



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:34 PM UTC

PDB ID : 9QM0 / pdb_00009qm0
Title : W-formate dehydrogenase U192C from *Desulfovibrio vulgaris*
Authors : Vilela-Alves, G.; Oliveira, A.R.; Pereira, I.C.; Romao, M.J.; Mota, C.
Deposited on : 2025-03-21
Resolution : 1.83 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

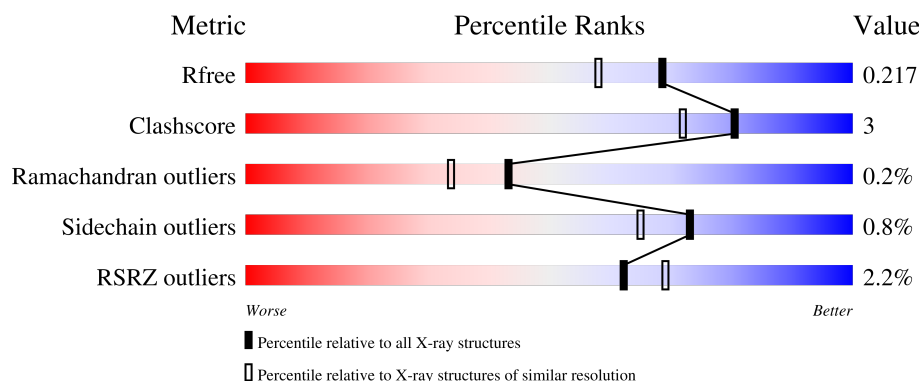
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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
4	EDO	A	1116	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9945 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	970	Total	C	N	O	S	0	2	0
			7605	4846	1325	1392	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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



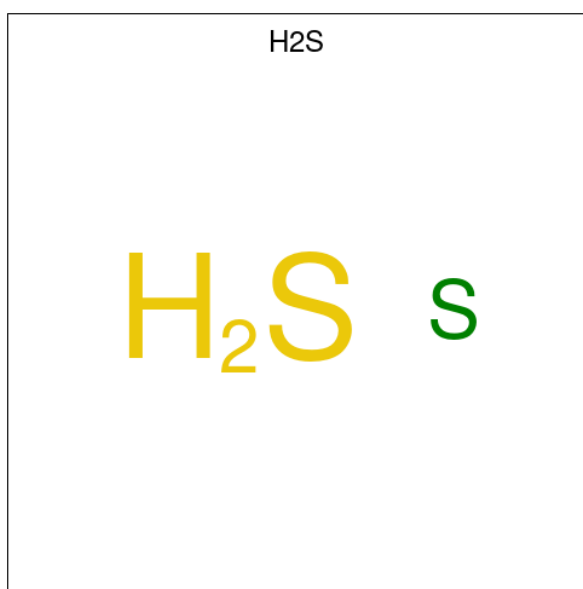
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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



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

- Molecule 6 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).

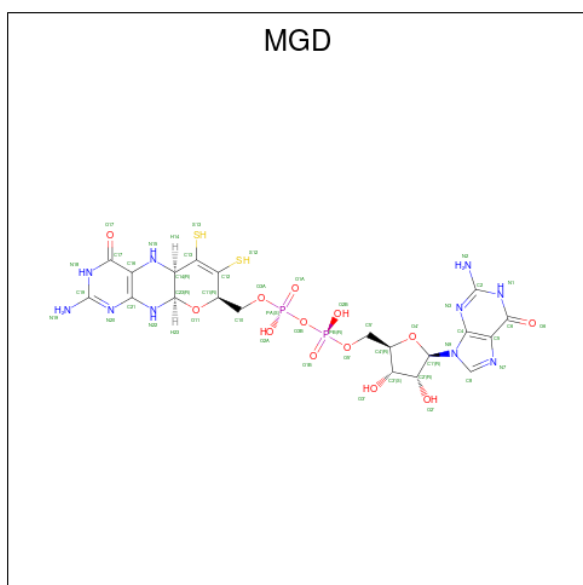


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total S 1 1	0	0

- Molecule 7 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

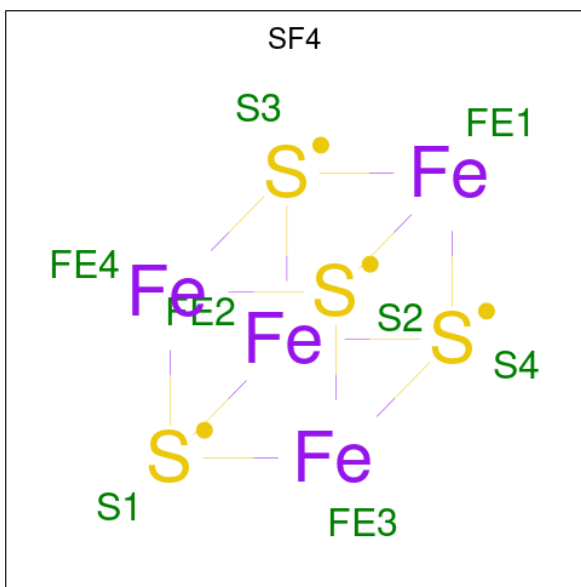
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total W 1 1	0	0

- Molecule 8 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	
8	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
8	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



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

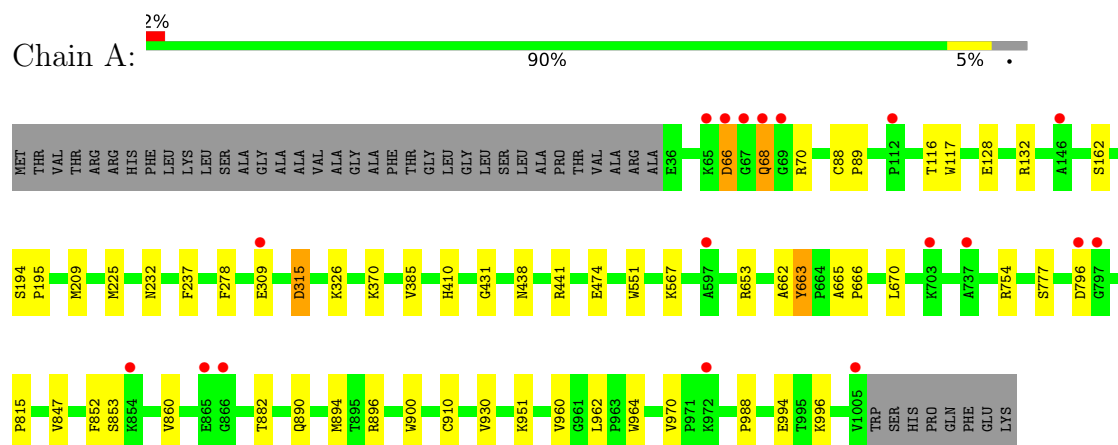
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	351	Total	O	0	0
			351	351		
10	B	80	Total	O	0	0
			80	80		

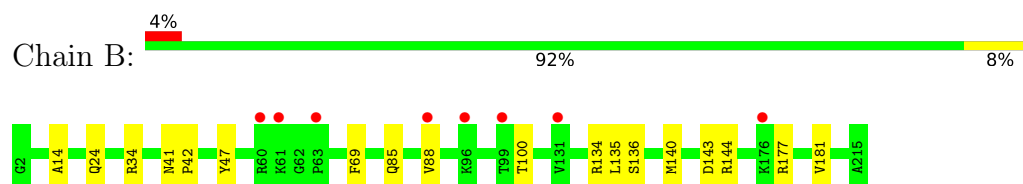
3 Residue-property plots [i](#)

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

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



- 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	62.40Å 123.10Å 147.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.17 – 1.83 63.17 – 1.83	Depositor EDS
% Data completeness (in resolution range)	74.4 (63.17-1.83) 73.3 (63.17-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.213 0.182 , 0.217	Depositor DCC
R_{free} test set	3891 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9945	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: EDO, W, PEG, SF4, MGD, H2S, GOL

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	0/7820	1.30	2/10608 (0.0%)
2	B	0.98	0/1699	1.33	0/2302
All	All	0.98	0/9519	1.31	2/12910 (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	66	ASP	CA-C-N	5.33	126.39	121.86
1	A	66	ASP	C-N-CA	5.33	126.39	121.86

