



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:21 AM UTC

PDB ID : 9RK1 / pdb_00009rk1
Title : W-formate dehydrogenase W491E from Nitratidesulfovibrio vulgaris (Desulfovibrio vulgaris)
Authors : Vilela-Alves, G.; Manuel, R.R.; Martins, G.; Pereira, I.C.; Romao, M.J.; Mota, C.
Deposited on : 2025-06-12
Resolution : 1.99 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

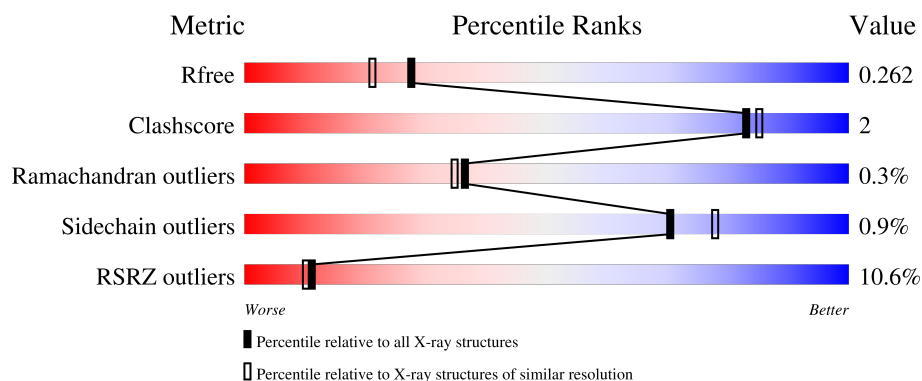
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1013	
2	B	214	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9585 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
			7572	4824	1319	1387	41	1			

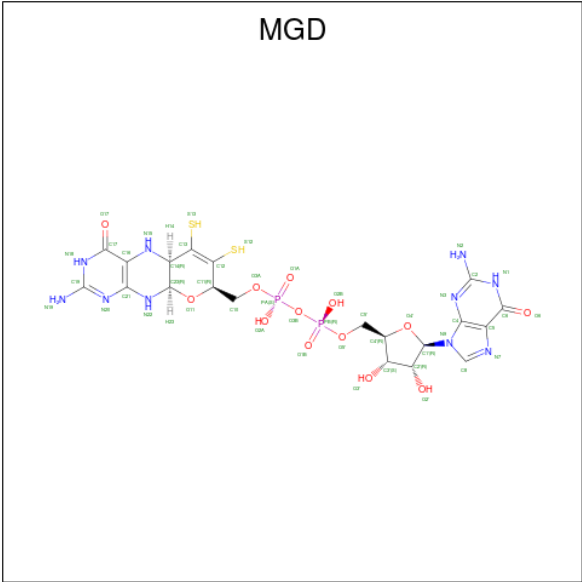
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	GLU	TRP	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.

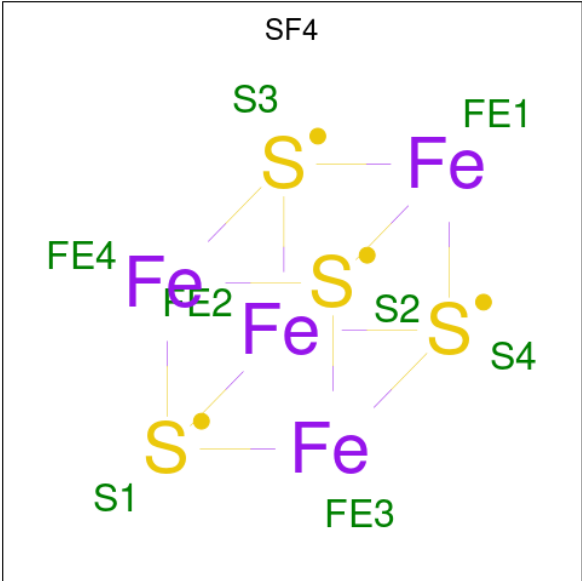
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			

- Molecule 3 is 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).



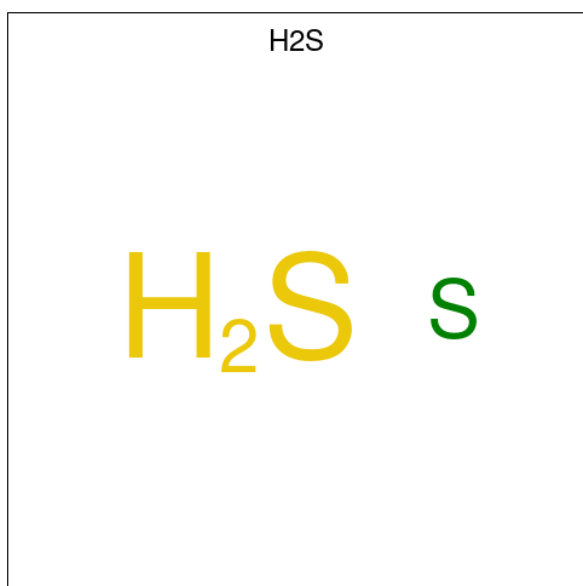
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

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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) (labeled as "Ligand of Interest" by depositor).



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

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

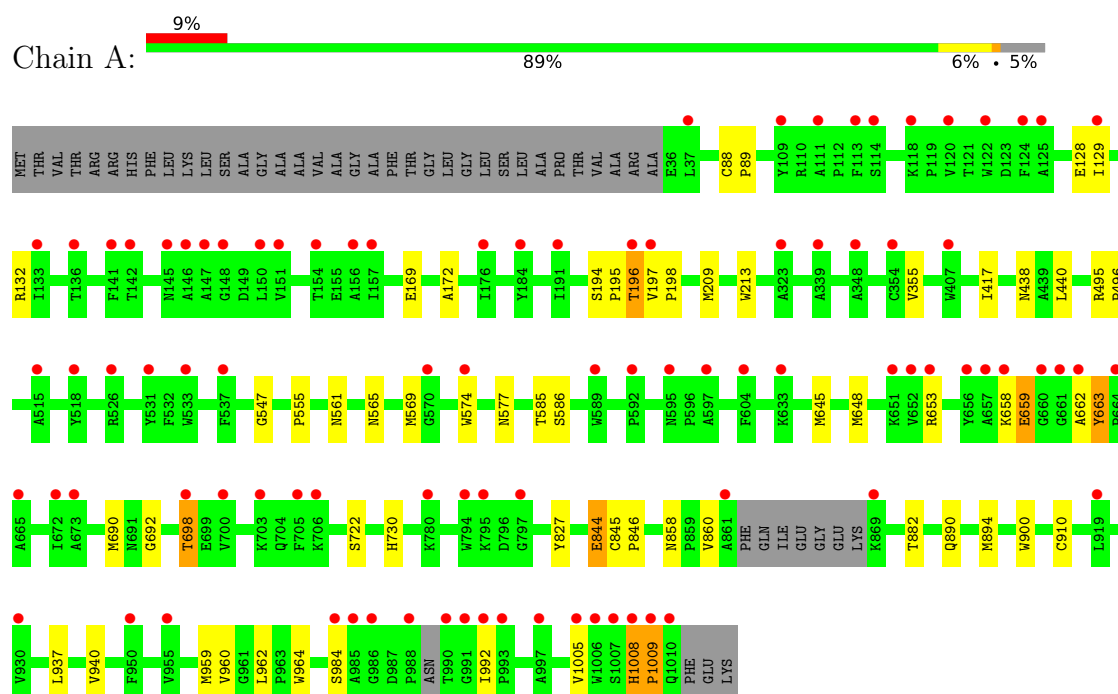
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	166	Total	O	0	0
			166	166		
9	B	33	Total	O	0	0
			33	33		

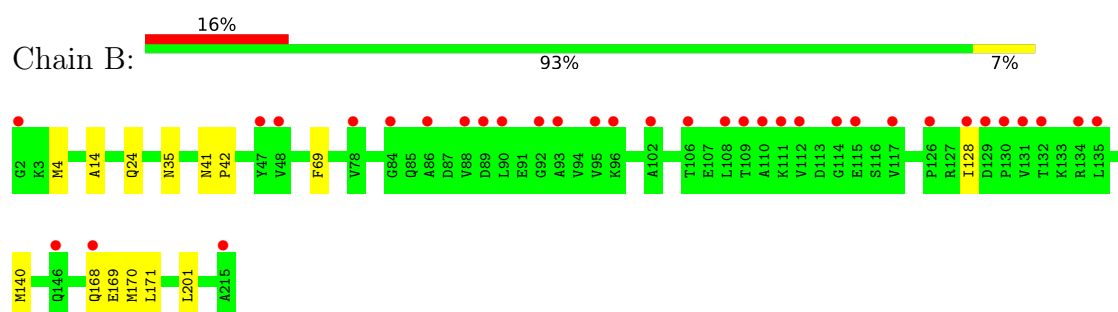
3 Residue-property plots [i](#)

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	64.82Å 128.04Å 148.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.37 – 1.99 74.37 – 1.99	Depositor EDS
% Data completeness (in resolution range)	81.6 (74.37-1.99) 81.4 (74.37-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.258 0.217 , 0.262	Depositor DCC
R_{free} test set	3530 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9585	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: W, SEC, MGD, EDO, SF4, 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	1.00	0/7776	1.37	3/10547 (0.0%)
2	B	1.01	0/1699	1.42	0/2302
All	All	1.00	0/9475	1.38	3/12849 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	GLY	CA-C-O	-5.30	118.77	122.22
1	A	844	GLU	CA-C-N	5.08	125.47	119.83
1	A	844	GLU	C-N-CA	5.08	125.47	119.83

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	7572	0	7398	36	0
2	B	1664	0	1633	10	0
3	A	94	0	44	1	0
4	A	8	0	0	0	0
4	B	24	0	0	0	0
5	A	1	0	0	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	6	0	8	0	0
8	A	4	0	6	0	0
8	B	12	0	18	0	0
9	A	166	0	0	0	0
9	B	33	0	0	0	0
All	All	9585	0	9107	44	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 2.

