



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:38 PM UTC

PDB ID : 8CH9 / pdb_00008ch9
Title : Crystal structure of arsenite oxidase from *Alcaligenes faecalis* (Af Aio) bound to arsenic oxyanion
Authors : Engrola, F.; Correia, M.A.S.; Romao, M.J.; Santos-Silva, T.
Deposited on : 2023-02-07
Resolution : 1.43 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

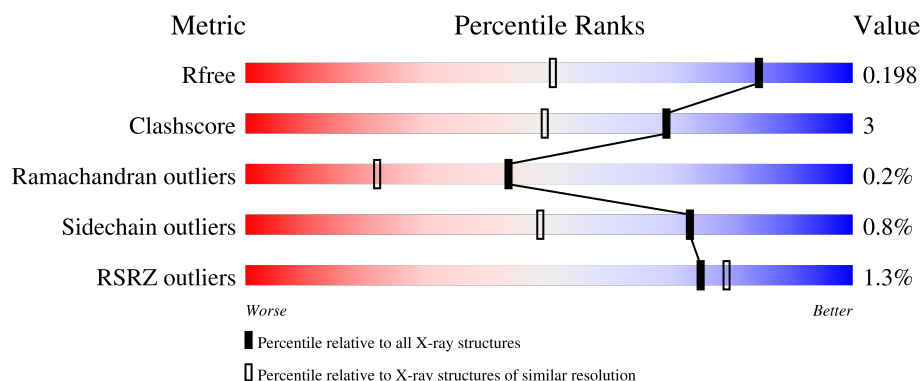
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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.



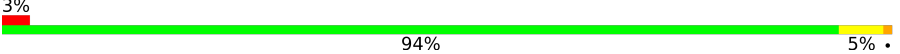
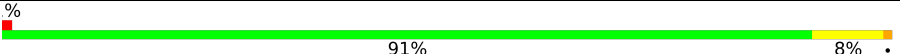
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	823	% 91% 8%
1	C	823	% 92% 7%
1	E	823	% 91% 8%
2	B	134	3% 91% 7%
2	D	134	4% 92% 7%

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Mol	Chain	Length	Quality of chain
2	F	134	
2	H	134	
3	G	823	

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
8	ART	A	906	-	X	-	-
8	ART	C	904	-	X	-	-
8	ART	E	904	-	X	-	-
8	ART	G	2407	-	X	-	-
9	GOL	E	909	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35090 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 Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	5	18	0
			6626	4166	1176	1242	42			
1	C	823	Total	C	N	O	S	7	19	0
			6636	4170	1173	1250	43			
1	E	822	Total	C	N	O	S	12	24	0
			6647	4174	1176	1253	44			

- Molecule 2 is a protein called Arsenite oxidase subunit AioB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	4	0
			1026	640	172	205	9			
2	D	133	Total	C	N	O	S	0	7	0
			1038	646	174	209	9			
2	F	134	Total	C	N	O	S	3	5	0
			1029	642	172	205	10			
2	H	133	Total	C	N	O	S	0	6	0
			1028	640	172	206	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q7SIF3
D	0	LEU	-	expression tag	UNP Q7SIF3
F	0	LEU	-	expression tag	UNP Q7SIF3
H	0	LEU	-	expression tag	UNP Q7SIF3

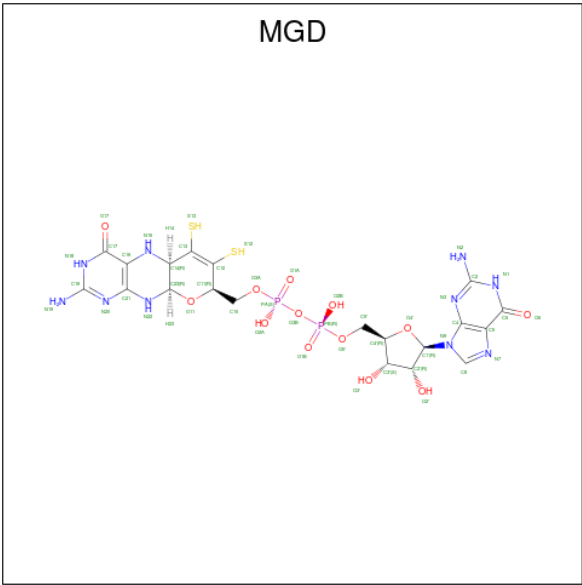
- Molecule 3 is a protein called Arsenite oxidase subunit AioA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	821	Total	C	N	O	S	0	20	0
			6619	4163	1173	1240	43			

There is a discrepancy between the modelled and reference sequences:

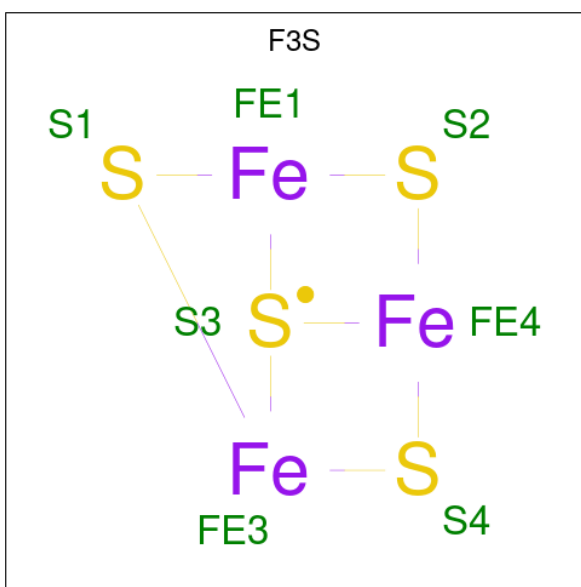
Chain	Residue	Modelled	Actual	Comment	Reference
G	280	ASP	GLU	conflict	UNP Q7SIF4

- Molecule 4 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).



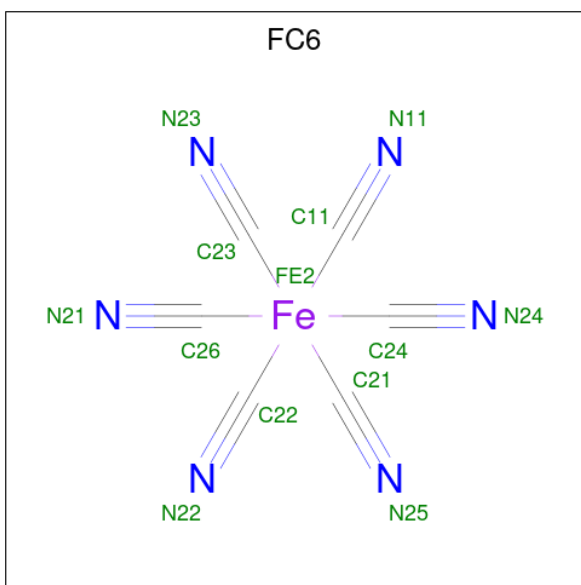
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P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

- Molecule 5 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		
5	C	1	Total	Fe	S	0	0
			7	3	4		
5	E	1	Total	Fe	S	0	0
			7	3	4		
5	G	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is HEXACYANOFERRATE(3-) (CCD ID: FC6) (formula: C_6FeN_6).