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	7605	0	7445	38	0
2	B	1664	0	1633	11	0
3	A	49	0	70	2	0
4	A	40	0	60	5	0
4	B	16	0	24	3	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	94	0	44	3	0
9	A	8	0	0	0	0
9	B	24	0	0	0	0
10	A	351	0	0	2	0
10	B	80	0	0	0	0
All	All	9945	0	9292	48	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 (48) 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:754:ARG:NH1	10:A:1201:HOH:O	2.15	0.78
2:B:143:ASP:OD1	2:B:144:ARG:N	2.25	0.67
1:A:653:ARG:NH2	1:A:670:LEU:O	2.28	0.67
2:B:177:ARG:HD2	4:B:1704:EDO:C2	2.31	0.60
2:B:134:ARG:NH1	2:B:135:LEU:O	2.36	0.59
1:A:116:THR:HA	4:A:1116:EDO:C2	2.33	0.58
1:A:116:THR:HA	4:A:1116:EDO:H21	1.85	0.58
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.48	0.54
2:B:41:ASN:HA	2:B:42:PRO:C	2.33	0.53
1:A:567:LYS:HE3	3:A:1107:PEG:H31	1.91	0.52
1:A:894:MET:SD	8:A:1122:MGD:H2'	2.50	0.52
1:A:951:LYS:HE2	3:A:1102:PEG:H42	1.92	0.51
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.93	0.50
1:A:474:GLU:HA	4:A:1117:EDO:H22	1.93	0.49
1:A:441[B]:ARG:NH1	10:A:1204:HOH:O	2.45	0.49
2:B:177:ARG:HD2	4:B:1704:EDO:H22	1.96	0.47
1:A:431:GLY:O	1:A:777:SER:HB3	2.13	0.47
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.50	0.46
1:A:128:GLU:O	1:A:132:ARG:HG2	2.17	0.45
1:A:162:SER:HB2	1:A:551:TRP:O	2.17	0.45
1:A:815:PRO:HB3	5:A:1109:GOL:H32	1.99	0.45
1:A:209:MET:HG3	1:A:438:ASN:HA	1.98	0.45
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.52	0.45
1:A:232:ASN:HA	8:A:1121:MGD:N20	2.32	0.44
2:B:85:GLN:O	2:B:88:VAL:HG22	2.18	0.44
1:A:116:THR:HA	4:A:1116:EDO:H22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ALA:HB3	1:A:666:PRO:HD3	1.98	0.44
1:A:860:VAL:O	1:A:988:PRO:HB3	2.17	0.44
1:A:441[A]:ARG:HA	1:A:441[A]:ARG:HD2	1.81	0.43
1:A:410:HIS:HA	1:A:994:GLU:HG3	2.01	0.43
1:A:225:MET:HE1	1:A:278:PHE:CD1	2.53	0.43
1:A:194:SER:N	1:A:195:PRO:CD	2.81	0.42
1:A:662:ALA:O	1:A:663:TYR:C	2.62	0.42
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.54	0.42
1:A:930:VAL:HG11	1:A:962:LEU:HD11	2.02	0.42
2:B:181:VAL:CG2	4:B:1704:EDO:H21	2.50	0.42
1:A:896:ARG:HD2	1:A:970:VAL:O	2.20	0.42
1:A:278:PHE:HZ	1:A:385:VAL:HG11	1.84	0.42
1:A:996:LYS:HD2	8:A:1121:MGD:C8	2.49	0.41
1:A:88:CYS:CB	1:A:89:PRO:HD2	2.50	0.41
1:A:68:GLN:H	1:A:68:GLN:HG3	1.61	0.41
2:B:47:TYR:HA	2:B:136:SER:OG	2.20	0.41
1:A:117:TRP:H	4:A:1116:EDO:H22	1.85	0.41
1:A:315:ASP:C	1:A:853:SER:HB2	2.45	0.41
2:B:100:THR:HB	2:B:140:MET:HE1	2.03	0.40
1:A:370:LYS:HD2	1:A:852:PHE:CE1	2.57	0.40
1:A:68:GLN:HB2	1:A:70:ARG:HG2	2.04	0.40
1:A:882:THR:HA	1:A:962:LEU:O	2.21	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%)	939 (97%)	29 (3%)	2 (0%)	43	34
2	B	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
All	All	1182/1227 (96%)	1141 (96%)	39 (3%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	796	ASP
1	A	663	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	791/820 (96%)	784 (99%)	7 (1%)	70	60
2	B	185/185 (100%)	184 (100%)	1 (0%)	81	75
All	All	976/1005 (97%)	968 (99%)	8 (1%)	73	65

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	68	GLN
1	A	237	PHE
1	A	309	GLU
1	A	315	ASP
1	A	326	LYS
1	A	847	VAL
2	B	34	ARG

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

Mol	Chain	Res	Type
1	A	340	ASN
1	A	381	GLN
1	A	383	GLN
1	A	857	HIS
1	A	973	ASN
2	B	194	ASN
2	B	212	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 29 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	$\# Z > 2$
9	SF4	B	1707	2	0,12,12	-	-	-		
4	EDO	A	1110	-	3,3,3	0.08	0	2,2,2	0.18	0
5	GOL	A	1109	-	5,5,5	0.10	0	5,5,5	0.17	0
3	PEG	A	1104	-	6,6,6	0.19	0	5,5,5	0.10	0
8	MGD	A	1122	7	47,52,52	0.77	2 (4%)	58,81,81	1.01	4 (6%)
3	PEG	A	1101	-	6,6,6	0.28	0	5,5,5	0.23	0
4	EDO	A	1118	-	3,3,3	0.07	0	2,2,2	0.18	0
4	EDO	A	1108	-	3,3,3	0.09	0	2,2,2	0.22	0
3	PEG	A	1102	-	6,6,6	0.17	0	5,5,5	0.10	0
4	EDO	A	1113	-	3,3,3	0.10	0	2,2,2	0.14	0
4	EDO	A	1114	-	3,3,3	0.12	0	2,2,2	0.18	0
4	EDO	B	1703	-	3,3,3	0.07	0	2,2,2	0.13	0
4	EDO	A	1117	-	3,3,3	0.06	0	2,2,2	0.17	0
9	SF4	B	1708	2	0,12,12	-	-	-		
3	PEG	A	1105	-	6,6,6	0.16	0	5,5,5	0.07	0
3	PEG	A	1107	-	6,6,6	0.15	0	5,5,5	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1704	-	3,3,3	0.11	0	2,2,2	0.23	0
4	EDO	A	1111	-	3,3,3	0.07	0	2,2,2	0.04	0
4	EDO	A	1116	-	3,3,3	0.15	0	2,2,2	0.28	0
5	GOL	B	1701	-	5,5,5	0.10	0	5,5,5	0.30	0
8	MGD	A	1121	7	47,52,52	0.50	0	58,81,81	1.03	4 (6%)
9	SF4	B	1706	2	0,12,12	-	-	-	-	-
3	PEG	A	1103	-	6,6,6	0.16	0	5,5,5	0.08	0
9	SF4	A	1123	1	0,12,12	-	-	-	-	-
3	PEG	A	1106	-	6,6,6	0.17	0	5,5,5	0.09	0
4	EDO	A	1115	-	3,3,3	0.03	0	2,2,2	0.25	0
4	EDO	B	1705	-	3,3,3	0.03	0	2,2,2	0.15	0
4	EDO	A	1112	-	3,3,3	0.09	0	2,2,2	0.11	0
4	EDO	B	1702	-	3,3,3	0.08	0	2,2,2	0.08	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
9	SF4	B	1707	2	-	-	0/6/5/5
4	EDO	A	1110	-	-	0/1/1/1	-
5	GOL	A	1109	-	-	2/4/4/4	-
3	PEG	A	1104	-	-	1/4/4/4	-
8	MGD	A	1122	7	-	3/22/66/66	0/6/6/6
3	PEG	A	1101	-	-	2/4/4/4	-
4	EDO	A	1118	-	-	0/1/1/1	-
4	EDO	A	1108	-	-	0/1/1/1	-
3	PEG	A	1102	-	-	2/4/4/4	-
4	EDO	A	1113	-	-	0/1/1/1	-
4	EDO	A	1114	-	-	1/1/1/1	-
4	EDO	B	1703	-	-	1/1/1/1	-
4	EDO	A	1117	-	-	1/1/1/1	-
9	SF4	B	1708	2	-	-	0/6/5/5
3	PEG	A	1105	-	-	1/4/4/4	-
3	PEG	A	1107	-	-	2/4/4/4	-
4	EDO	B	1704	-	-	1/1/1/1	-
4	EDO	A	1111	-	-	1/1/1/1	-
4	EDO	A	1116	-	-	1/1/1/1	-
5	GOL	B	1701	-	-	2/4/4/4	-
8	MGD	A	1121	7	-	3/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	1706	2	-	-	0/6/5/5
3	PEG	A	1103	-	-	3/4/4/4	-
9	SF4	A	1123	1	-	-	0/6/5/5
3	PEG	A	1106	-	-	3/4/4/4	-
4	EDO	A	1115	-	-	0/1/1/1	-
4	EDO	B	1705	-	-	0/1/1/1	-
4	EDO	A	1112	-	-	1/1/1/1	-
4	EDO	B	1702	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1122	MGD	C23-C14	3.27	1.56	1.53
8	A	1122	MGD	PA-O3B	2.21	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1122	MGD	O11-C23-C14	3.21	111.10	108.96
8	A	1122	MGD	C19-N20-C21	3.00	118.66	113.36
8	A	1121	MGD	C19-N20-C21	2.98	118.61	113.36
8	A	1121	MGD	O11-C23-N22	2.89	111.23	108.61
8	A	1121	MGD	C23-C14-N15	2.86	110.67	107.87
8	A	1122	MGD	C17-C16-N15	2.33	122.62	116.27
8	A	1122	MGD	C23-C14-N15	2.17	109.99	107.87
8	A	1121	MGD	C17-C16-N15	2.07	121.92	116.27