All (44) 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:1008:HIS:CG	1:A:1009:PRO:HA	2.19	0.76
2:B:4:MET:HE2	2:B:170:MET:HB2	1.75	0.67
1:A:569:MET:HE1	1:A:585:THR:HG23	1.78	0.64
1:A:129:ILE:HG21	1:A:648:MET:HE2	1.81	0.62
2:B:4:MET:HE1	2:B:171:LEU:HG	1.83	0.59
1:A:172:ALA:HB3	1:A:645:MET:CE	2.36	0.55
2:B:41:ASN:HA	2:B:42:PRO:C	2.32	0.54
2:B:140:MET:CG	2:B:140:MET:O	2.56	0.53
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.91	0.51
1:A:698:THR:HG21	1:A:722:SER:CB	2.41	0.51
2:B:168:GLN:HG2	2:B:169:GLU:OE1	2.10	0.50
1:A:128:GLU:O	1:A:132:ARG:HG2	2.12	0.49
2:B:4:MET:HE2	2:B:170:MET:CB	2.43	0.48
1:A:698:THR:HG21	1:A:722:SER:HB3	1.96	0.48
2:B:201:LEU:C	2:B:201:LEU:HD23	2.38	0.47
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.55	0.47
1:A:197:VAL:N	1:A:198:PRO:CD	2.78	0.46
1:A:658:LYS:O	1:A:659:GLU:HB2	2.15	0.46
1:A:355:VAL:HG13	1:A:827:TYR:HB2	1.97	0.46
1:A:172:ALA:HB3	1:A:645:MET:HE1	1.98	0.45
1:A:894:MET:SD	3:A:1102:MGD:H2'	2.56	0.45
1:A:940:VAL:HG11	2:B:35:ASN:HB3	1.98	0.45
1:A:565:ASN:O	1:A:569:MET:HG3	2.17	0.45
1:A:937:LEU:C	1:A:937:LEU:HD12	2.42	0.45
1:A:209:MET:HG3	1:A:438:ASN:HA	1.99	0.45
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.52	0.45
1:A:197:VAL:HG22	1:A:198:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:OE1	1:A:132:ARG:NH2	2.50	0.43
1:A:845:CYS:HB2	1:A:846:PRO:HD3	2.00	0.43
1:A:690:MET:HE2	1:A:730:HIS:CE1	2.54	0.43
1:A:858:ASN:OD1	1:A:860:VAL:HG22	2.17	0.43
1:A:882:THR:HA	1:A:962:LEU:O	2.18	0.43
1:A:196:THR:OG1	1:A:417:ILE:HG13	2.19	0.42
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.55	0.42
1:A:555:PRO:HD2	1:A:585:THR:HG21	2.02	0.42
1:A:662:ALA:O	1:A:663:TYR:C	2.63	0.41
1:A:169:GLU:O	1:A:645:MET:HE1	2.20	0.41
1:A:577:ASN:OD1	1:A:586:SER:HB3	2.21	0.41
1:A:213:TRP:CH2	1:A:440:LEU:HD22	2.56	0.41
1:A:495:ARG:N	1:A:496:PRO:CD	2.84	0.40
1:A:561:ASN:HD22	1:A:984:SER:HB2	1.86	0.40
1:A:194:SER:N	1:A:195:PRO:CD	2.84	0.40
1:A:547:GLY:HA3	1:A:574:TRP:CZ2	2.56	0.40
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.56	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	961/1013 (95%)	922 (96%)	36 (4%)	3 (0%)	36	35
2	B	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	1173/1227 (96%)	1129 (96%)	41 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	GLU

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Mol	Chain	Res	Type
1	A	663	TYR
1	A	1009	PRO

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%)	779 (99%)	8 (1%)	68	75
2	B	185/185 (100%)	184 (100%)	1 (0%)	81	87
All	All	972/1004 (97%)	963 (99%)	9 (1%)	70	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	THR
1	A	653	ARG
1	A	698	THR
1	A	844	GLU
1	A	959	MET
1	A	992	ILE
1	A	1005	VAL
1	A	1008	HIS
2	B	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	45	GLN
1	A	175	ASN
1	A	482	GLN
1	A	561	ASN
1	A	671	ASN
1	A	814	HIS

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Mol	Chain	Res	Type
1	A	855	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 11 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	A	1103	1	0,12,12	-	-	-		
4	SF4	B	302	2	0,12,12	-	-	-		
8	EDO	A	1107	-	3,3,3	0.05	0	2,2,2	0.13	0
3	MGD	A	1102	6	47,52,52	0.63	1 (2%)	58,81,81	0.91	3 (5%)
3	MGD	A	1101	6	47,52,52	0.59	1 (2%)	58,81,81	0.92	3 (5%)
8	EDO	B	304	-	3,3,3	0.09	0	2,2,2	0.20	0
4	SF4	B	301	2	0,12,12	-	-	-		
4	SF4	B	303	2	0,12,12	-	-	-		
8	EDO	B	305	-	3,3,3	0.07	0	2,2,2	0.19	0
8	EDO	B	306	-	3,3,3	0.07	0	2,2,2	0.13	0
7	GOL	A	1106	-	5,5,5	0.09	0	5,5,5	0.30	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
4	SF4	A	1103	1	-	-	0/6/5/5
8	EDO	A	1107	-	-	1/1/1/1	-
4	SF4	B	302	2	-	-	0/6/5/5
3	MGD	A	1102	6	-	5/22/66/66	0/6/6/6
8	EDO	B	304	-	-	0/1/1/1	-
3	MGD	A	1101	6	-	1/22/66/66	0/6/6/6
4	SF4	B	301	2	-	-	0/6/5/5
4	SF4	B	303	2	-	-	0/6/5/5
8	EDO	B	305	-	-	1/1/1/1	-
8	EDO	B	306	-	-	1/1/1/1	-
7	GOL	A	1106	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	MGD	C23-C14	2.50	1.55	1.53
3	A	1101	MGD	PB-O3B	2.01	1.61	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	C19-N20-C21	3.08	118.80	113.36
3	A	1102	MGD	C19-N20-C21	2.99	118.64	113.36
3	A	1101	MGD	C23-C14-N15	2.26	110.09	107.87
3	A	1102	MGD	C23-C14-N15	2.23	110.06	107.87
3	A	1101	MGD	O11-C23-N22	2.21	110.61	108.61
3	A	1102	MGD	C17-C16-N15	2.14	122.11	116.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C4'-C5'-O5'-PB
3	A	1102	MGD	O4'-C4'-C5'-O5'
8	A	1107	EDO	O1-C1-C2-O2
3	A	1102	MGD	C3'-C4'-C5'-O5'
3	A	1101	MGD	PA-O3B-PB-O5'