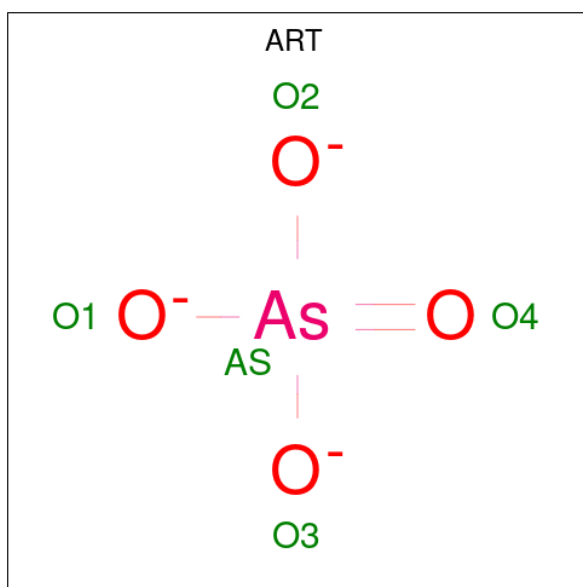


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	0	0
			13	6	1	6		
6	C	1	Total	C	Fe	N	0	0
			13	6	1	6		
6	E	1	Total	C	Fe	N	0	0
			13	6	1	6		
6	G	1	Total	C	Fe	N	0	0
			13	6	1	6		

- Molecule 7 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mo	0	0
			1	1		
7	C	1	Total	Mo	0	0
			1	1		
7	E	1	Total	Mo	0	0
			1	1		
7	G	1	Total	Mo	0	0
			1	1		

- Molecule 8 is ARSENATE (CCD ID: ART) (formula: AsO₄) (labeled as "Ligand of Interest" by depositor).



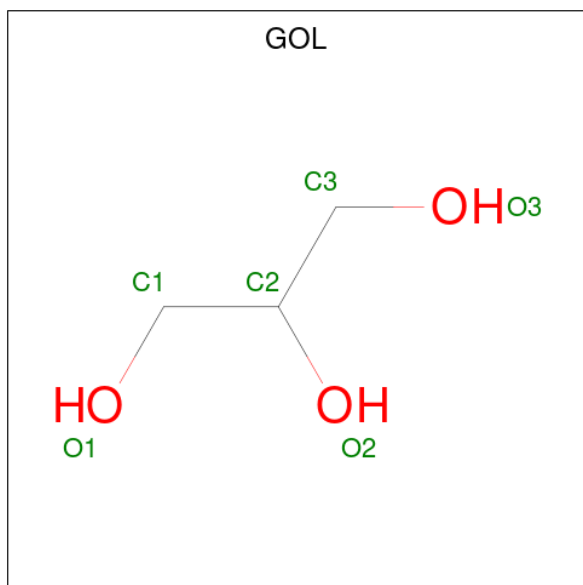
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	As	O	0	0
			5	1	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	As	O	0	0
			5	1	4		
8	E	1	Total	As	O	0	0
			5	1	4		
8	G	1	Total	As	O	0	0
			5	1	4		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



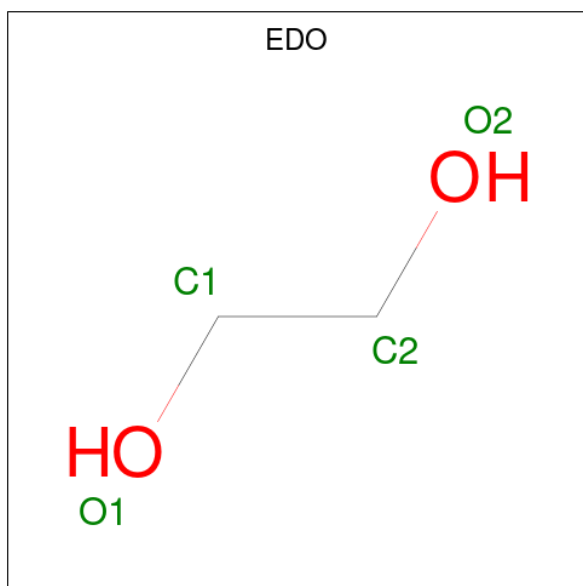
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



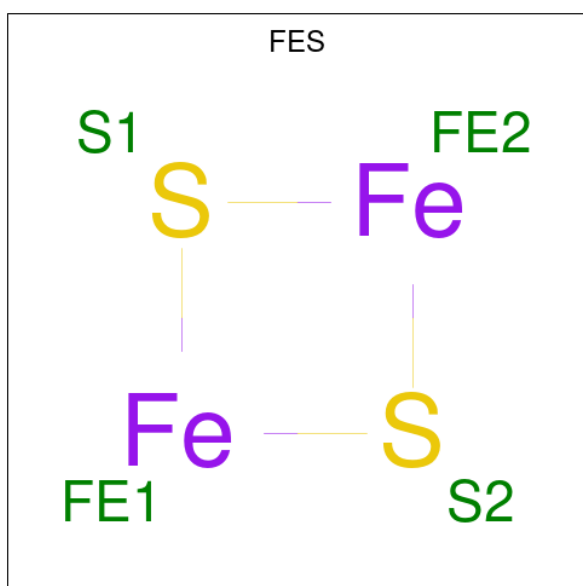
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		

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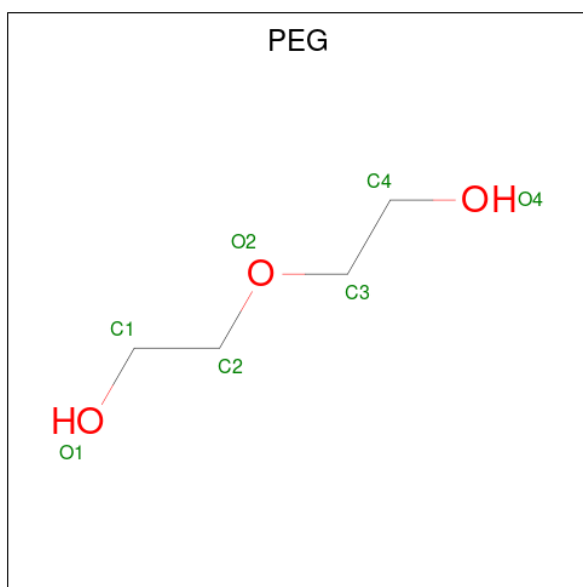
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 4 2 2	0	0
10	C	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	E	1	Total C O 4 2 2	0	0
10	G	1	Total C O 4 2 2	0	0

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Fe S 4 2 2	0	0
11	D	1	Total Fe S 4 2 2	0	0
11	F	1	Total Fe S 4 2 2	0	0
11	H	1	Total Fe S 4 2 2	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