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1122	MGD	C4'-C5'-O5'-PB
3	A	1103	PEG	O2-C3-C4-O4
5	A	1109	GOL	O1-C1-C2-O2
8	A	1122	MGD	O4'-C4'-C5'-O5'
3	A	1102	PEG	O2-C3-C4-O4
3	A	1105	PEG	O2-C3-C4-O4
3	A	1106	PEG	O2-C3-C4-O4
3	A	1107	PEG	O2-C3-C4-O4
5	A	1109	GOL	O1-C1-C2-C3
5	B	1701	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	1701	GOL	O2-C2-C3-O3
3	A	1101	PEG	O1-C1-C2-O2
4	A	1116	EDO	O1-C1-C2-O2
3	A	1102	PEG	O1-C1-C2-O2
4	A	1111	EDO	O1-C1-C2-O2
4	A	1114	EDO	O1-C1-C2-O2
4	B	1702	EDO	O1-C1-C2-O2
4	B	1703	EDO	O1-C1-C2-O2
4	B	1704	EDO	O1-C1-C2-O2
8	A	1122	MGD	C3'-C4'-C5'-O5'
4	A	1112	EDO	O1-C1-C2-O2
8	A	1121	MGD	PA-O3B-PB-O5'
3	A	1101	PEG	C1-C2-O2-C3
3	A	1106	PEG	O1-C1-C2-O2
3	A	1104	PEG	C4-C3-O2-C2
3	A	1107	PEG	C4-C3-O2-C2
3	A	1103	PEG	C4-C3-O2-C2
4	A	1117	EDO	O1-C1-C2-O2
3	A	1106	PEG	C4-C3-O2-C2
3	A	1103	PEG	O1-C1-C2-O2
8	A	1121	MGD	PA-O3B-PB-O1B
8	A	1121	MGD	PA-O3B-PB-O2B

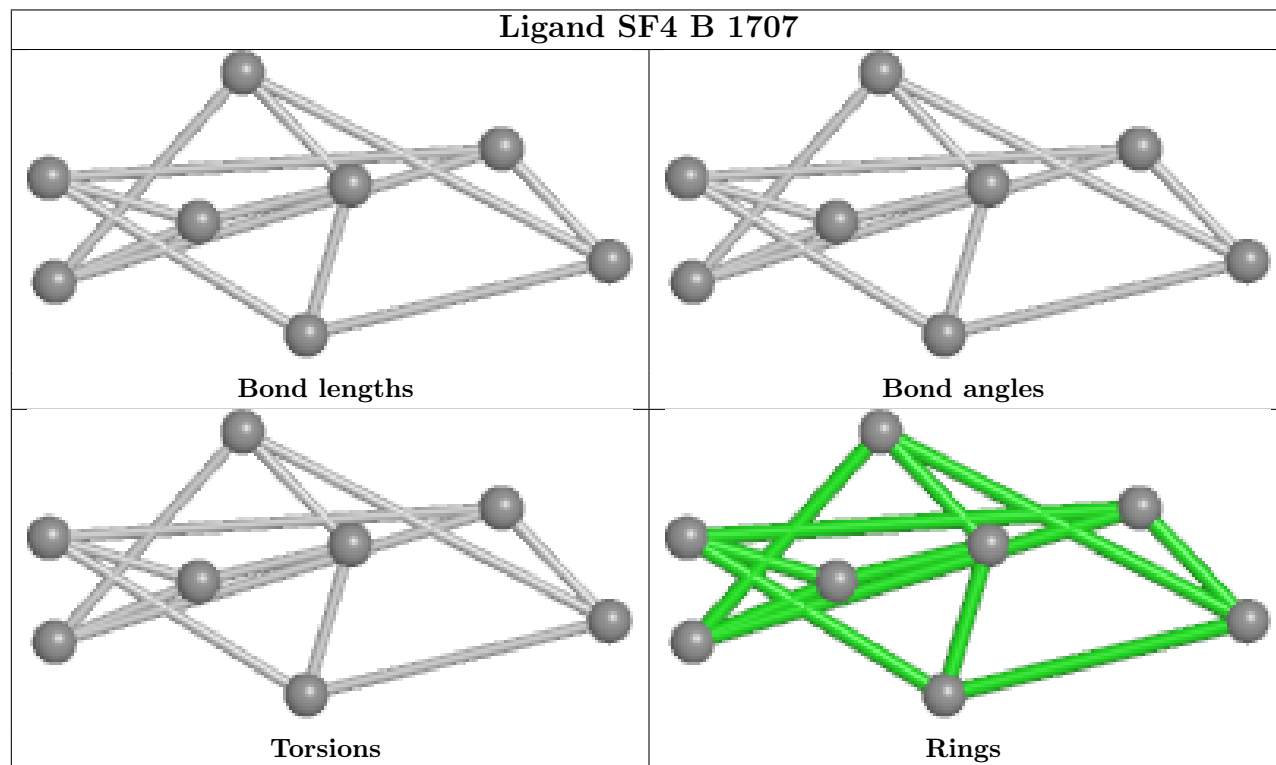
There are no ring outliers.

8 monomers are involved in 14 short contacts:

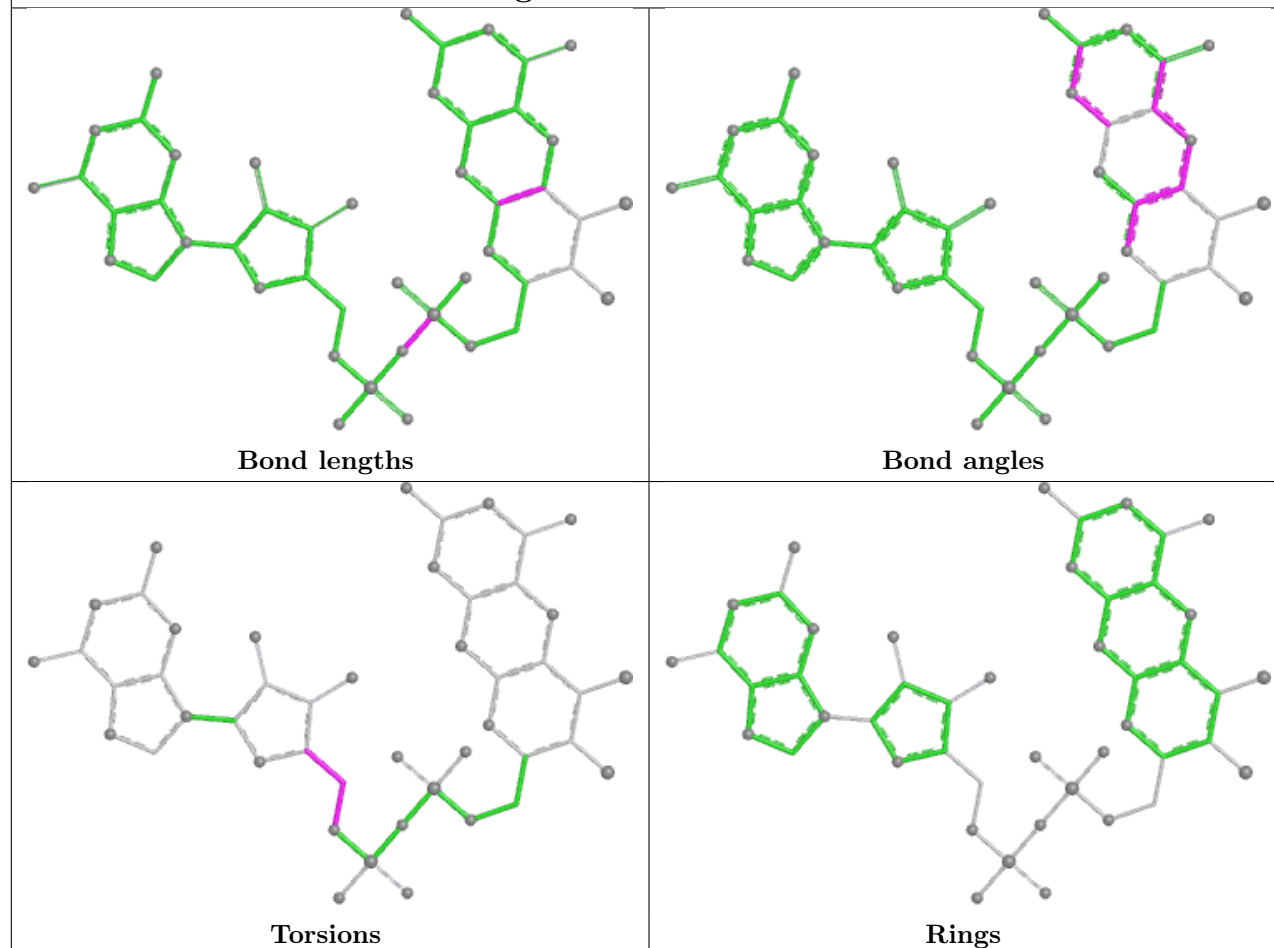
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1109	GOL	1	0
8	A	1122	MGD	1	0
3	A	1102	PEG	1	0
4	A	1117	EDO	1	0
3	A	1107	PEG	1	0
4	B	1704	EDO	3	0
4	A	1116	EDO	4	0
8	A	1121	MGD	2	0