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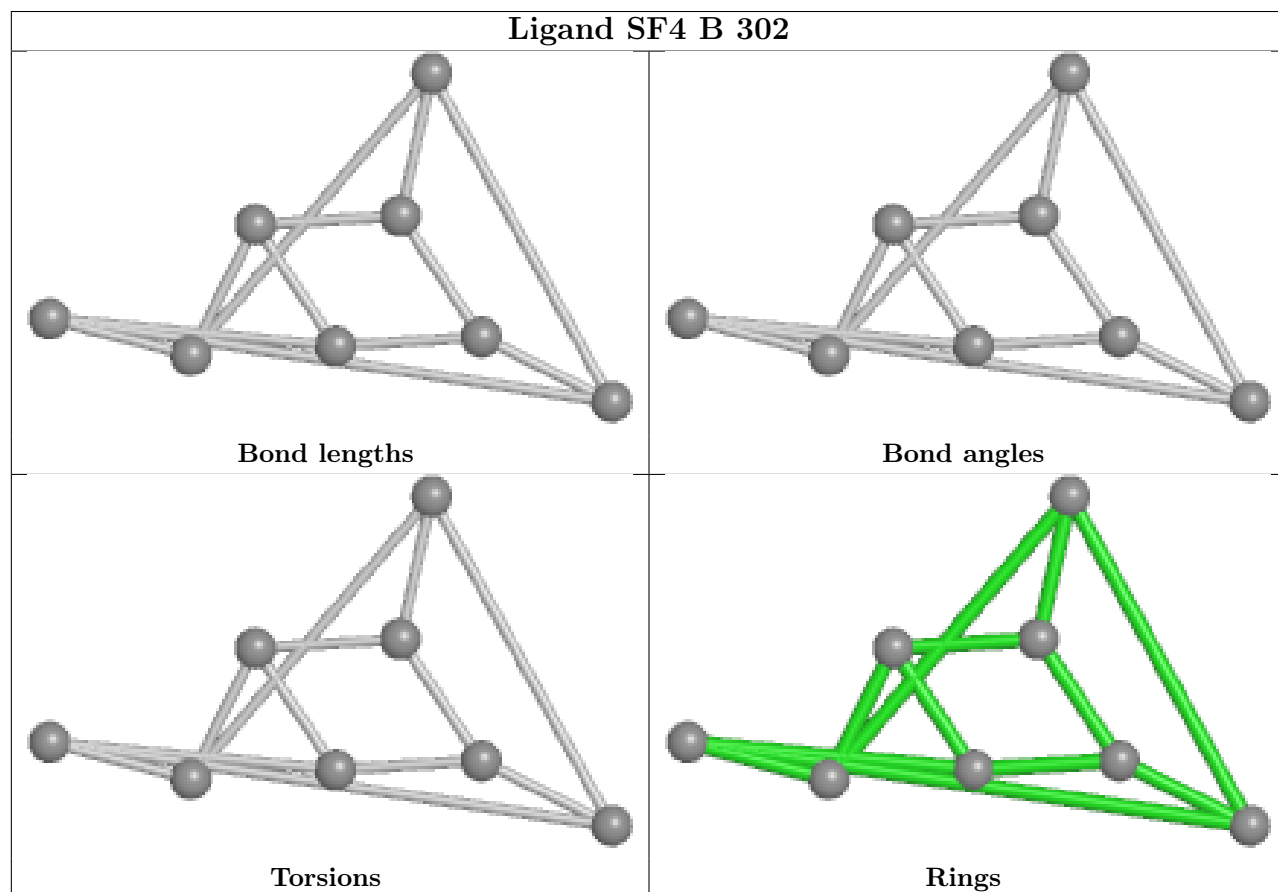
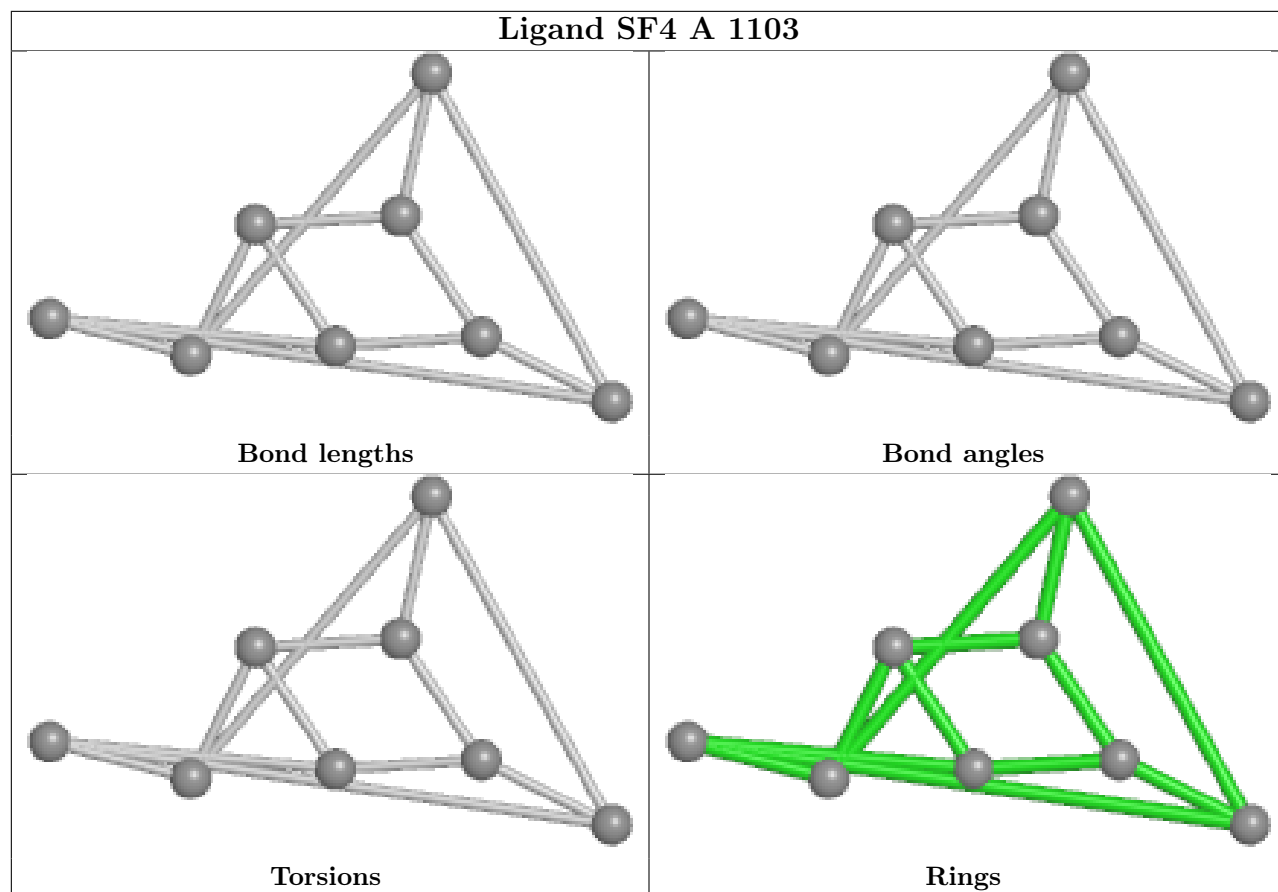
Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	PA-O3B-PB-O1B
3	A	1102	MGD	PA-O3B-PB-O2B
8	B	305	EDO	O1-C1-C2-O2
8	B	306	EDO	O1-C1-C2-O2

There are no ring outliers.

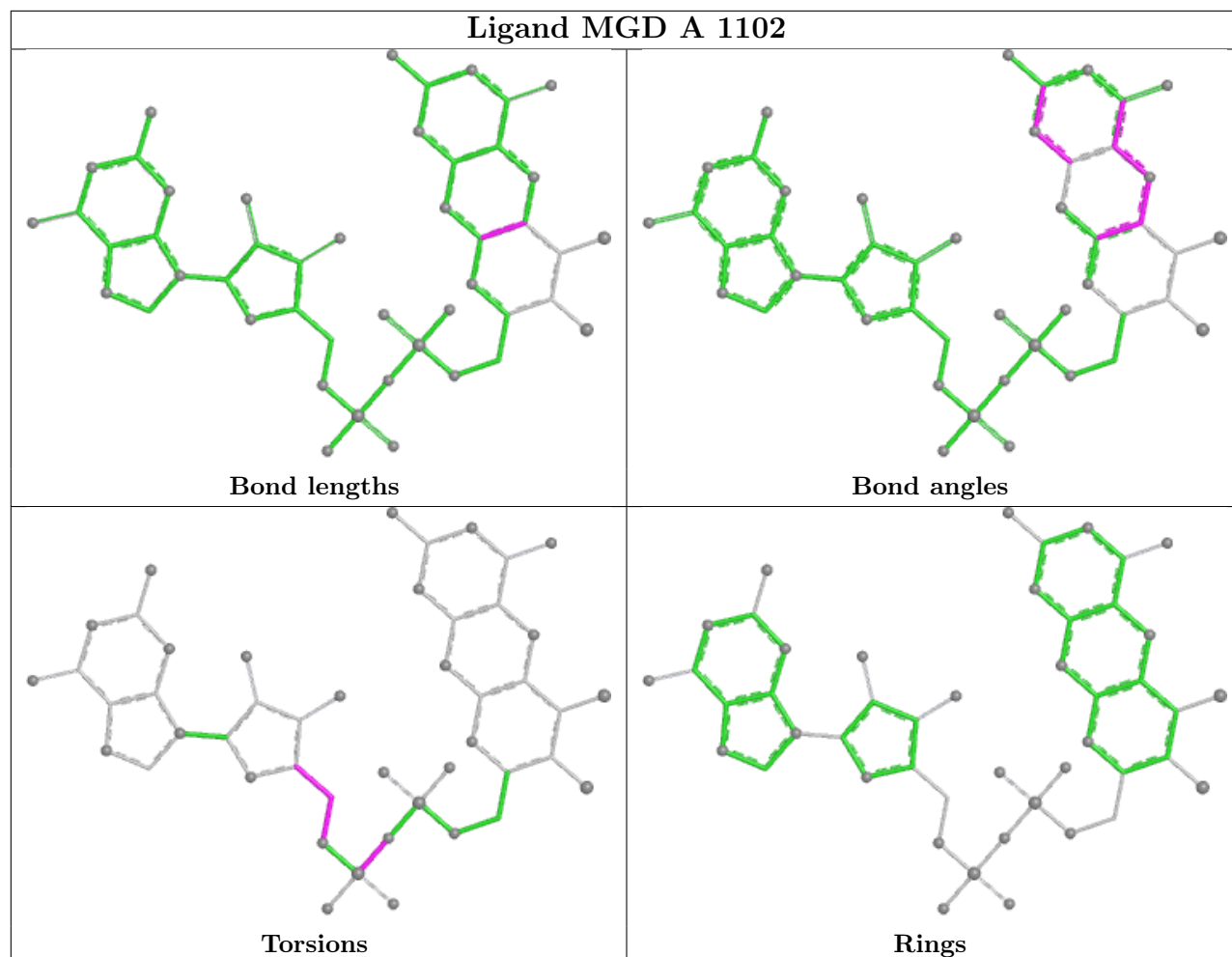
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	MGD	1	0