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

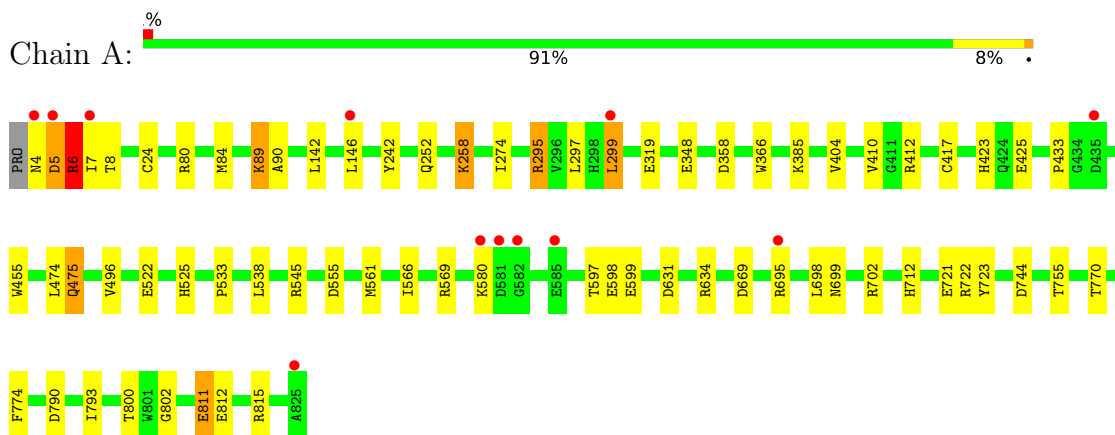
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	866	Total	O	0	0
			866	866		
13	B	143	Total	O	0	0
			143	143		
13	C	770	Total	O	0	0
			770	770		
13	D	154	Total	O	0	0
			154	154		
13	E	830	Total	O	0	0
			830	830		
13	F	134	Total	O	0	0
			134	134		
13	G	771	Total	O	0	0
			771	771		
13	H	137	Total	O	0	0
			137	137		

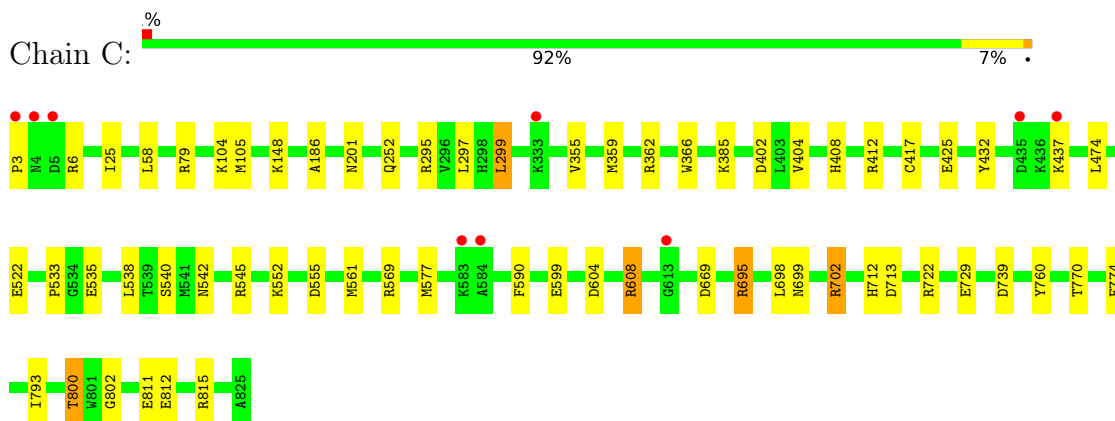
3 Residue-property plots [i](#)

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.

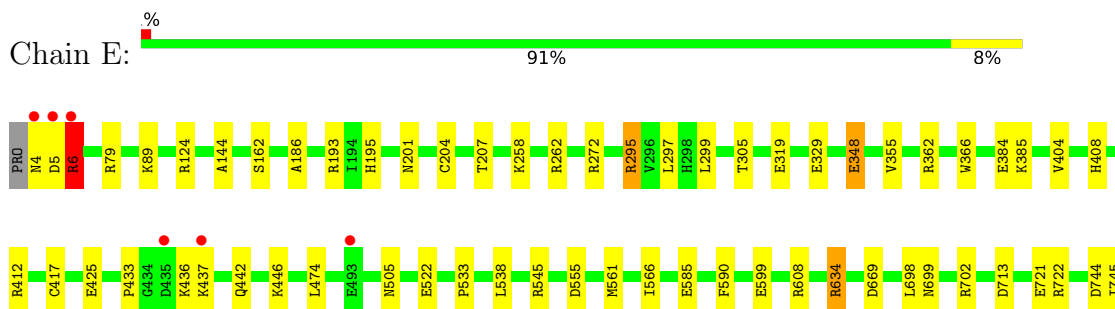
• Molecule 1: Arsenite oxidase subunit AioA



• Molecule 1: Arsenite oxidase subunit AioA

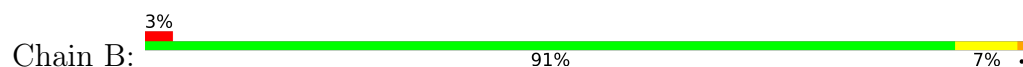


• Molecule 1: Arsenite oxidase subunit AioA

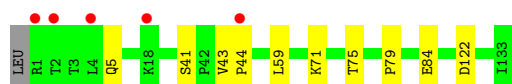




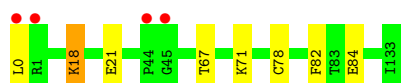
- Molecule 2: Arsenite oxidase subunit AioB



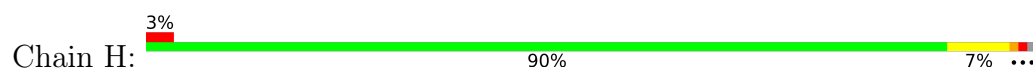
- Molecule 2: Arsenite oxidase subunit AioB



- Molecule 2: Arsenite oxidase subunit AioB



- Molecule 2: Arsenite oxidase subunit AioB



- Molecule 3: Arsenite oxidase subunit AioA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.29Å 109.95Å 117.42Å 98.33° 89.97° 96.58°	Depositor
Resolution (Å)	65.47 – 1.43 65.47 – 1.43	Depositor EDS
% Data completeness (in resolution range)	73.0 (65.47-1.43) 73.0 (65.47-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.167 , 0.195 0.172 , 0.198	Depositor DCC
R_{free} test set	29766 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35090	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, 4MO, MGD, FES, FC6, ART, GOL, F3S

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	0.95	3/6790 (0.0%)	1.20	28/9199 (0.3%)
1	C	0.91	1/6803 (0.0%)	1.18	11/9216 (0.1%)
1	E	0.95	5/6813 (0.1%)	1.20	14/9228 (0.2%)
2	B	0.88	0/1047	1.21	3/1426 (0.2%)
2	D	0.89	0/1060	1.19	2/1444 (0.1%)
2	F	0.90	0/1053	1.21	3/1435 (0.2%)
2	H	0.82	0/1052	1.23	5/1432 (0.3%)
3	G	0.93	4/6786 (0.1%)	1.18	18/9196 (0.2%)
All	All	0.93	13/31404 (0.0%)	1.19	84/42576 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	6
1	E	0	6
3	G	0	5
All	All	0	23