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

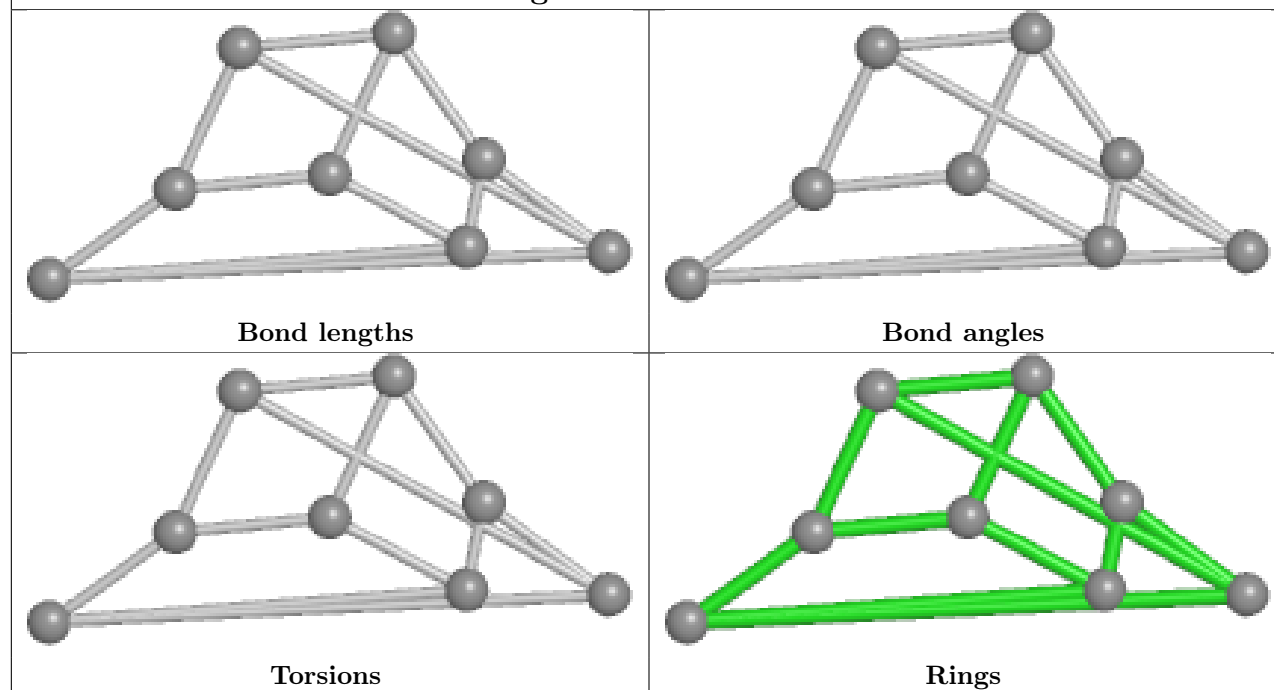
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