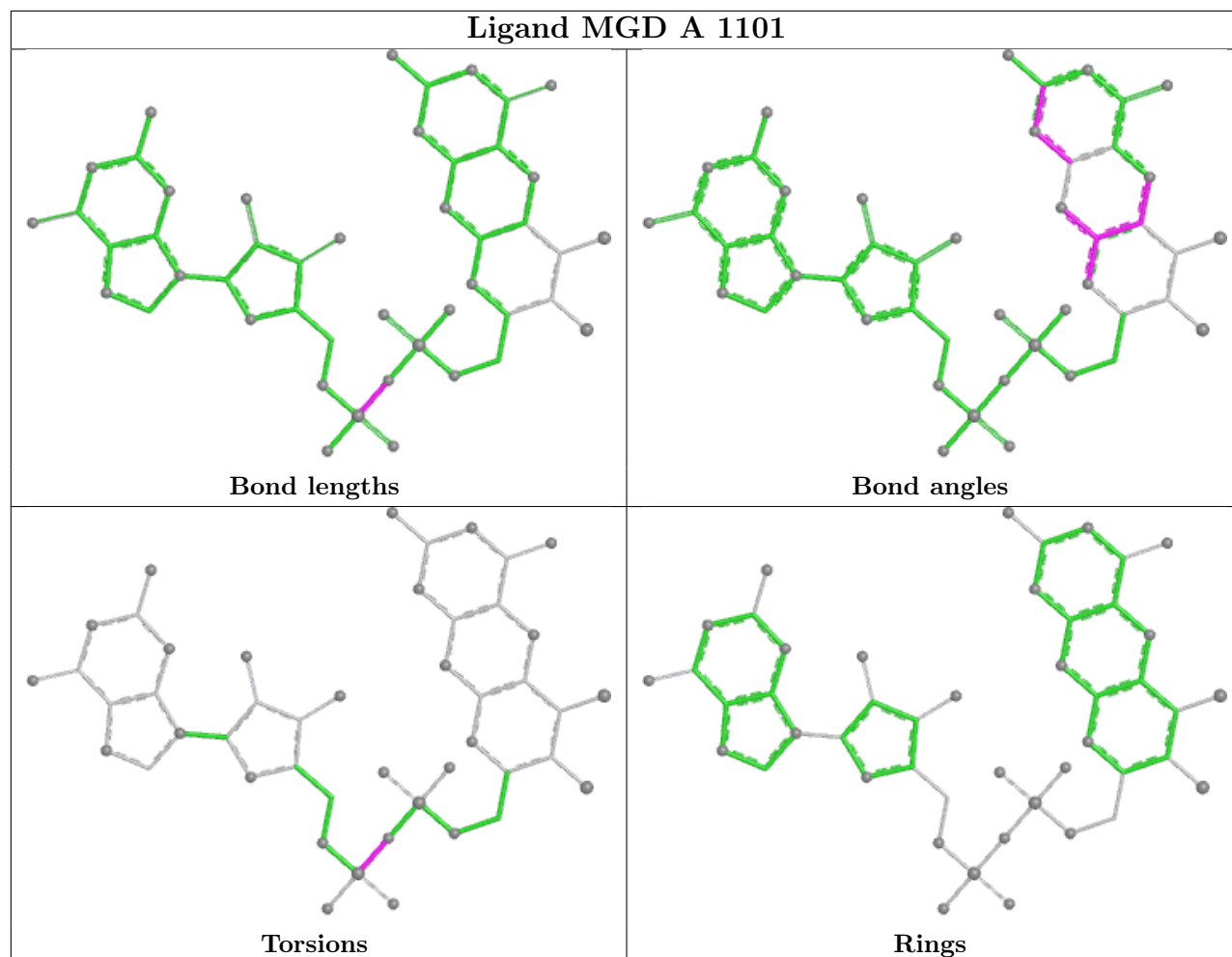
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

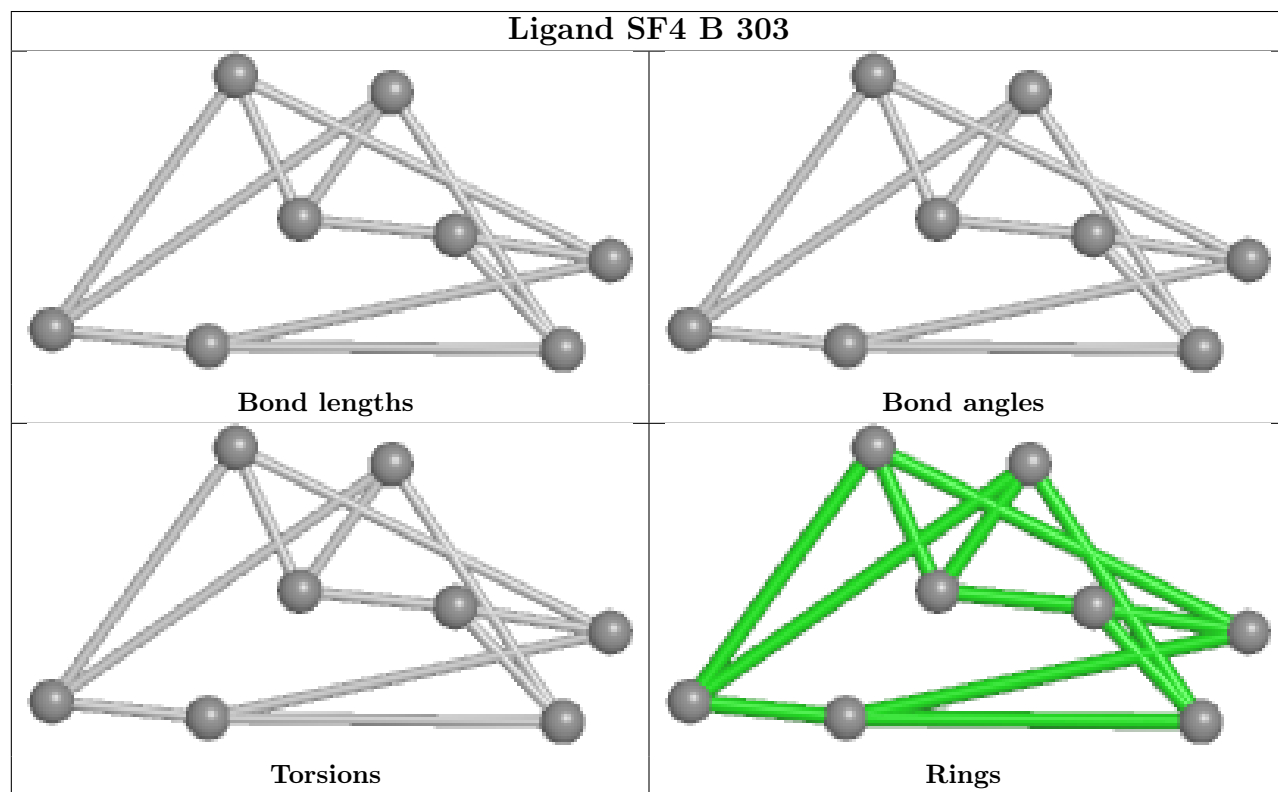
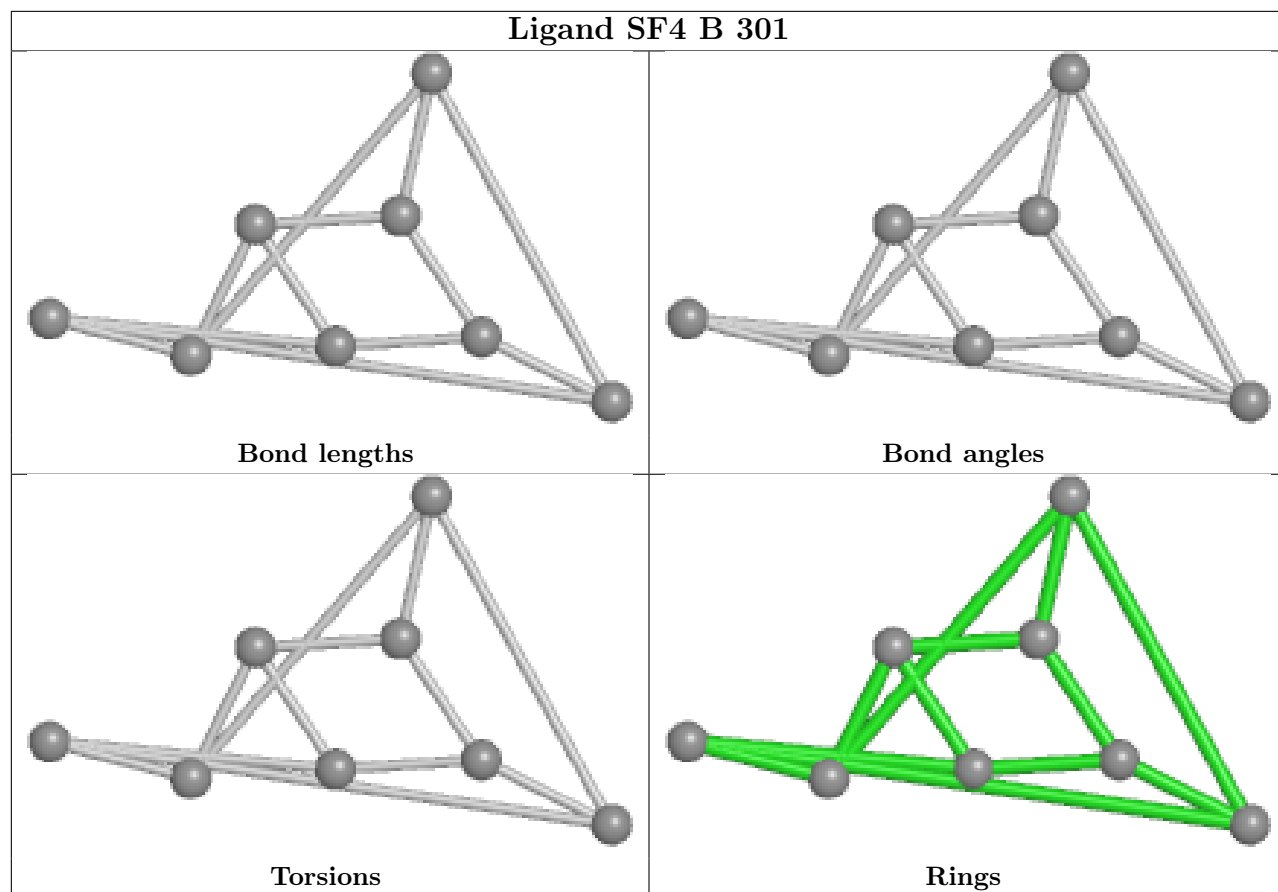