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	348	GLU	C-O	-14.26	1.07	1.24
3	G	280	ASP	CG-OD1	8.96	1.42	1.25
3	G	529	PRO	CA-CB	-8.42	1.43	1.53
3	G	272	ARG	NE-CZ	7.10	1.40	1.33
3	G	525	HIS	CE1-NE2	6.81	1.39	1.32
1	E	272	ARG	NE-CZ	6.74	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	423	HIS	CE1-NE2	6.37	1.39	1.32
1	C	712	HIS	CE1-NE2	5.49	1.38	1.32
1	A	525	HIS	CG-CD2	-5.41	1.29	1.35
1	A	455	TRP	C-O	5.31	1.29	1.23
1	E	195	HIS	ND1-CE1	5.27	1.37	1.32
1	E	124	ARG	NE-CZ	5.08	1.38	1.33
1	E	144	ALA	CA-CB	-5.05	1.45	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	GLN	OE1-CD-NE2	14.31	136.91	122.60
2	H	44	PRO	N-CA-CB	-12.96	89.64	103.25
1	A	555	ASP	CA-CB-CG	9.05	121.66	112.60
1	E	555	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	412	ARG	CD-NE-CZ	8.64	136.50	124.40
1	C	555	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	5	ASP	CA-CB-CG	7.54	120.14	112.60
1	C	599	GLU	CB-CG-CD	7.46	125.29	112.60
3	G	669	ASP	CA-CB-CG	7.30	119.90	112.60
3	G	555	ASP	CA-CB-CG	7.29	119.89	112.60
1	A	599	GLU	CB-CG-CD	7.26	124.94	112.60
1	C	713	ASP	CA-CB-CG	7.21	119.81	112.60
3	G	569	ARG	CG-CD-NE	-7.18	96.21	112.00
1	A	669	ASP	CA-CB-CG	7.13	119.73	112.60
1	E	669	ASP	CA-CB-CG	7.13	119.73	112.60
2	D	122	ASP	CA-CB-CG	7.12	119.72	112.60
1	C	669	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	6	ARG	N-CA-C	6.91	119.37	108.79
1	C	811	GLU	CB-CG-CD	6.91	124.35	112.60
1	E	319	GLU	CB-CG-CD	6.83	124.20	112.60
1	A	258	LYS	CB-CG-CD	-6.67	95.97	111.30
1	E	599	GLU	CB-CG-CD	6.64	123.89	112.60
3	G	6	ARG	N-CA-C	6.56	118.44	108.47
2	H	71	LYS	CB-CA-C	-6.54	98.11	110.67
3	G	599	GLU	CB-CG-CD	6.54	123.71	112.60
1	A	423	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
2	H	122	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	695	ARG	CB-CG-CD	6.37	125.95	111.30
2	F	84	GLU	CB-CG-CD	6.29	123.29	112.60
1	E	6	ARG	N-CA-C	6.13	118.17	108.79
3	G	713	ASP	CA-CB-CG	6.11	118.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	295	ARG	CA-CB-CG	-6.11	101.89	114.10
3	G	295	ARG	CD-NE-CZ	6.08	132.91	124.40
3	G	569	ARG	CB-CG-CD	5.99	125.07	111.30
1	E	634	ARG	CD-NE-CZ	5.97	132.76	124.40
3	G	384	GLU	CB-CA-C	5.95	122.27	110.42
2	F	71	LYS	CB-CA-C	-5.94	99.26	110.67
1	C	702	ARG	NE-CZ-NH1	-5.88	115.62	121.50
2	D	71	LYS	CB-CA-C	-5.85	99.44	110.67
2	B	84	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	295	ARG	CA-CB-CG	-5.81	102.47	114.10
1	C	402	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	6	ARG	N-CA-C	5.74	118.00	108.99
2	B	71	LYS	CB-CA-C	-5.74	99.66	110.67
1	A	723	TYR	O-C-N	-5.72	116.25	121.34
1	A	348	GLU	CG-CD-OE1	5.71	131.53	118.40
1	E	752	PHE	CA-CB-CG	-5.63	108.17	113.80
3	G	634	ARG	CD-NE-CZ	5.59	132.23	124.40
1	A	597	THR	OG1-CB-CG2	-5.58	98.13	109.30
1	E	608	ARG	CG-CD-NE	-5.55	99.80	112.00
2	H	44	PRO	N-CA-C	5.53	123.87	112.47
1	A	295	ARG	NE-CZ-NH1	5.53	127.03	121.50
2	F	82	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	598	GLU	CB-CA-C	5.50	121.22	110.67
1	E	295	ARG	CD-NE-CZ	5.49	132.09	124.40
1	A	475	GLN	CG-CD-OE1	-5.44	109.93	120.80
1	A	423	HIS	CG-CD2-NE2	5.41	112.61	107.20
1	A	348	GLU	CG-CD-OE2	-5.40	105.97	118.40
1	A	811	GLU	CB-CG-CD	5.40	121.77	112.60
1	E	305	THR	CA-CB-OG1	5.39	117.69	109.60
1	A	790	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	89	LYS	CB-CG-CD	5.39	123.69	111.30
1	C	695	ARG	NE-CZ-NH1	-5.38	116.11	121.50
1	A	258	LYS	CA-CB-CG	5.37	124.84	114.10
3	G	598	GLU	CB-CA-C	5.36	120.96	110.67
2	H	20	ASN	CA-CB-CG	-5.35	107.25	112.60
1	E	89	LYS	CB-CG-CD	5.34	123.57	111.30
2	B	82	PHE	CA-CB-CG	-5.30	108.50	113.80
3	G	295	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	E	384	GLU	CB-CA-C	5.24	120.86	110.42
3	G	348	GLU	N-CA-CB	5.24	117.92	110.16
1	A	295	ARG	CD-NE-CZ	5.23	131.72	124.40
1	A	597	THR	CA-CB-CG2	5.20	119.35	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	713	ASP	CA-CB-CG	5.16	117.76	112.60
3	G	608	ARG	CG-CD-NE	-5.15	100.67	112.00
3	G	425	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	242	TYR	N-CA-C	-5.14	105.59	111.14
1	A	24	CYS	N-CA-CB	5.13	117.42	110.38
1	A	712	HIS	CA-CB-CG	5.13	118.93	113.80
3	G	712	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	755	THR	CA-CB-OG1	-5.08	101.99	109.60
3	G	295	ARG	CA-CB-CG	-5.05	103.99	114.10
3	G	800	THR	CA-CB-OG1	-5.03	102.05	109.60
1	E	295	ARG	CA-CB-CG	-5.03	104.05	114.10

