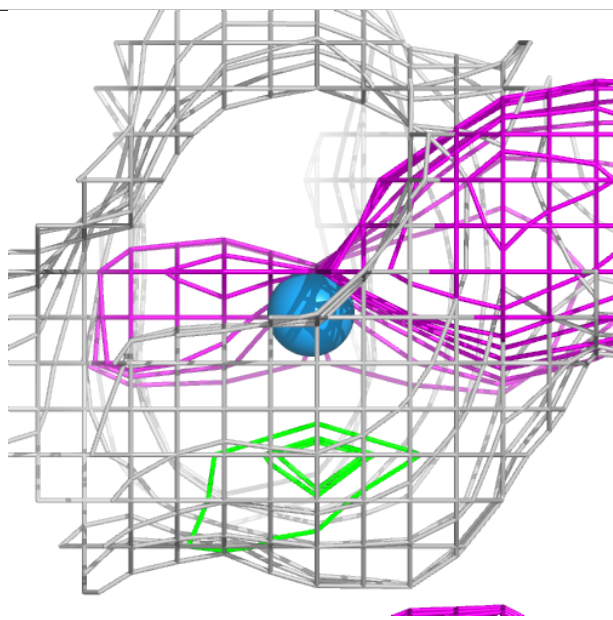
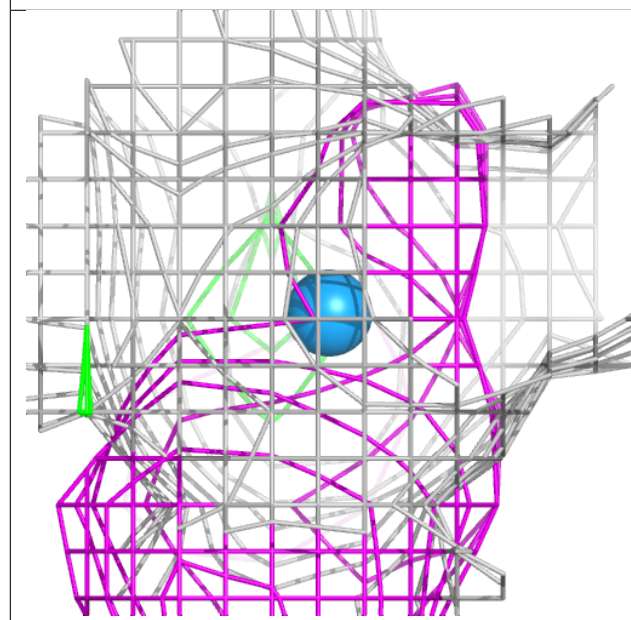
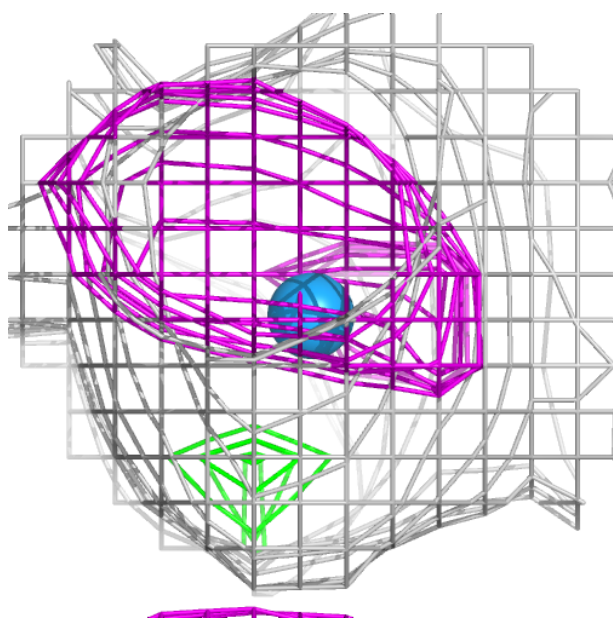