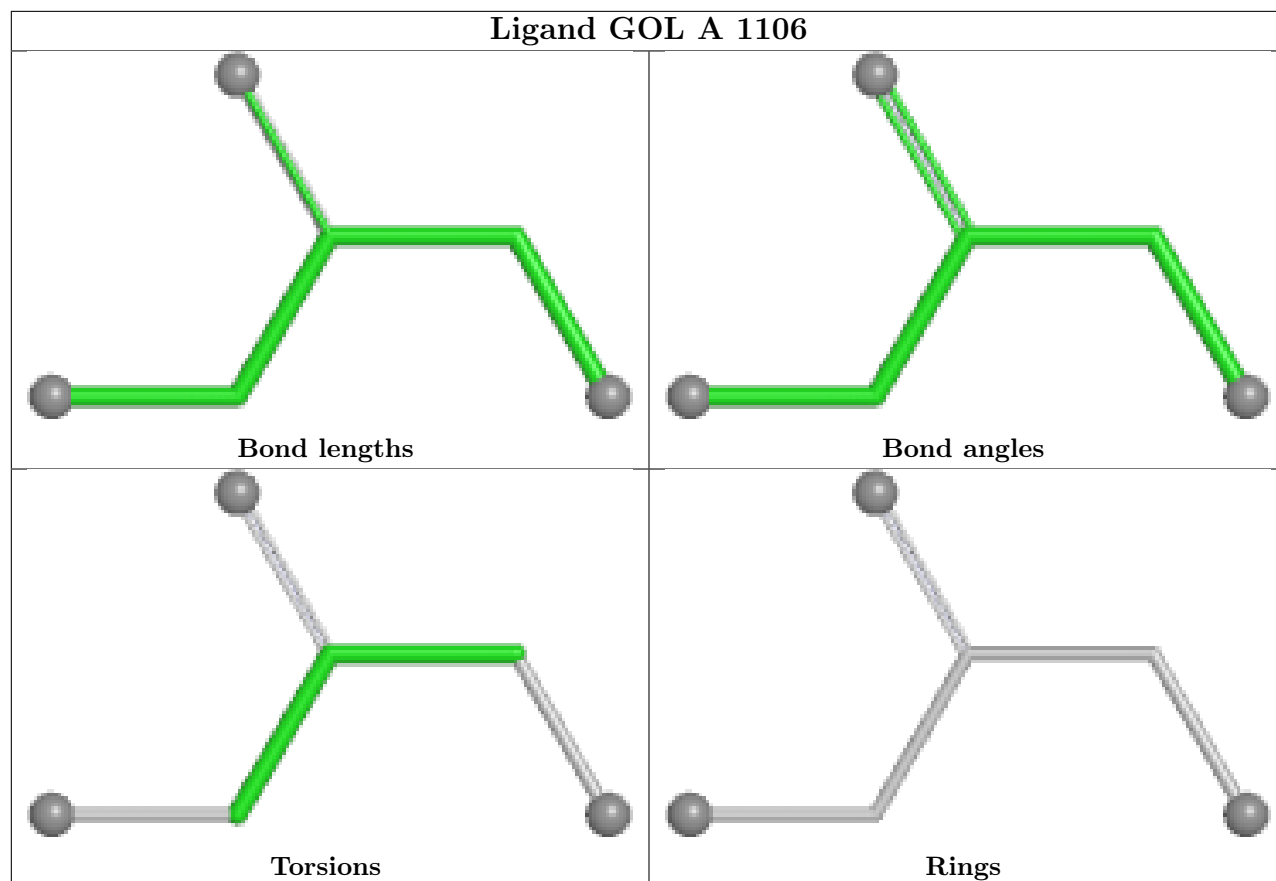
Ligand MGD A 1102



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 [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	966/1013 (95%)	0.81	91 (9%)	14 13	16, 34, 59, 105	1 (0%)
2	B	214/214 (100%)	0.98	34 (15%)	5 4	21, 39, 73, 86	0
All	All	1180/1227 (96%)	0.84	125 (10%)	11 10	16, 35, 65, 105	1 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1009	PRO	6.8
1	A	597	ALA	5.6
1	A	1008	HIS	5.1
1	A	1005	VAL	4.9
1	A	993	PRO	4.8
1	A	122	TRP	4.7
1	A	660	GLY	4.6
1	A	196	THR	4.3
2	B	132	THR	4.3
2	B	112	VAL	4.3
1	A	988	PRO	4.2
2	B	108	LEU	4.2
1	A	992	ILE	4.2
1	A	1006	TRP	4.2
1	A	125	ALA	4.1
2	B	131	VAL	4.1
1	A	986	GLY	4.1
1	A	129	ILE	4.0
2	B	126	PRO	4.0
1	A	1010	GLN	4.0
1	A	661	GLY	3.6
1	A	861	ALA	3.6
1	A	113	PHE	3.6
1	A	133	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	589	TRP	3.5
2	B	135	LEU	3.5
1	A	869	LYS	3.4
2	B	128	ILE	3.4
1	A	570	GLY	3.4
1	A	990	THR	3.4
2	B	88	VAL	3.3
1	A	985	ALA	3.3
1	A	574	TRP	3.3
1	A	705	PHE	3.2
1	A	950	PHE	3.2
2	B	90	LEU	3.1
2	B	146	GLN	3.1
2	B	130	PRO	3.1
2	B	110	ALA	3.1
1	A	533	TRP	3.0
2	B	106	THR	3.0
1	A	664	PRO	3.0
1	A	120	VAL	3.0
2	B	117	VAL	2.9
1	A	109	TYR	2.9
1	A	154	THR	2.9
1	A	111	ALA	2.9
1	A	657	ALA	2.9
1	A	354	CYS	2.9
1	A	604	PHE	2.9
1	A	919	LEU	2.9
1	A	700	VAL	2.8
1	A	339	ALA	2.8
1	A	984	SER	2.8
1	A	142	THR	2.8
1	A	651	LYS	2.8
1	A	698	THR	2.8
2	B	86	ALA	2.8
1	A	176	ILE	2.8
2	B	92	GLY	2.7
1	A	407	TRP	2.7
1	A	662	ALA	2.7
2	B	47	TYR	2.7
2	B	114	GLY	2.7
1	A	114	SER	2.7
1	A	526	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	672	ILE	2.7
1	A	348	ALA	2.6
2	B	134	ARG	2.6
1	A	997	ALA	2.6
1	A	633	LYS	2.6
1	A	652	VAL	2.6
1	A	673	ALA	2.6
2	B	102	ALA	2.6
1	A	658	LYS	2.5
1	A	665	ALA	2.5
2	B	109	THR	2.5
1	A	141	PHE	2.5
2	B	93	ALA	2.4
1	A	991	GLY	2.4
1	A	955	VAL	2.4
1	A	537	PHE	2.4
2	B	215	ALA	2.4
1	A	145	ASN	2.4
2	B	48	VAL	2.4
1	A	191	ILE	2.3
2	B	78	VAL	2.3
1	A	595	ASN	2.3
1	A	146	ALA	2.3
1	A	147	ALA	2.3
2	B	96	LYS	2.3
1	A	653	ARG	2.3
1	A	151	VAL	2.3
1	A	124	PHE	2.3
1	A	518	TYR	2.3
2	B	168	GLN	2.3
1	A	706	LYS	2.3
1	A	156	ALA	2.2
1	A	797	GLY	2.2
1	A	930	VAL	2.2
1	A	323	ALA	2.2
2	B	84	GLY	2.2
1	A	197	VAL	2.2
2	B	89	ASP	2.2
2	B	2	GLY	2.2
1	A	656	TYR	2.1
1	A	37	LEU	2.1
1	A	780	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	THR	2.1
2	B	95	VAL	2.1
1	A	703	LYS	2.1
1	A	515	ALA	2.1
1	A	184	TYR	2.1
2	B	129	ASP	2.1
1	A	118	LYS	2.1
1	A	794	TRP	2.1
1	A	592	PRO	2.1
1	A	157	ILE	2.0
2	B	111	LYS	2.0
2	B	115	GLU	2.0
1	A	148	GLY	2.0
1	A	150	LEU	2.0
1	A	795	LYS	2.0
1	A	1007	SER	2.0
1	A	531	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