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Mainchain
1	A	433	PRO	Peptide
1	A	545	ARG	Sidechain
1	A	695	ARG	Sidechain
1	A	702	ARG	Sidechain
1	A	722	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	545	ARG	Sidechain
1	C	608	ARG	Sidechain
1	C	695	ARG	Sidechain
1	C	702	ARG	Sidechain
1	C	722	ARG	Sidechain
1	E	295	ARG	Mainchain
1	E	433	PRO	Peptide
1	E	545	ARG	Sidechain
1	E	6	ARG	Sidechain
1	E	702	ARG	Sidechain
1	E	722	ARG	Sidechain
3	G	295	ARG	Mainchain
3	G	362	ARG	Sidechain
3	G	569	ARG	Sidechain
3	G	702	ARG	Sidechain
3	G	722	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	6626	0	6406	47	0
1	C	6636	0	6405	44	0
1	E	6647	0	6409	40	0
2	B	1026	0	1000	9	0
2	D	1038	0	1005	7	0
2	F	1029	0	1006	4	0
2	H	1028	0	999	8	0
3	G	6619	0	6407	51	0
4	A	94	0	44	1	0
4	C	94	0	44	1	0
4	E	94	0	44	2	0
4	G	94	0	44	1	0
5	A	7	0	0	0	0
5	C	7	0	0	0	0
5	E	7	0	0	0	0
5	G	7	0	0	0	0
6	A	13	0	0	1	0
6	C	13	0	0	1	0
6	E	13	0	0	1	0
6	G	13	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	A	5	0	0	0	0
8	C	5	0	0	0	0
8	E	5	0	0	1	0
8	G	5	0	0	0	0
9	A	18	0	24	4	0
9	B	6	0	8	1	0
9	C	18	0	24	3	0
9	E	24	0	32	8	0
9	G	24	0	32	1	0
10	A	12	0	18	2	0
10	C	12	0	18	2	0
10	D	4	0	6	1	0
10	E	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	G	4	0	6	2	0
11	B	4	0	0	0	0
11	D	4	0	0	0	0
11	F	4	0	0	0	0
11	H	4	0	0	0	0
12	C	7	0	10	2	0
12	H	7	0	10	3	0
13	A	866	0	0	11	0
13	B	143	0	0	5	0
13	C	770	0	0	12	0
13	D	154	0	0	3	0
13	E	830	0	0	13	0
13	F	134	0	0	0	0
13	G	771	0	0	16	0
13	H	137	0	0	2	0
All	All	35090	0	30007	213	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 (213) 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:C:425[B]:GLU:OE1	9:C:906:GOL:O1	1.70	1.08
1:A:4:ASN:O	1:A:6:ARG:N	1.88	1.07
1:A:425[B]:GLU:OE1	9:A:912:GOL:O3	1.77	1.03
1:A:569[B]:ARG:NH1	13:A:1001:HOH:O	1.95	0.99
3:G:273[A]:ILE:HD12	3:G:275:PHE:CE1	2.02	0.95
1:A:142:LEU:O	1:A:146[A]:LEU:HD23	1.71	0.91
1:E:425[A]:GLU:OE1	9:E:907:GOL:O3	1.89	0.90
1:A:274:ILE:HG23	1:A:299[A]:LEU:HD21	1.55	0.89
1:C:299[A]:LEU:CD2	1:C:359[A]:MET:SD	2.61	0.88
1:E:442:GLN:HG3	13:E:1363:HOH:O	1.73	0.88
3:G:273[A]:ILE:HD13	3:G:274:ILE:N	1.94	0.82
2:F:67:THR:HG22	2:F:78[B]:CYS:SG	2.20	0.81
10:A:910:EDO:H22	13:A:1082:HOH:O	1.82	0.80
1:C:299[A]:LEU:HD22	1:C:359[A]:MET:SD	2.23	0.79
1:A:7[B]:ILE:HD11	1:A:84:MET:CE	2.13	0.79
1:C:58:LEU:O	10:C:913:EDO:H21	1.83	0.78
3:G:289:HIS:NE2	12:H:202:PEG:H41	1.98	0.78
1:A:7[B]:ILE:HD11	1:A:84:MET:HE1	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:PRO:O	10:D:202:EDO:H22	1.86	0.75
1:A:146[A]:LEU:HD22	1:A:496:VAL:HG13	1.69	0.74
1:A:358:ASP:HB2	13:A:1633:HOH:O	1.85	0.74
1:C:299[A]:LEU:CD2	1:C:359[A]:MET:HG2	2.18	0.73
10:G:2401:EDO:C2	13:G:2543:HOH:O	2.36	0.73
1:C:299[A]:LEU:HD23	1:C:359[A]:MET:SD	2.29	0.72
1:C:299[A]:LEU:HD21	1:C:359[A]:MET:HG2	1.72	0.72
3:G:359[B]:MET:HG3	13:G:3039:HOH:O	1.91	0.71
1:A:425[B]:GLU:CD	9:A:912:GOL:HO3	1.93	0.70
9:E:909:GOL:H12	13:E:1557:HOH:O	1.90	0.70
1:E:4:ASN:N	13:E:1004:HOH:O	2.24	0.69
1:C:604:ASP:O	1:C:608:ARG:HD3	1.92	0.69
3:G:474:LEU:HD21	3:G:522[A]:GLU:HG3	1.76	0.68
1:A:474:LEU:HD21	1:A:522[A]:GLU:HG3	1.76	0.67
1:C:359[C]:MET:SD	13:C:1734:HOH:O	2.52	0.67
1:A:146[A]:LEU:CD2	1:A:496:VAL:HG22	2.24	0.67
3:G:561[B]:MET:HE1	13:G:3168:HOH:O	1.95	0.67
2:B:80:CYS:HA	9:B:202:GOL:H2	1.75	0.67
1:A:561[B]:MET:HE1	1:A:569[B]:ARG:HD2	1.77	0.67
2:D:5:GLN:NE2	13:D:302:HOH:O	2.28	0.66
1:C:359[C]:MET:HE1	13:C:1380:HOH:O	1.95	0.66
1:E:474:LEU:HD21	1:E:522[B]:GLU:HG3	1.78	0.66
3:G:248[B]:LEU:HD23	13:G:2522:HOH:O	1.96	0.65
2:B:122[B]:ASP:OD2	13:B:301:HOH:O	2.15	0.65
2:H:68:SER:OG	12:H:202:PEG:H11	1.96	0.65
1:C:299[A]:LEU:CD2	1:C:359[A]:MET:CG	2.75	0.64
3:G:273[A]:ILE:CD1	3:G:275:PHE:CE1	2.78	0.64
2:B:122[B]:ASP:OD1	13:B:302:HOH:O	2.15	0.64
1:A:299[A]:LEU:HD22	1:A:299[A]:LEU:N	2.13	0.64
1:C:359[C]:MET:HG3	13:C:1590:HOH:O	1.97	0.64
1:C:3:PRO:HG3	13:C:1700:HOH:O	1.99	0.63
2:B:100:GLU:HG3	13:B:405:HOH:O	1.99	0.62
1:C:474:LEU:HD21	1:C:522[A]:GLU:HG3	1.80	0.62
2:H:79:PRO:HD3	12:H:202:PEG:H12	1.81	0.62
1:A:299[A]:LEU:HD22	1:A:299[A]:LEU:H	1.66	0.61
1:A:4:ASN:C	1:A:6:ARG:H	2.04	0.61
1:E:366:TRP:HE1	9:E:909:GOL:C3	2.13	0.61
3:G:695:ARG:NH2	13:G:2506:HOH:O	2.33	0.60
1:E:258[A]:LYS:HE3	1:E:262:ARG:HE	1.66	0.60
3:G:345:SER:OG	3:G:348:GLU:HG3	2.01	0.60
2:D:75:THR:HG21	13:D:401:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HG23	1:A:299[A]:LEU:CD2	2.30	0.59
1:A:631:ASP:OD1	1:A:634[B]:ARG:NH2	2.29	0.59
3:G:248[B]:LEU:HD12	3:G:290:VAL:HG11	1.85	0.58
1:E:366:TRP:HE1	9:E:909:GOL:H32	1.69	0.58
1:E:362:ARG:HD3	9:E:909:GOL:H31	1.87	0.56
2:B:43:VAL:HB	2:B:44:PRO:HD2	1.88	0.56
3:G:273[A]:ILE:HD12	3:G:275:PHE:CD1	2.40	0.56
1:A:274:ILE:CG2	1:A:299[A]:LEU:HD21	2.31	0.56
3:G:89:LYS:O	9:G:2408:GOL:H12	2.05	0.56
1:A:721[B]:GLU:HG3	13:A:1274:HOH:O	2.05	0.55
3:G:7[B]:ILE:HD11	3:G:84:MET:HE1	1.88	0.55
1:A:475:GLN:HG2	3:G:482:GLN:NE2	2.21	0.55
2:H:18:LYS:HE2	13:H:406:HOH:O	2.07	0.55
2:D:43:VAL:HB	2:D:44[A]:PRO:HD2	1.89	0.55
1:C:437:LYS:HG3	13:C:1490:HOH:O	2.06	0.55
1:E:561[A]:MET:HE3	1:E:566:ILE:HG12	1.89	0.55
3:G:585:GLU:OE2	13:G:2501:HOH:O	2.17	0.55
1:C:3:PRO:CG	13:C:1700:HOH:O	2.55	0.54
1:A:812:GLU:HG2	13:A:1596:HOH:O	2.07	0.54
1:A:7[B]:ILE:HD13	1:A:8:THR:C	2.32	0.54
2:B:75:THR:HG21	13:B:404:HOH:O	2.08	0.54
3:G:332:THR:O	3:G:333:LYS:HE3	2.07	0.54
3:G:404:VAL:HG11	3:G:417:CYS:HB2	1.89	0.54
1:C:404:VAL:HG11	1:C:417:CYS:HB2	1.89	0.54
1:E:810[B]:MET:HE1	13:E:1508:HOH:O	2.08	0.53
3:G:299[A]:LEU:CD2	3:G:359[A]:MET:SD	2.97	0.53
1:E:201:ASN:HB3	1:E:437:LYS:HE2	1.91	0.53
1:C:359[C]:MET:CE	13:C:1380:HOH:O	2.55	0.52
2:H:75:THR:HG21	13:H:401:HOH:O	2.09	0.52
1:E:425[A]:GLU:OE1	9:E:907:GOL:C3	2.57	0.52
2:F:67:THR:CG2	2:F:78[B]:CYS:SG	2.95	0.52
1:E:404:VAL:HG11	1:E:417:CYS:HB2	1.91	0.52
1:A:258:LYS:HG3	13:A:1553:HOH:O	2.08	0.51
1:C:812:GLU:OE2	1:C:815:ARG:NH2	2.32	0.51
3:G:273[A]:ILE:HD13	3:G:273[A]:ILE:C	2.35	0.51