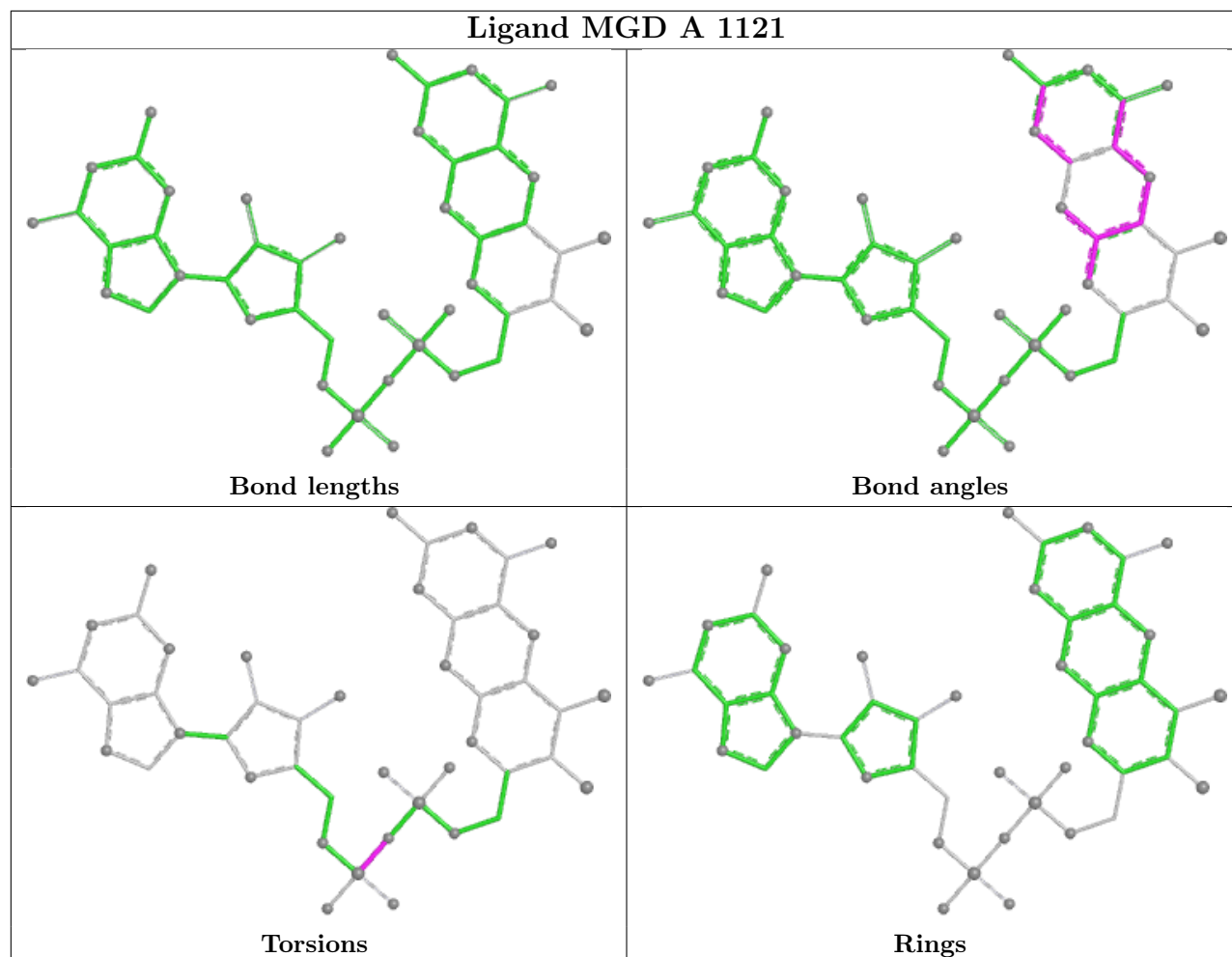
Ligand MGD A 1122

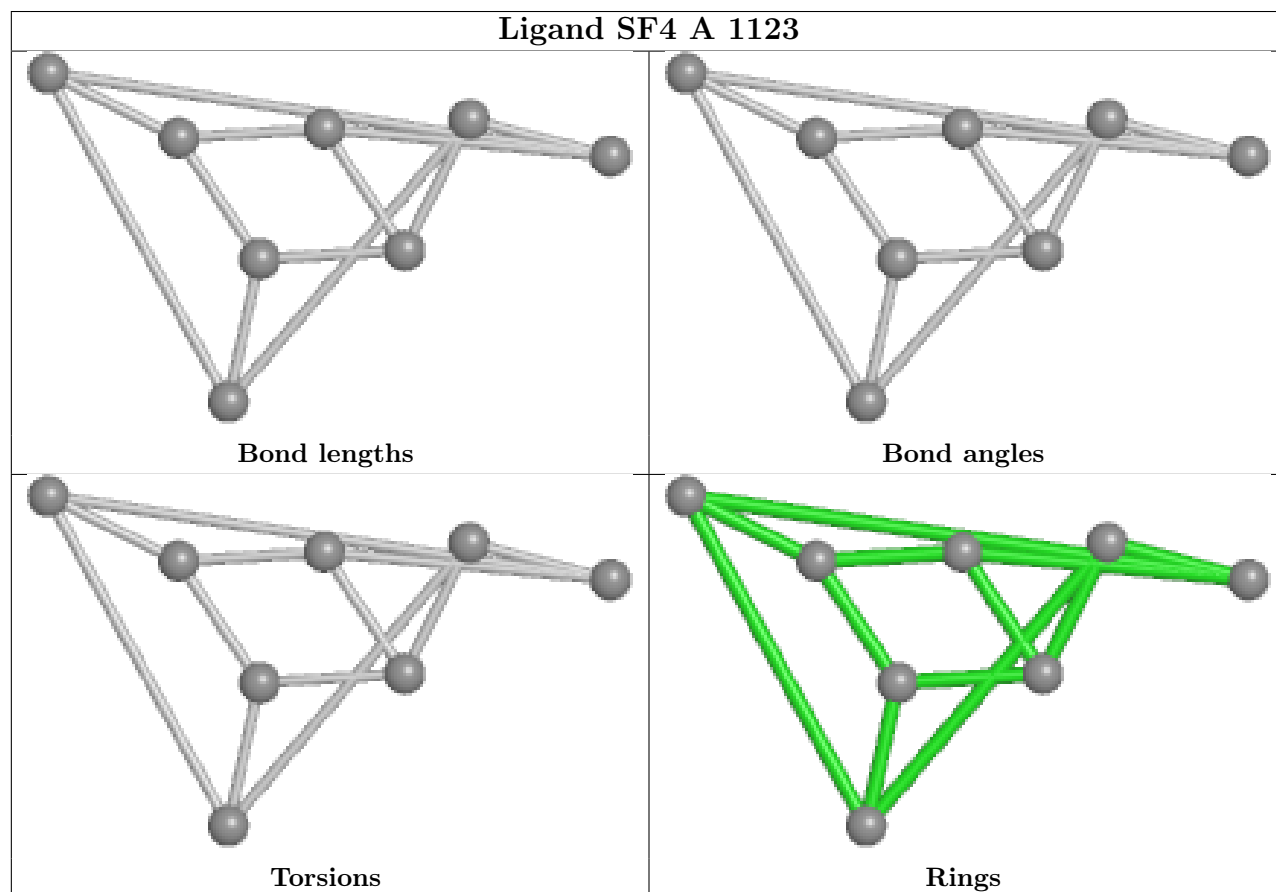
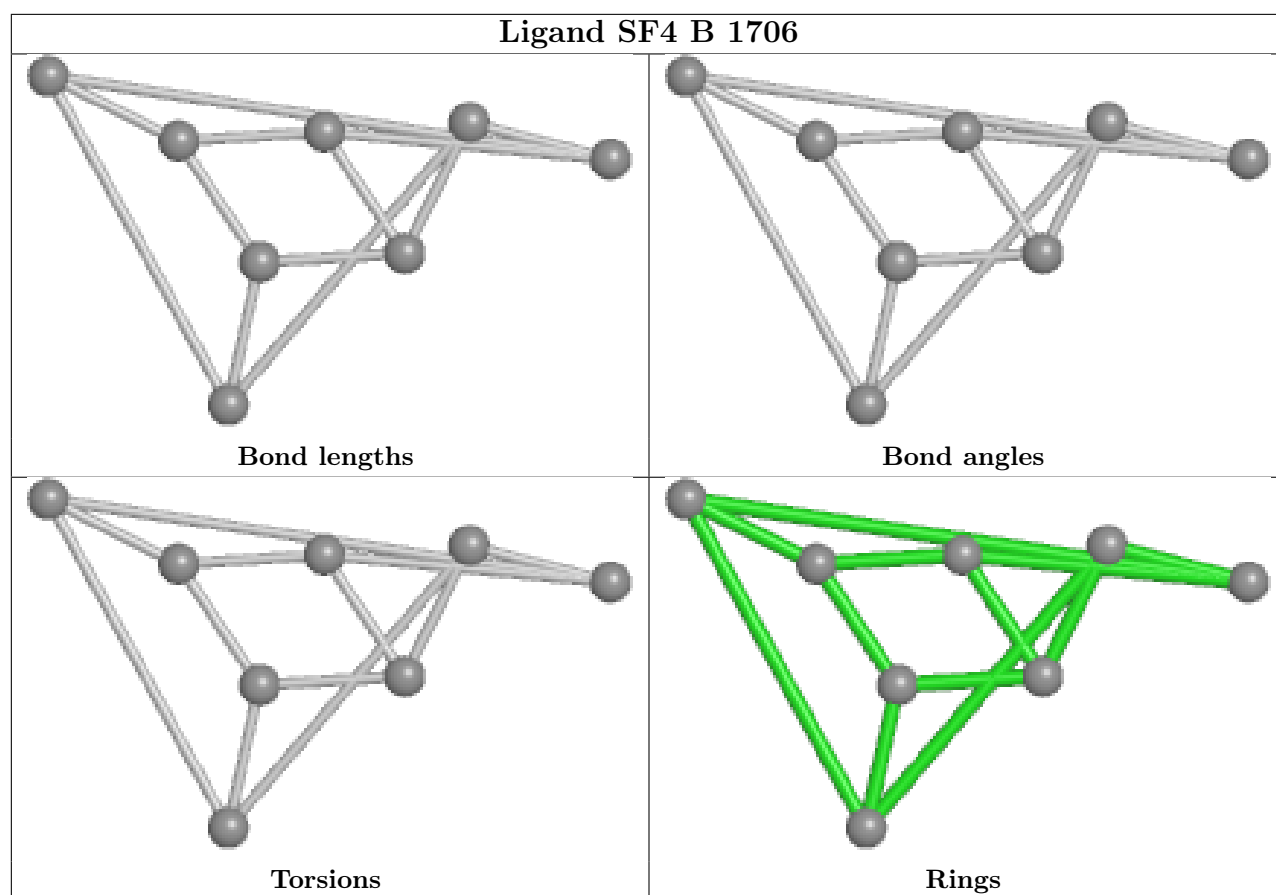


Ligand SF4 B 1708



Ligand MGD A 1121





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	970/1013 (95%)	0.17	18 (1%) 66 73	10, 24, 44, 96	2 (0%)
2	B	214/214 (100%)	0.28	8 (3%) 45 48	15, 24, 47, 66	0
All	All	1184/1227 (96%)	0.19	26 (2%) 62 69	10, 24, 45, 96	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	ASP	3.8
1	A	67	GLY	3.5
2	B	88	VAL	3.4
2	B	131	VAL	3.4
1	A	146	ALA	3.4
1	A	68	GLN	3.2
2	B	63	PRO	3.1
1	A	1005	VAL	3.0
1	A	796	ASP	3.0
1	A	69	GLY	2.8
2	B	96	LYS	2.7
1	A	866	GLY	2.6
1	A	865	GLU	2.5
1	A	854	LYS	2.5
2	B	61	LYS	2.5
1	A	65	LYS	2.4
1	A	703	LYS	2.4
1	A	597	ALA	2.3
1	A	309	GLU	2.3
1	A	737	ALA	2.2
2	B	176	LYS	2.1
1	A	797	GLY	2.1
2	B	99	THR	2.1
1	A	112	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	972	LYS	2.0
2	B	60	ARG	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	1111	4/4	0.68	0.18	54,59,60,64	0
3	PEG	A	1101	7/7	0.75	0.17	28,32,37,47	0
4	EDO	A	1117	4/4	0.75	0.19	42,45,47,51	0
4	EDO	B	1703	4/4	0.78	0.17	47,50,52,58	0
3	PEG	A	1107	7/7	0.79	0.15	42,47,49,50	0
3	PEG	A	1105	7/7	0.79	0.18	48,55,62,64	0
4	EDO	B	1702	4/4	0.82	0.14	36,45,46,50	0
4	EDO	A	1116	4/4	0.83	0.18	43,49,52,66	0
4	EDO	A	1112	4/4	0.84	0.12	39,43,46,51	0
4	EDO	A	1115	4/4	0.84	0.14	41,42,43,48	0
4	EDO	A	1108	4/4	0.84	0.12	36,36,38,38	0
4	EDO	B	1704	4/4	0.84	0.18	35,37,42,44	0
3	PEG	A	1104	7/7	0.85	0.15	39,44,54,56	0
4	EDO	A	1113	4/4	0.85	0.16	41,43,50,52	0
4	EDO	A	1114	4/4	0.85	0.14	49,50,55,55	0
4	EDO	B	1705	4/4	0.85	0.14	40,40,46,51	0
5	GOL	A	1109	6/6	0.85	0.22	51,53,63,71	0
5	GOL	B	1701	6/6	0.85	0.20	52,58,65,75	0
3	PEG	A	1102	7/7	0.86	0.12	38,41,44,48	0
4	EDO	A	1118	4/4	0.86	0.15	40,41,42,47	0
3	PEG	A	1103	7/7	0.87	0.12	37,44,48,54	0