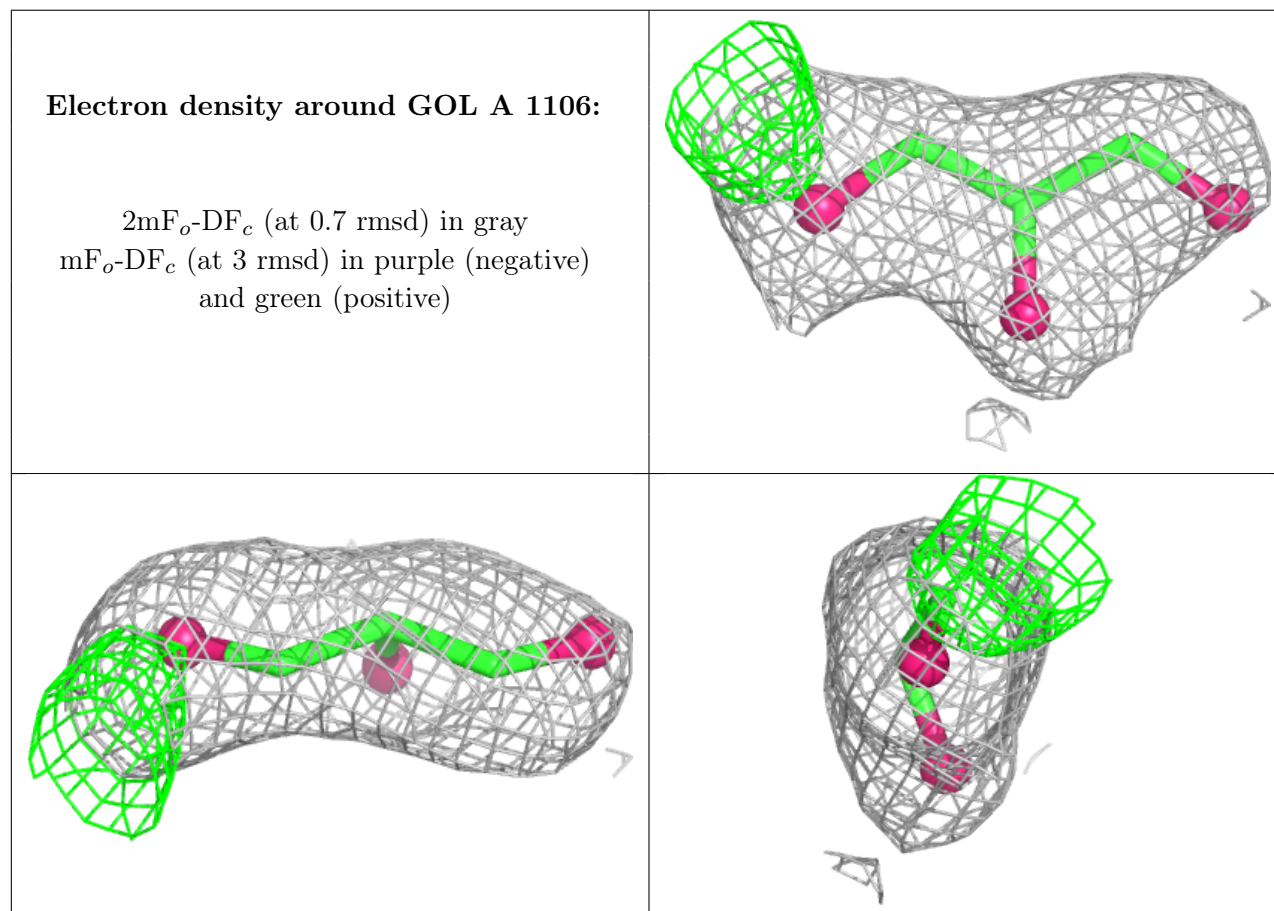
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	EDO	A	1107	4/4	0.79	0.17	36,39,43,46	0
8	EDO	B	305	4/4	0.82	0.19	47,48,49,59	0
7	GOL	A	1106	6/6	0.83	0.15	37,39,42,47	0
8	EDO	B	304	4/4	0.88	0.15	28,37,38,44	0
8	EDO	B	306	4/4	0.89	0.19	41,46,50,54	0
3	MGD	A	1102	47/47	0.97	0.06	18,24,31,41	0

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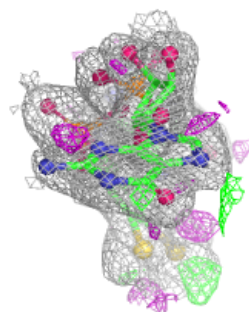
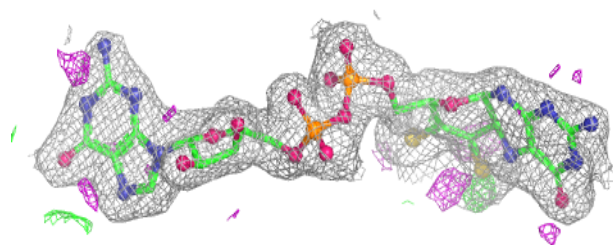
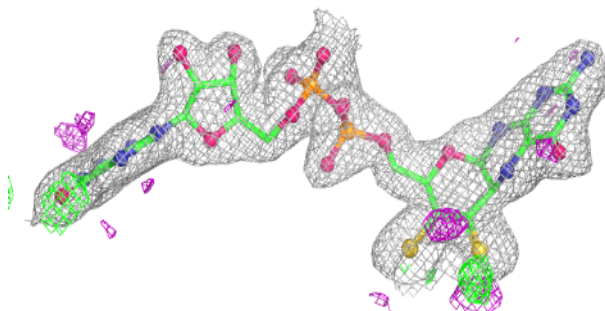
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SF4	B	302	8/8	0.97	0.05	40,42,44,49	0
5	H2S	A	1104	1/1	0.97	0.07	18,18,18,18	0
3	MGD	A	1101	47/47	0.97	0.06	16,21,25,26	0
4	SF4	B	303	8/8	0.98	0.04	32,35,37,38	0
4	SF4	A	1103	8/8	0.99	0.03	19,20,21,22	0
4	SF4	B	301	8/8	0.99	0.03	21,22,25,26	0
6	W	A	1105	1/1	1.00	0.01	22,22,22,22	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.



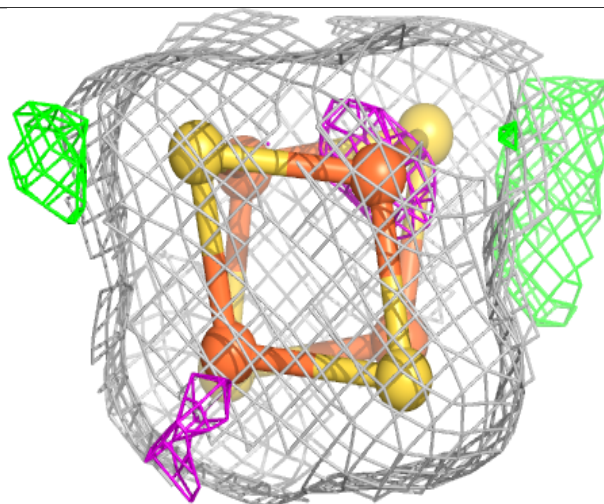
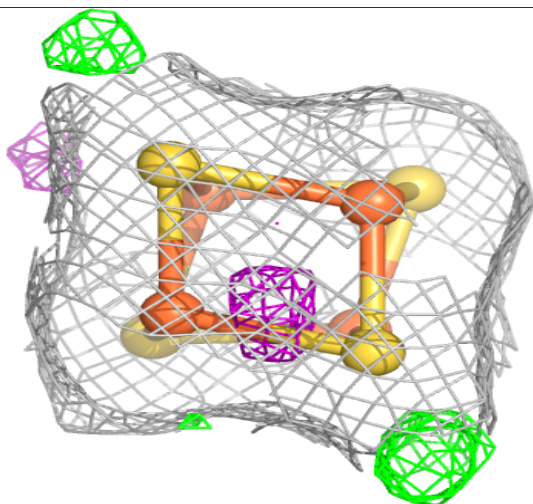
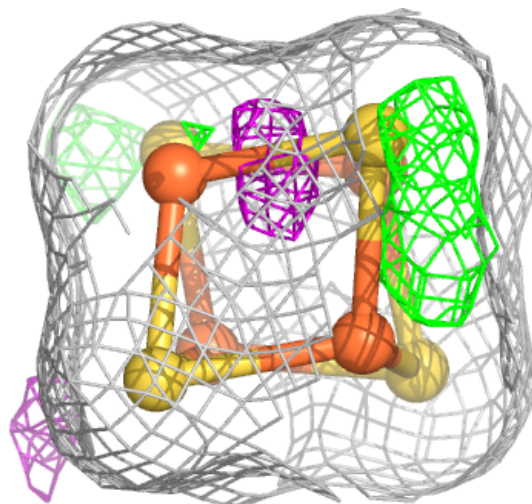
Electron density around MGD A 1102:

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



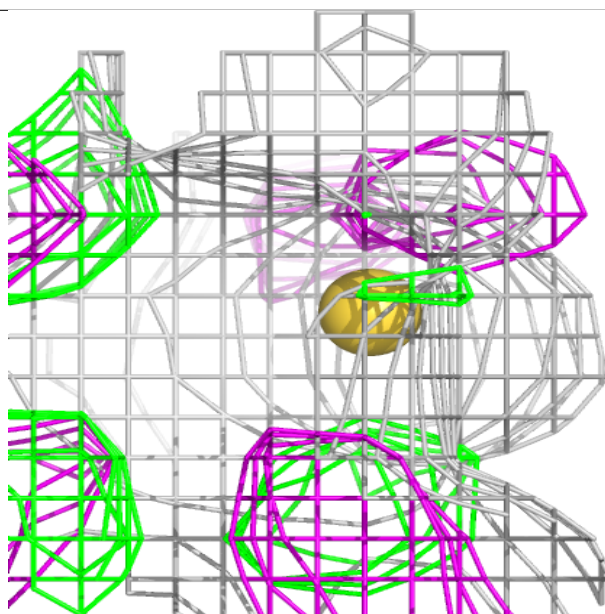
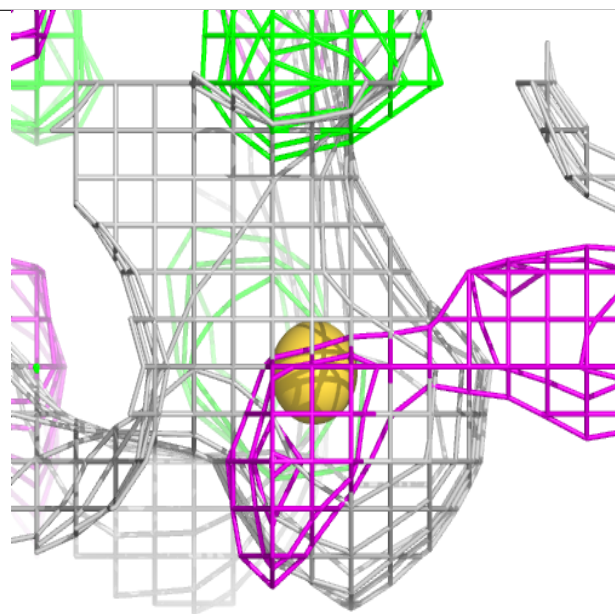
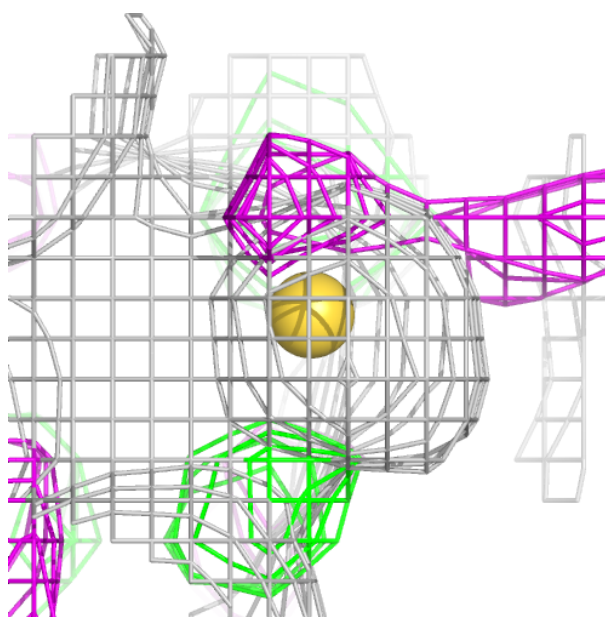
Electron density around SF4 B 302:

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



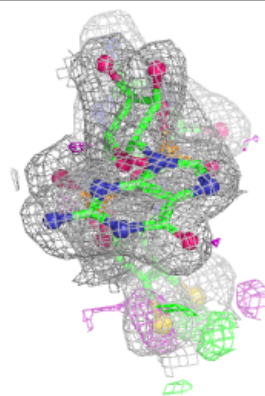
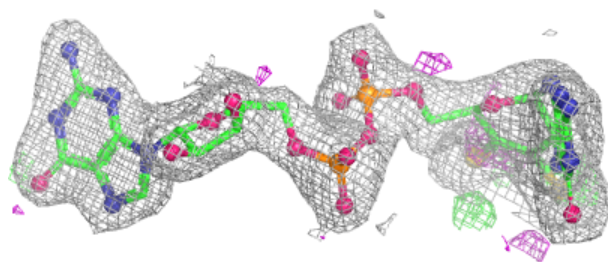
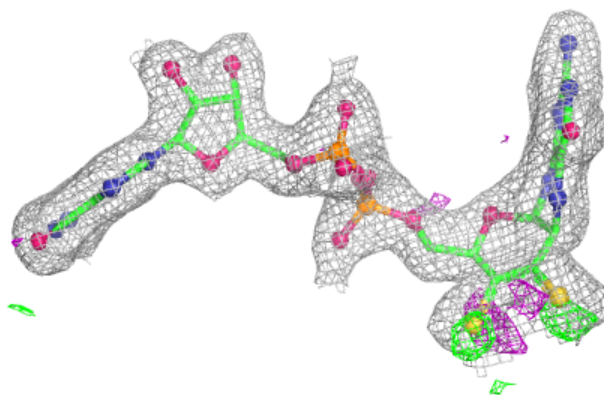
Electron density around H2S A 1104:

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



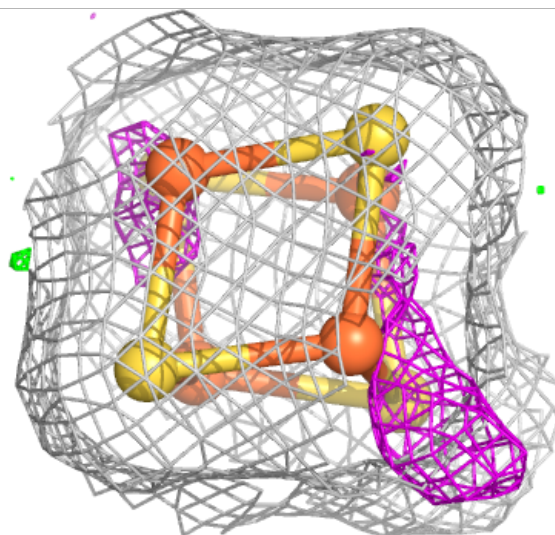
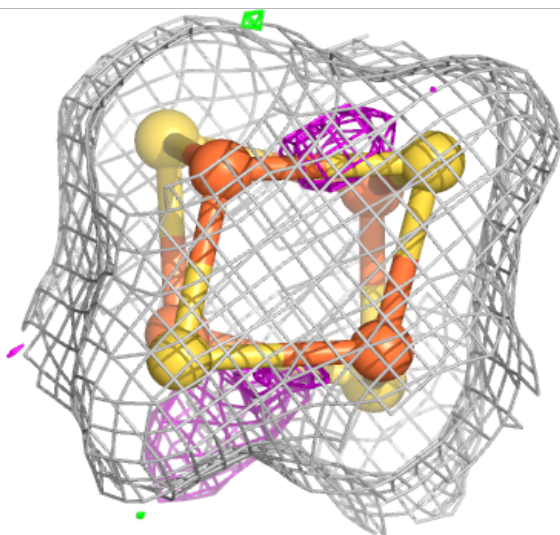
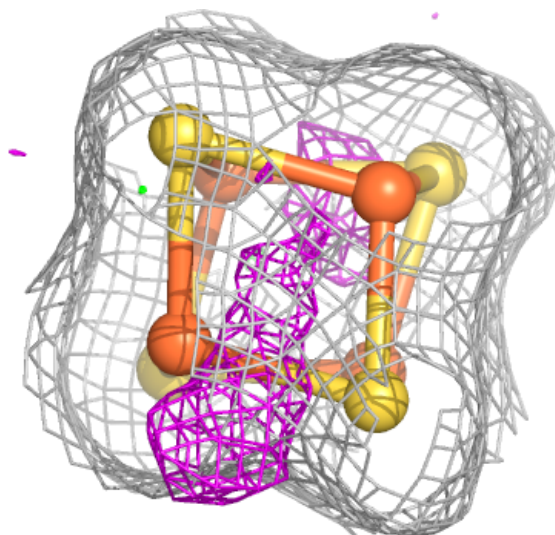
Electron density around MGD A 1101:

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



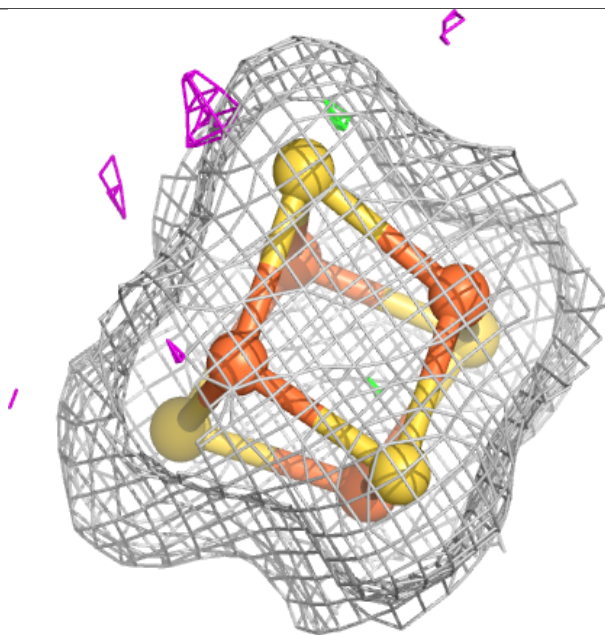
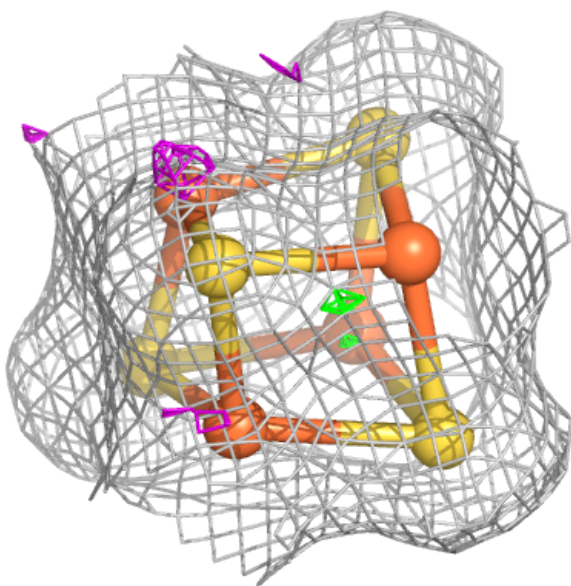
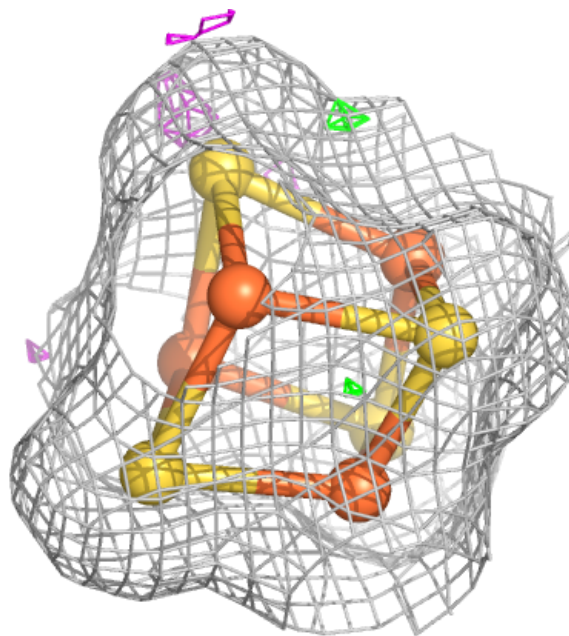
Electron density around SF4 B 303:

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



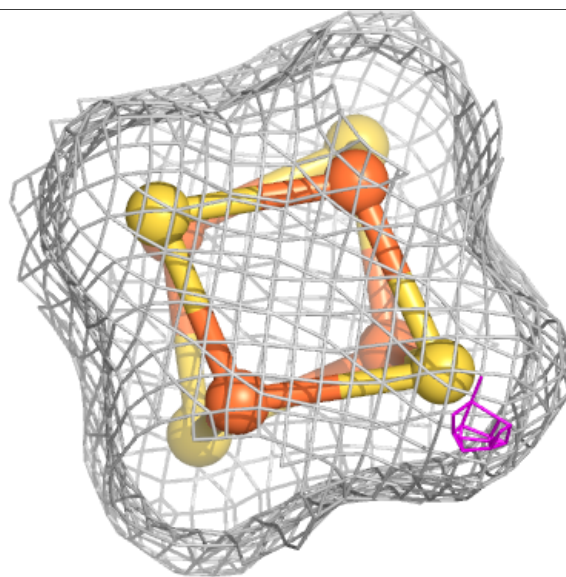
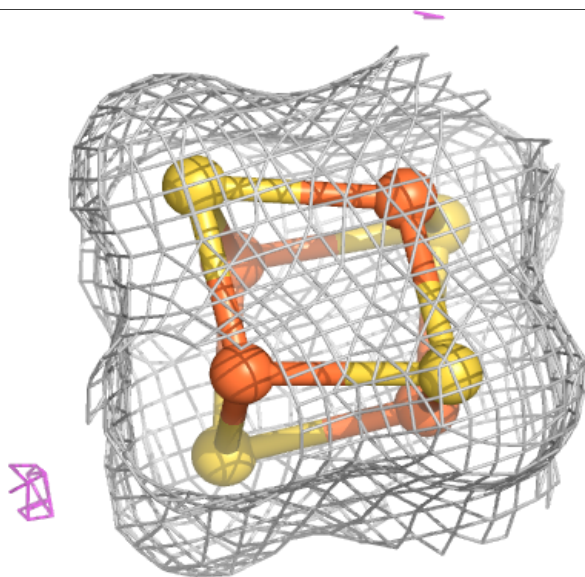
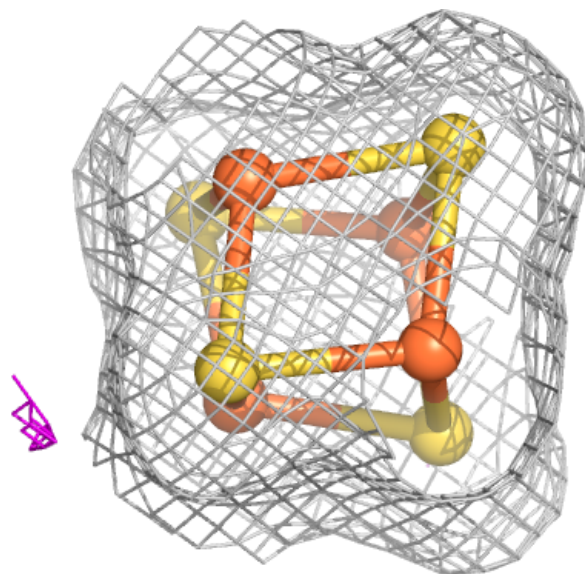
Electron density around SF4 A 1103:

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



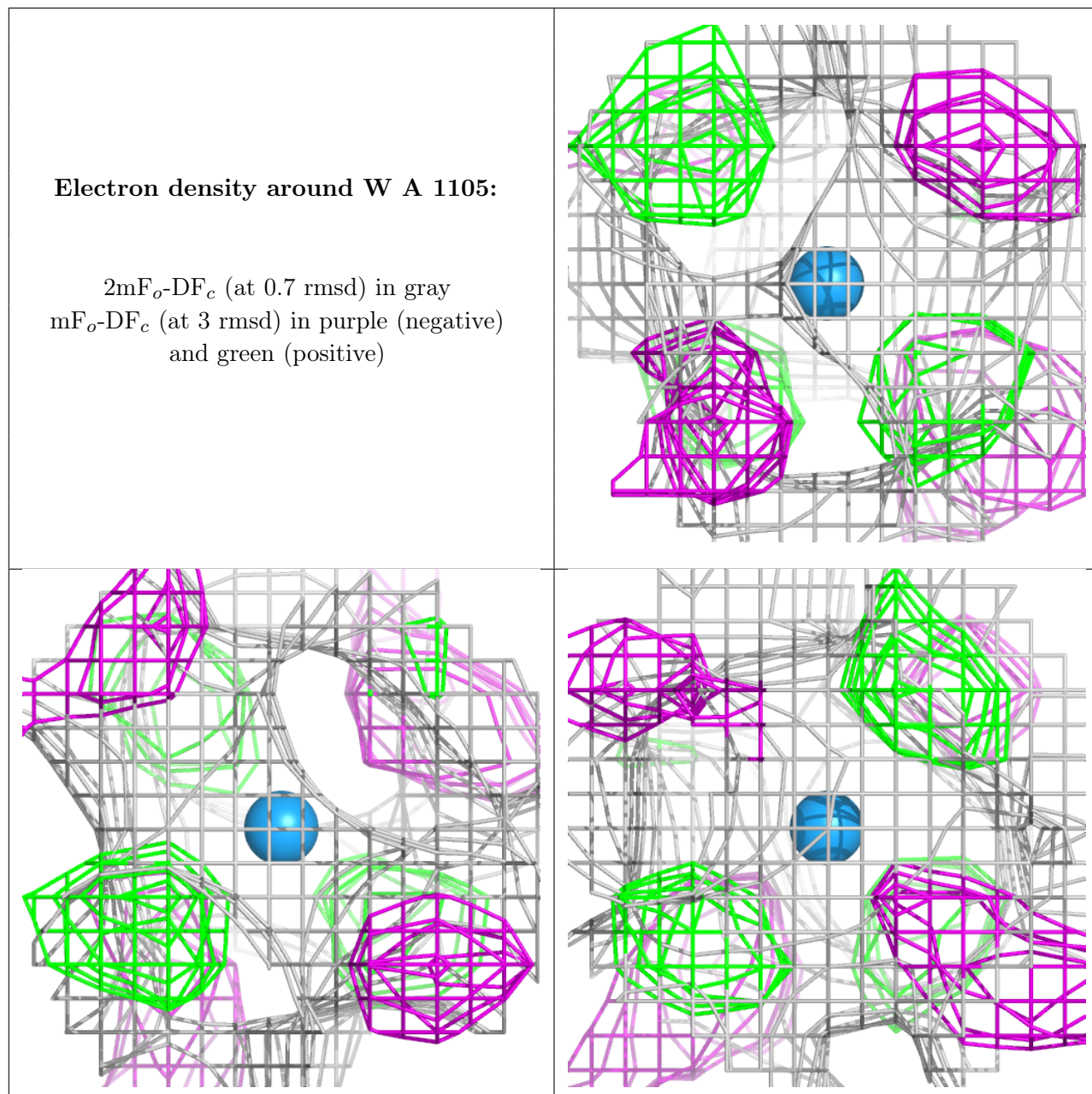
Electron density around SF4 B 301:

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



Electron density around 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.