1:C:535:GLU:O	1:C:552[A]:LYS:NZ	2.40	0.51
3:G:149:LYS:NZ	13:G:2518:HOH:O	2.42	0.51
3:G:575:ARG:HD3	13:G:2936:HOH:O	2.10	0.51
1:A:146[A]:LEU:HD21	1:A:496:VAL:HG22	1.93	0.51
1:C:739[A]:ASP:OD2	6:C:905:FC6:N21	2.44	0.51
1:A:319:GLU:OE1	13:A:1003:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:PRO:HG3	1:C:538:LEU:HD13	1.92	0.50
12:C:911:PEG:H42	13:C:1083:HOH:O	2.11	0.50
2:D:41[A]:SER:OG	13:D:301:HOH:O	2.20	0.50
1:E:299[A]:LEU:HD23	1:E:355:VAL:HG11	1.94	0.50
3:G:201:ASN:HB3	3:G:437:LYS:HE2	1.94	0.50
3:G:721:GLU:HG3	13:G:2698:HOH:O	2.11	0.50
4:E:902:MGD:S12	8:E:904:ART:O1	2.70	0.49
3:G:248[B]:LEU:CD1	3:G:290:VAL:HG21	2.41	0.49
1:E:810[B]:MET:HE3	1:E:810[B]:MET:C	2.37	0.49
3:G:299[A]:LEU:HD23	3:G:359[A]:MET:SD	2.52	0.49
3:G:812:GLU:HG2	13:G:3009:HOH:O	2.12	0.49
1:A:404:VAL:HG11	1:A:417:CYS:HB2	1.94	0.49
1:A:811:GLU:HG2	13:A:1492:HOH:O	2.12	0.49
1:A:561[B]:MET:HE3	1:A:566:ILE:HG12	1.94	0.49
3:G:7[B]:ILE:HD13	3:G:7[B]:ILE:C	2.37	0.49
3:G:408:HIS:O	3:G:412[A]:ARG:HD3	2.13	0.48
1:C:408:HIS:O	1:C:412[A]:ARG:HD3	2.14	0.48
1:C:355:VAL:HG13	1:C:359[C]:MET:HE2	1.96	0.48
1:E:201:ASN:O	9:E:910:GOL:H31	2.13	0.48
2:F:18:LYS:HG3	2:F:21:GLU:HG3	1.95	0.48
2:H:65:CYS:SG	2:H:80[B]:CYS:HB2	2.54	0.47
1:C:437:LYS:HG3	13:C:1489:HOH:O	2.14	0.47
1:A:252:GLN:NE2	13:A:1009:HOH:O	2.39	0.47
1:A:812:GLU:OE2	1:A:815:ARG:NH2	2.35	0.47
1:C:252:GLN:OE1	13:C:1001:HOH:O	2.20	0.47
1:E:329:GLU:HG3	13:E:1630:HOH:O	2.15	0.46
10:G:2401:EDO:H22	13:G:2543:HOH:O	2.08	0.46
2:H:43:VAL:HB	2:H:44:PRO:HD2	1.96	0.46
1:A:80:ARG:HD2	10:A:911:EDO:H22	1.96	0.46
1:E:204:CYS:HB3	1:E:207:THR:HG22	1.97	0.46
3:G:248[B]:LEU:HB3	3:G:249:PRO:HD3	1.98	0.46
2:B:44:PRO:HG2	13:B:365:HOH:O	2.15	0.46
1:C:425[B]:GLU:OE2	9:C:906:GOL:H2	2.16	0.46
3:G:385:LYS:HE2	4:G:2403:MGD:S13	2.56	0.46
3:G:299[B]:LEU:HD23	3:G:355:VAL:HG11	1.98	0.46
3:G:533:PRO:HG3	3:G:538:LEU:HD13	1.96	0.46
1:A:297:LEU:HG	1:A:366:TRP:CH2	2.51	0.46
1:A:533:PRO:HG3	1:A:538:LEU:HD13	1.97	0.46
2:D:44[A]:PRO:HB3	13:E:1450:HOH:O	2.16	0.46
1:C:385:LYS:HE2	4:C:902:MGD:S13	2.56	0.46
1:E:533:PRO:HG3	1:E:538:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:NZ	13:A:1004:HOH:O	2.31	0.45
1:E:162[B]:SER:OG	1:E:193:ARG:HD3	2.16	0.45
1:E:385:LYS:HE2	4:E:902:MGD:S13	2.56	0.45
3:G:569:ARG:HD3	13:G:2968:HOH:O	2.16	0.45
1:C:148:LYS:HD3	1:C:577:MET:HE2	1.98	0.45
1:A:425[B]:GLU:OE2	9:A:912:GOL:H31	2.16	0.45
1:E:745:ILE:HD11	1:E:810[B]:MET:HG3	1.98	0.45
1:E:6:ARG:NH1	13:E:1002:HOH:O	2.12	0.45
1:E:744:ASP:OD2	6:E:905:FC6:N24	2.50	0.45
3:G:5:ASP:OD1	3:G:5:ASP:N	2.50	0.45
3:G:374:GLY:O	13:G:2502:HOH:O	2.20	0.45
1:E:186:ALA:HB1	1:E:590:PHE:CD2	2.52	0.44
1:C:201:ASN:HB3	1:C:437:LYS:HE2	1.98	0.44
1:E:810[B]:MET:CE	13:E:1508:HOH:O	2.65	0.44
1:C:561[B]:MET:HE2	1:C:561[B]:MET:HB3	1.85	0.44
1:E:698:LEU:HD11	1:E:802:GLY:HA3	1.99	0.44
1:E:425[A]:GLU:OE2	9:E:907:GOL:H31	2.18	0.43
2:F:18:LYS:H	2:F:18:LYS:HG2	1.63	0.43
3:G:699:ASN:HB3	3:G:770:THR:O	2.18	0.43
1:A:90:ALA:HB3	9:A:908:GOL:C1	2.48	0.43
13:A:1489:HOH:O	2:H:44:PRO:HB3	2.18	0.43
1:A:475:GLN:HG2	3:G:482:GLN:HE22	1.82	0.43
1:E:408:HIS:O	1:E:412[A]:ARG:HD3	2.17	0.43
3:G:89:LYS:HE3	13:G:2857:HOH:O	2.17	0.43
3:G:729:GLU:HA	3:G:760:TYR:O	2.18	0.43
1:C:699:ASN:HB3	1:C:770:THR:O	2.18	0.43
1:E:79:ARG:NH1	13:E:1018:HOH:O	2.45	0.43
3:G:204:CYS:HB3	3:G:207:THR:HG22	2.01	0.43
1:C:297:LEU:HG	1:C:366:TRP:CH2	2.53	0.43
1:E:446:LYS:HG3	13:E:1029:HOH:O	2.18	0.43
3:G:299[A]:LEU:CD2	3:G:359[A]:MET:HG2	2.47	0.43
1:A:385:LYS:HE2	4:A:902:MGD:S13	2.58	0.43
1:A:699:ASN:HB3	1:A:770:THR:O	2.18	0.43
1:E:297:LEU:HG	1:E:366:TRP:CH2	2.54	0.43
1:A:580[A]:LYS:HE3	1:A:580[A]:LYS:HB2	1.74	0.42
1:C:425[B]:GLU:CD	9:C:906:GOL:HO1	2.02	0.42
1:C:698:LEU:HD11	1:C:802:GLY:HA3	2.00	0.42
3:G:248[B]:LEU:HD11	3:G:290:VAL:HG21	2.00	0.42
1:C:608:ARG:HD2	13:C:1060:HOH:O	2.18	0.42
3:G:698:LEU:HD11	3:G:802:GLY:HA3	2.00	0.42
1:E:204:CYS:HB3	1:E:207:THR:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146[A]:LEU:HD22	1:A:496:VAL:CG1	2.46	0.42
1:C:729:GLU:HA	1:C:760:TYR:O	2.20	0.42
10:C:913:EDO:H12	2:D:59:LEU:HD13	2.01	0.42
3:G:812:GLU:OE2	3:G:815:ARG:NH2	2.40	0.42
1:A:146[A]:LEU:CD2	1:A:146[A]:LEU:N	2.82	0.42
1:C:432:TYR:HB2	12:C:911:PEG:H41	2.02	0.42
1:E:699:ASN:HB3	1:E:770:THR:O	2.19	0.42
1:E:505:ASN:OD1	13:E:1003:HOH:O	2.21	0.41
1:A:698:LEU:HD11	1:A:802:GLY:HA3	2.01	0.41
1:C:561[C]:MET:HE2	13:C:1280:HOH:O	2.20	0.41
1:E:4:ASN:C	1:E:6:ARG:H	2.27	0.41
3:G:104:LYS:O	3:G:105:MET:C	2.64	0.41
3:G:273[A]:ILE:CD1	3:G:275:PHE:CD1	3.04	0.41
1:E:162[B]:SER:OG	1:E:193:ARG:CG	2.68	0.41
1:A:7[B]:ILE:HG22	2:B:129:GLN:HA	2.02	0.41
1:E:721:GLU:HG3	13:E:1348:HOH:O	2.19	0.41
1:A:698:LEU:HB2	1:A:800:THR:HG23	2.02	0.41
1:E:348:GLU:HB3	13:E:1597:HOH:O	2.21	0.41
1:E:698:LEU:HB2	1:E:800:THR:HG23	2.02	0.41
2:B:69:TYR:CE2	2:B:71:LYS:HA	2.56	0.41
3:G:410[B]:VAL:HG13	13:G:2855:HOH:O	2.21	0.41
3:G:561[B]:MET:HE3	13:G:3232:HOH:O	2.21	0.41
2:H:69:TYR:CE2	2:H:71:LYS:HA	2.55	0.41
3:G:248[B]:LEU:CD1	3:G:290:VAL:HG11	2.50	0.41
3:G:532:HIS:HB2	3:G:533:PRO:CD	2.51	0.41
1:C:25:ILE:O	1:C:542:ASN:HB2	2.20	0.40
1:C:698:LEU:HB2	1:C:800:THR:HG23	2.03	0.40
1:A:744:ASP:OD2	6:A:904:FC6:N11	2.55	0.40
1:C:104:LYS:O	1:C:105:MET:C	2.65	0.40
1:C:186:ALA:HB1	1:C:590:PHE:CD1	2.56	0.40
1:C:299[A]:LEU:HD22	1:C:359[A]:MET:CG	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	839/823 (102%)	811 (97%)	26 (3%)	2 (0%)	43	22
1	C	841/823 (102%)	811 (96%)	29 (3%)	1 (0%)	48	23
1	E	843/823 (102%)	817 (97%)	24 (3%)	2 (0%)	43	22
2	B	136/134 (102%)	129 (95%)	6 (4%)	1 (1%)	18	4
2	D	138/134 (103%)	129 (94%)	9 (6%)	0	100	100
2	F	137/134 (102%)	130 (95%)	7 (5%)	0	100	100
2	H	137/134 (102%)	130 (95%)	6 (4%)	1 (1%)	18	4
3	G	840/823 (102%)	814 (97%)	26 (3%)	0	100	100
All	All	3911/3828 (102%)	3771 (96%)	133 (3%)	7 (0%)	43	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
2	H	44	PRO
2	B	44	PRO
1	E	5	ASP
1	C	793	ILE
1	A	793	ILE
1	E	793	ILE