Electron density around SF4 B 301:

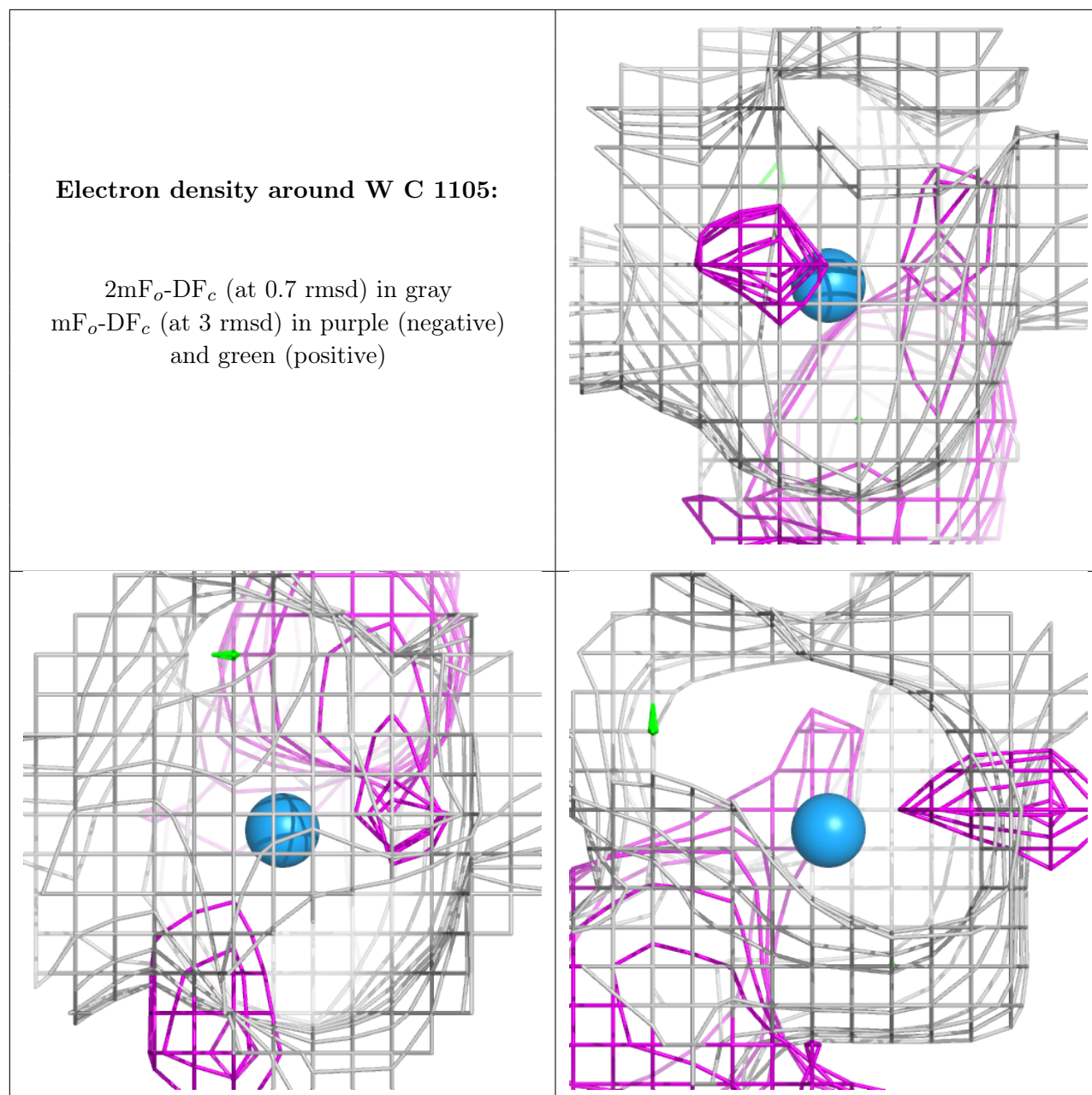
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.