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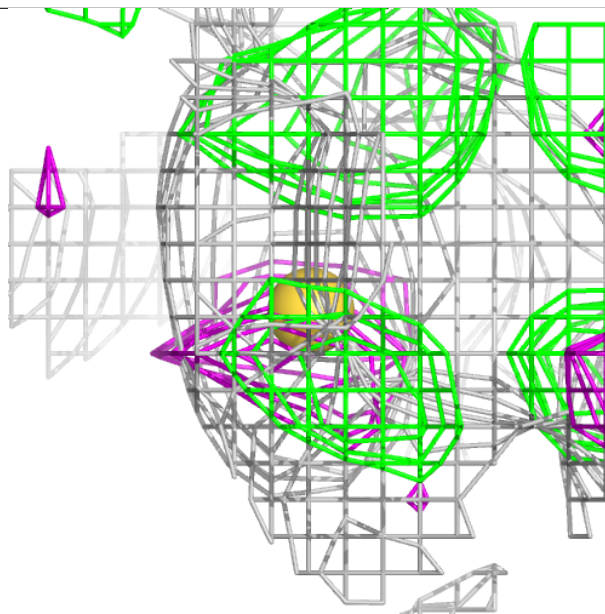
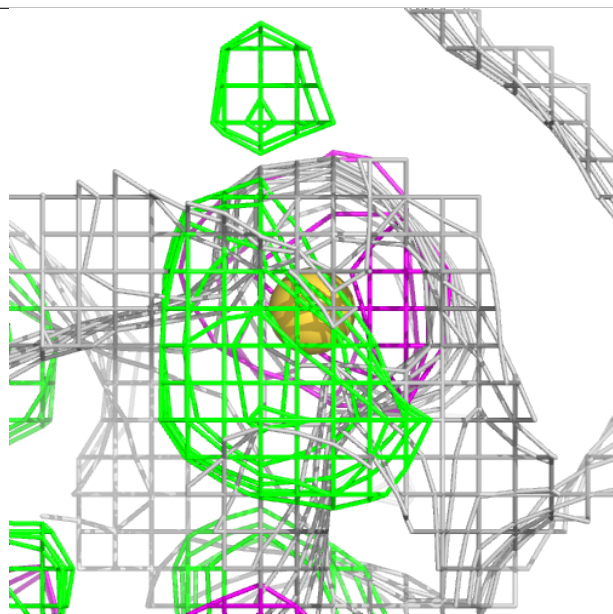
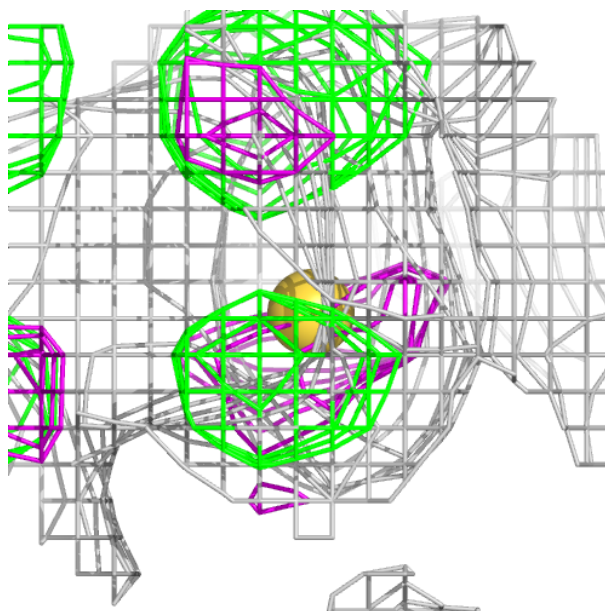
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	1106	7/7	0.87	0.14	37,41,46,46	0
4	EDO	A	1110	4/4	0.90	0.12	41,42,45,47	0
6	H2S	A	1119	1/1	0.93	0.13	23,23,23,23	0
8	MGD	A	1121	47/47	0.97	0.06	13,16,20,23	0
8	MGD	A	1122	47/47	0.97	0.06	14,20,23,25	0
9	SF4	A	1123	8/8	0.99	0.02	15,16,17,17	0
9	SF4	B	1706	8/8	0.99	0.02	15,17,18,20	0
9	SF4	B	1707	8/8	0.99	0.03	19,21,22,23	0
9	SF4	B	1708	8/8	0.99	0.03	18,20,21,24	0
7	W	A	1120	1/1	1.00	0.01	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

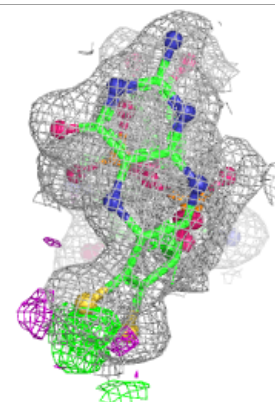
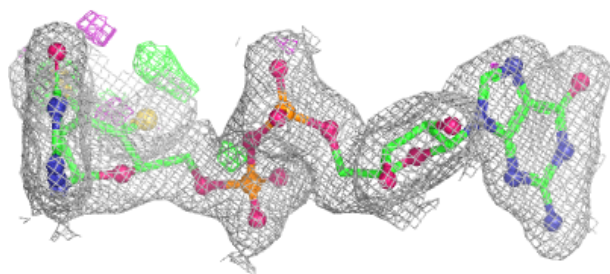
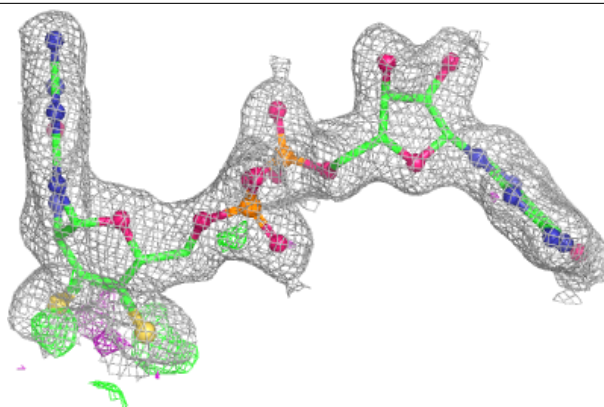
Electron density around H2S A 1119:

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

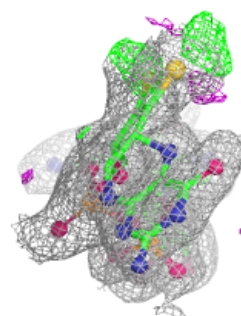
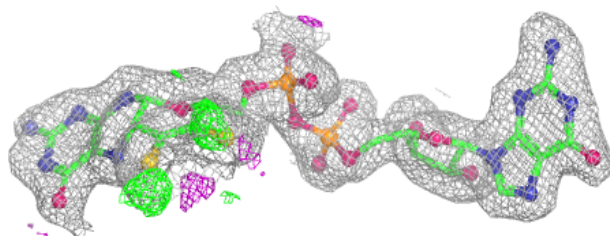
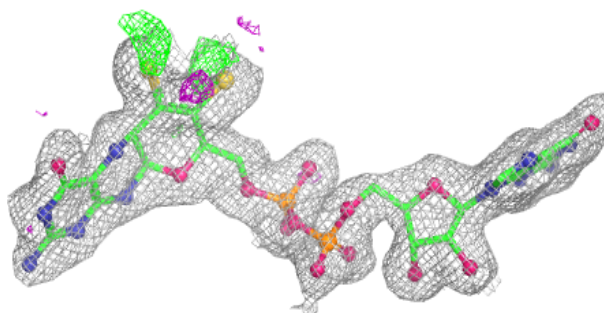


Electron density around MGD A 1121:

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

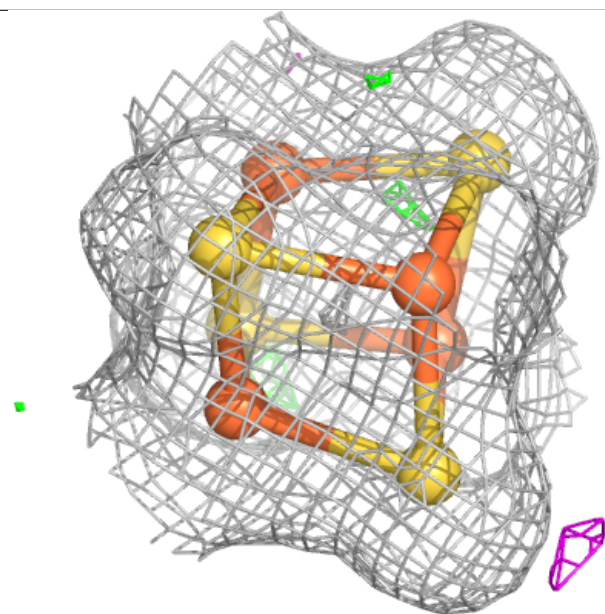
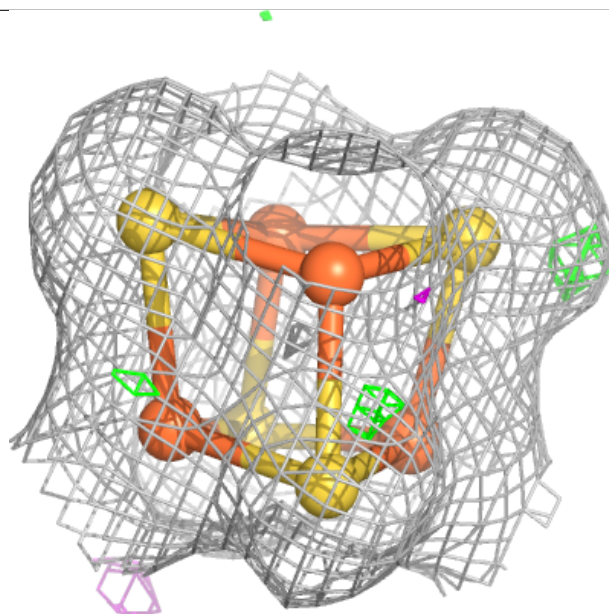
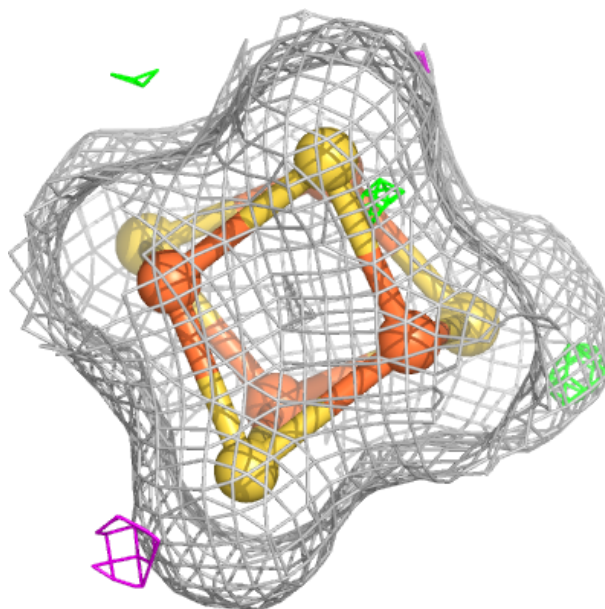
**Electron density around MGD A 1122:**

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



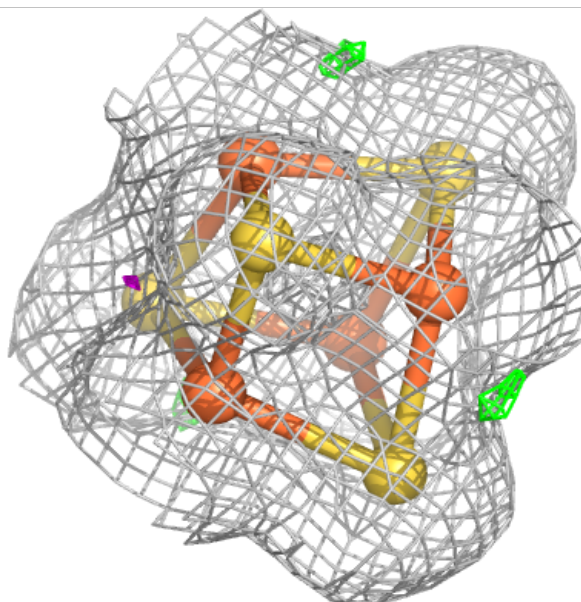
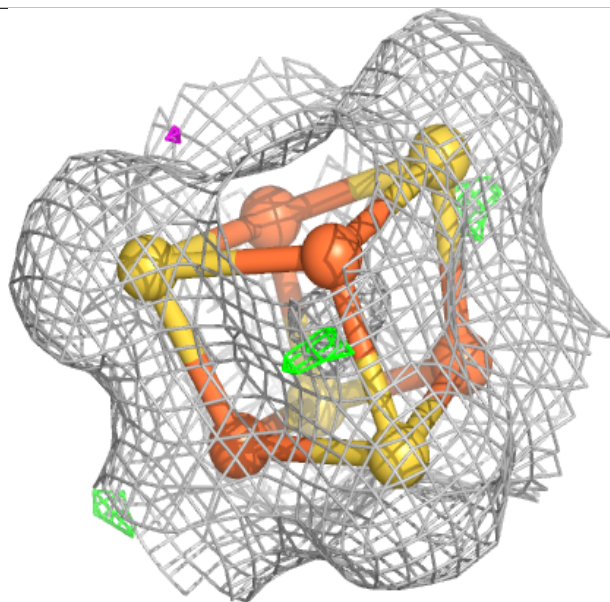
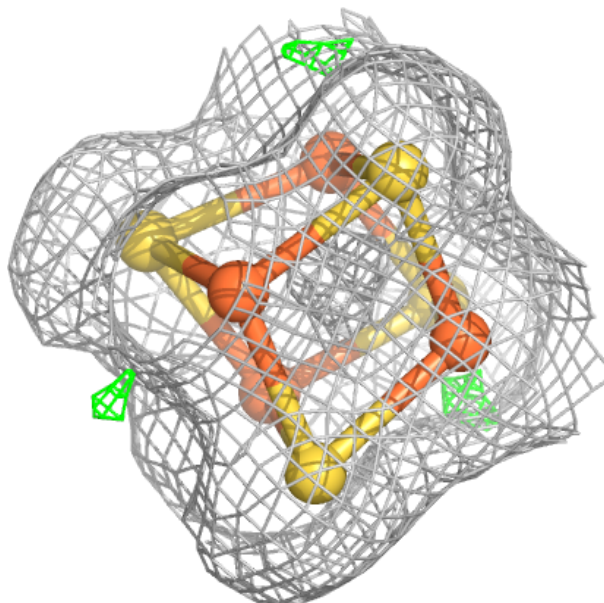
Electron density around SF4 A 1123:

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



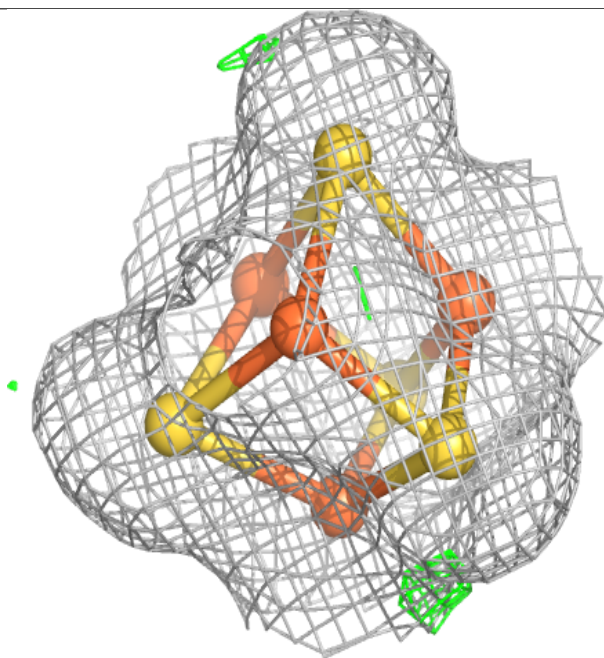
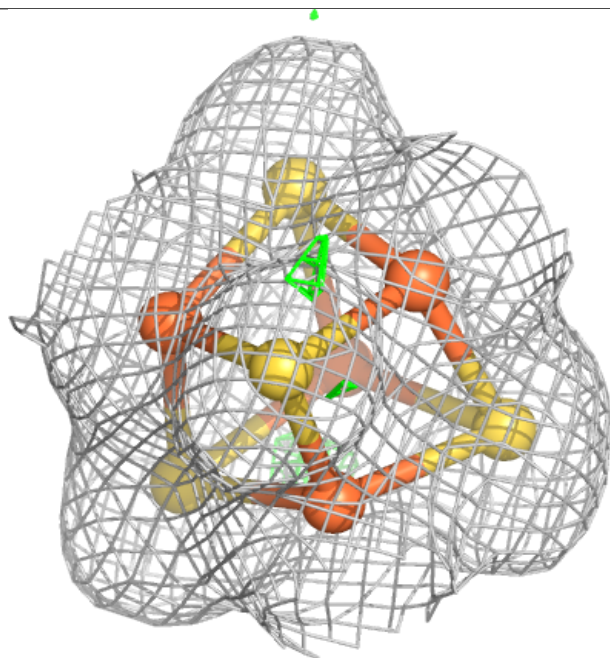
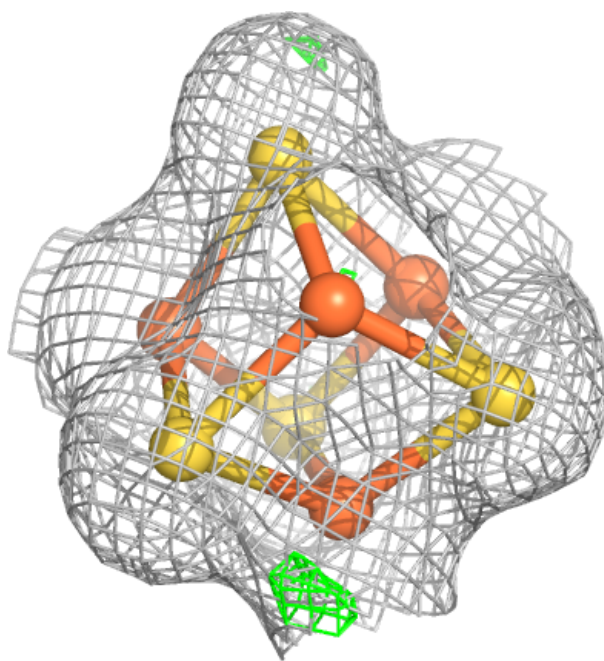
Electron density around SF4 B 1706:

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



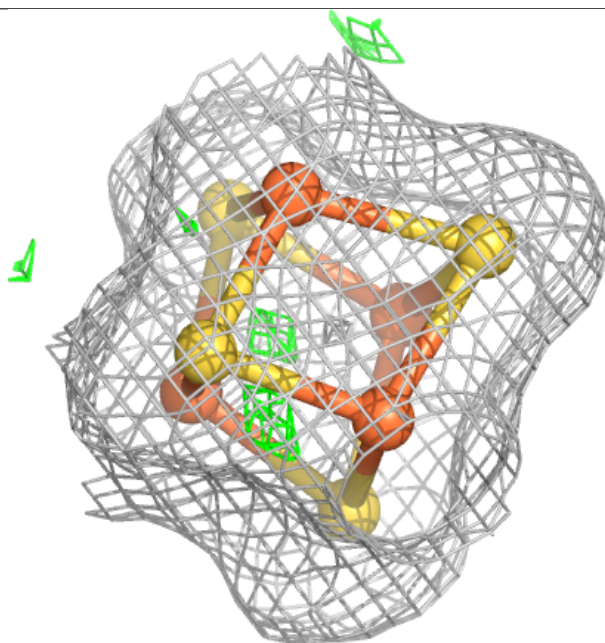
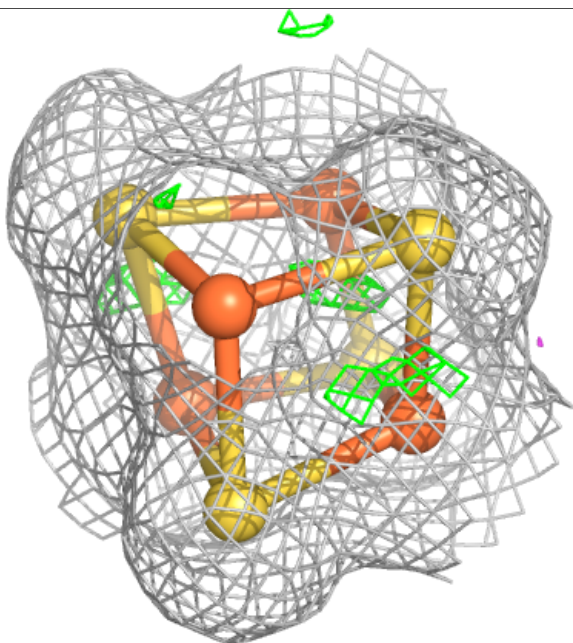
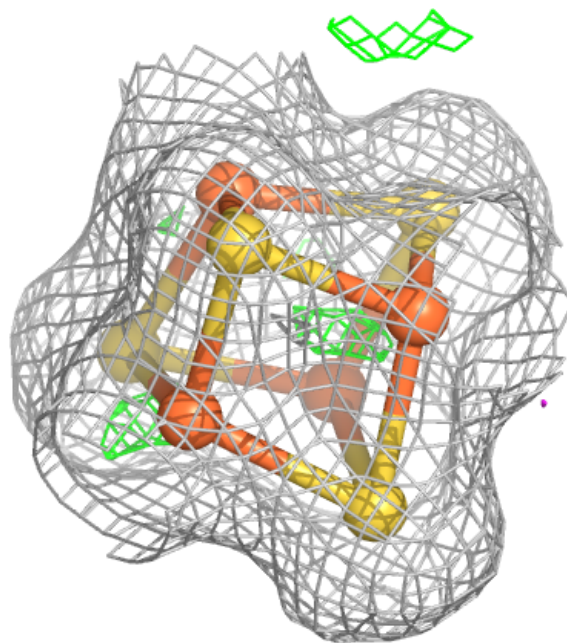
Electron density around SF4 B 1707:

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



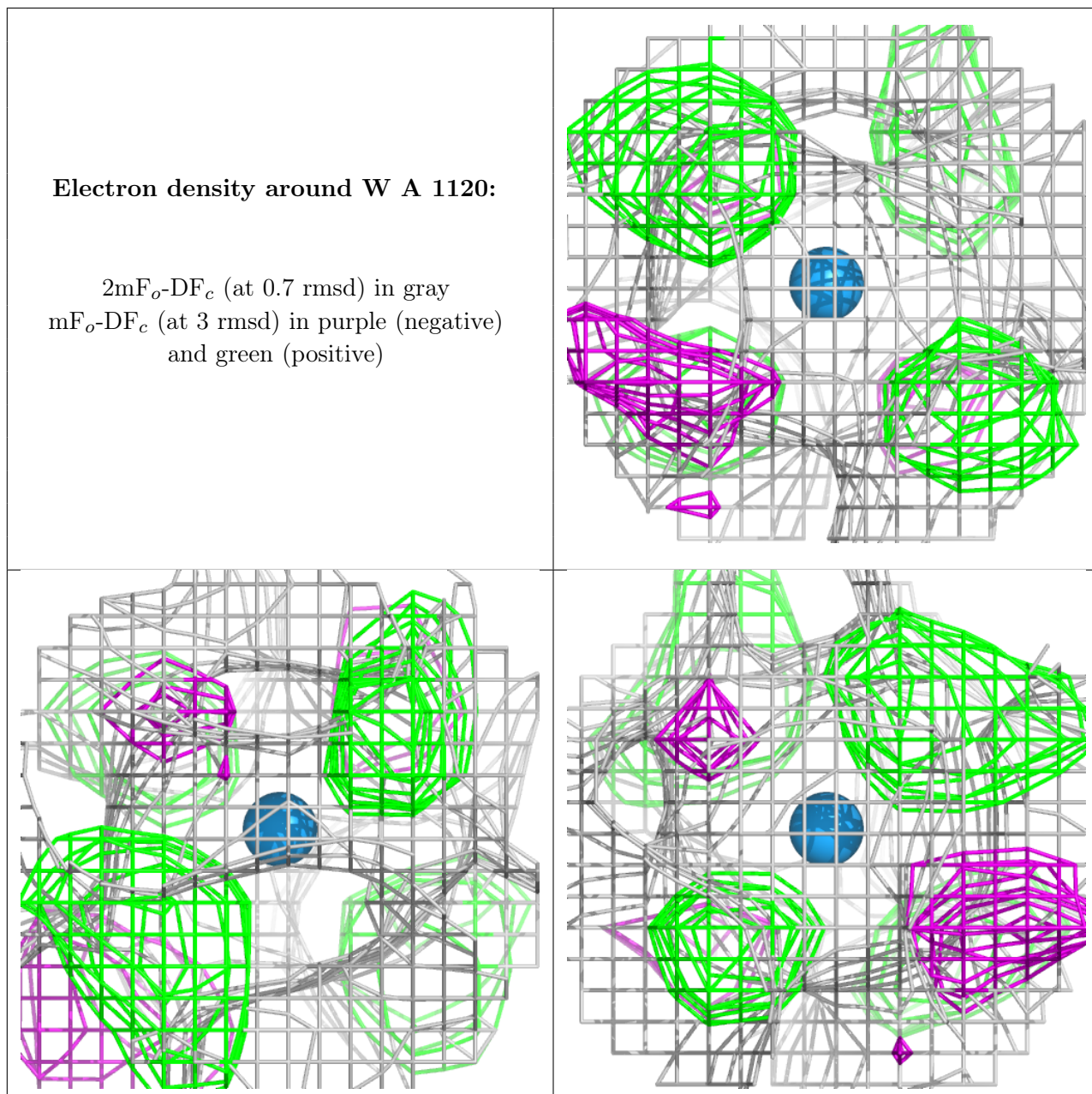
Electron density around SF4 B 1708:

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



Electron density around W A 1120:

$2mF_o-DF_c$ (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.