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	694/676 (103%)	688 (99%)	6 (1%)	70	44
1	C	696/676 (103%)	686 (99%)	10 (1%)	59	26
1	E	698/676 (103%)	693 (99%)	5 (1%)	76	53
2	B	116/112 (104%)	115 (99%)	1 (1%)	70	44
2	D	118/112 (105%)	116 (98%)	2 (2%)	53	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	117/112 (104%)	115 (98%)	2 (2%)	53	20
2	H	117/112 (104%)	113 (97%)	4 (3%)	32	4
3	G	695/676 (103%)	689 (99%)	6 (1%)	70	44
All	All	3251/3152 (103%)	3215 (99%)	36 (1%)	73	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	299[A]	LEU
1	A	299[B]	LEU
1	A	299[C]	LEU
1	A	410	VAL
1	A	774	PHE
2	B	18	LYS
1	C	79	ARG
1	C	299[A]	LEU
1	C	299[B]	LEU
1	C	540[A]	SER
1	C	540[B]	SER
1	C	540[C]	SER
1	C	569[A]	ARG
1	C	569[B]	ARG
1	C	774	PHE
1	C	800	THR
2	D	84[A]	GLU
2	D	84[B]	GLU
1	E	436	LYS
1	E	585	GLU
1	E	634	ARG
1	E	774	PHE
1	E	800	THR
2	F	0	LEU
2	F	18	LYS
3	G	6	ARG
3	G	273[A]	ILE
3	G	273[B]	ILE
3	G	410[A]	VAL
3	G	410[B]	VAL
3	G	774	PHE
2	H	18	LYS

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Mol	Chain	Res	Type
2	H	44	PRO
2	H	84[A]	GLU
2	H	84[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	505	ASN
1	A	769	GLN
1	C	611	GLN
1	C	688	GLN
1	C	720	GLN
2	D	5	GLN
1	E	157	GLN
1	E	216	ASN
1	E	505	ASN
1	E	611	GLN
1	E	688	GLN
1	E	769	GLN
3	G	216	ASN
3	G	482	GLN
3	G	611	GLN
3	G	792	ASN

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 54 ligands modelled in this entry, 4 are monoatomic - leaving 50 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	GOL	E	909	-	5,5,5	0.17	0	5,5,5	0.67	0
9	GOL	A	907	-	5,5,5	0.25	0	5,5,5	0.41	0
9	GOL	E	908	-	5,5,5	0.36	0	5,5,5	1.06	0
10	EDO	A	910	-	3,3,3	0.38	0	2,2,2	0.53	0
10	EDO	C	912	-	3,3,3	0.46	0	2,2,2	0.48	0
6	FC6	C	905	-	12,12,12	3.75	8 (66%)	-		
11	FES	H	201	2	0,4,4	-	-	-		
11	FES	B	201	2	0,4,4	-	-	-		
9	GOL	E	907	-	5,5,5	0.14	0	5,5,5	0.42	0
5	F3S	A	903	1	0,9,9	-	-	-		
6	FC6	A	904	-	12,12,12	4.01	8 (66%)	-		
10	EDO	A	911	-	3,3,3	1.23	0	2,2,2	0.98	0
12	PEG	C	911	-	6,6,6	0.17	0	5,5,5	0.29	0
5	F3S	C	903	1	0,9,9	-	-	-		
10	EDO	C	913	-	3,3,3	0.57	0	2,2,2	0.32	0
4	MGD	E	901	7	47,52,52	1.50	2 (4%)	58,81,81	1.26	6 (10%)
10	EDO	G	2401	-	3,3,3	0.30	0	2,2,2	0.24	0
4	MGD	E	902	7	47,52,52	0.92	1 (2%)	58,81,81	1.21	7 (12%)
9	GOL	E	910	-	5,5,5	0.21	0	5,5,5	0.71	0
6	FC6	E	905	-	12,12,12	3.47	7 (58%)	-		
9	GOL	G	2408	-	5,5,5	0.66	0	5,5,5	1.36	1 (20%)
9	GOL	G	2410	-	5,5,5	0.27	0	5,5,5	0.50	0
10	EDO	E	911	-	3,3,3	0.91	0	2,2,2	0.40	0
4	MGD	G	2402	7	47,52,52	1.50	3 (6%)	58,81,81	1.09	5 (8%)
4	MGD	A	902	7	47,52,52	0.91	2 (4%)	58,81,81	1.22	4 (6%)
10	EDO	A	909	-	3,3,3	0.18	0	2,2,2	0.77	0
8	ART	A	906	-	3,4,4	2.74	2 (66%)	6,6,6	8.72	5 (83%)
4	MGD	C	902	7	47,52,52	1.13	3 (6%)	58,81,81	1.48	5 (8%)
4	MGD	C	901	7	47,52,52	1.27	2 (4%)	58,81,81	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ART	E	904	-	3,4,4	3.04	1 (33%)	6,6,6	6.93	4 (66%)
9	GOL	A	908	-	5,5,5	0.28	0	5,5,5	0.56	0
10	EDO	D	202	-	3,3,3	0.07	0	2,2,2	0.07	0
9	GOL	A	912	-	5,5,5	0.24	0	5,5,5	0.97	0
11	FES	D	201	2	0,4,4	-	-	-	-	-
8	ART	C	904	-	3,4,4	1.21	0	6,6,6	9.78	6 (100%)
9	GOL	C	907	-	5,5,5	0.22	0	5,5,5	0.72	0
9	GOL	G	2411	-	5,5,5	0.54	0	5,5,5	0.99	0
10	EDO	C	910	-	3,3,3	0.17	0	2,2,2	0.12	0
4	MGD	A	901	7	47,52,52	1.26	4 (8%)	58,81,81	1.12	4 (6%)
5	F3S	G	2404	3	0,9,9	-	-	-	-	-
12	PEG	H	202	-	6,6,6	0.69	0	5,5,5	0.30	0
6	FC6	G	2405	-	12,12,12	3.18	7 (58%)	-	-	-
5	F3S	E	903	1	0,9,9	-	-	-	-	-
8	ART	G	2407	-	3,4,4	3.04	2 (66%)	6,6,6	9.23	5 (83%)
9	GOL	B	202	-	5,5,5	0.16	0	5,5,5	0.37	0
4	MGD	G	2403	7	47,52,52	0.82	1 (2%)	58,81,81	1.34	5 (8%)
11	FES	F	201	2	0,4,4	-	-	-	-	-
9	GOL	G	2409	-	5,5,5	0.31	0	5,5,5	1.14	0
9	GOL	C	908	-	5,5,5	0.51	0	5,5,5	1.48	1 (20%)
9	GOL	C	906	-	5,5,5	0.43	0	5,5,5	0.77	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	GOL	E	909	-	-	3/4/4/4	-
9	GOL	A	907	-	-	0/4/4/4	-
9	GOL	E	908	-	-	2/4/4/4	-
10	EDO	A	910	-	-	1/1/1/1	-
10	EDO	C	912	-	-	1/1/1/1	-
11	FES	H	201	2	-	-	0/1/1/1
11	FES	B	201	2	-	-	0/1/1/1
9	GOL	E	907	-	-	0/4/4/4	-
5	F3S	A	903	1	-	-	0/3/3/3
10	EDO	A	911	-	-	1/1/1/1	-
12	PEG	C	911	-	-	2/4/4/4	-
5	F3S	C	903	1	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	C	913	-	-	1/1/1/1	-
4	MGD	E	901	7	-	4/22/66/66	0/6/6/6
10	EDO	G	2401	-	-	0/1/1/1	-
4	MGD	E	902	7	-	5/22/66/66	0/6/6/6
9	GOL	E	910	-	-	2/4/4/4	-
9	GOL	G	2410	-	-	2/4/4/4	-
9	GOL	G	2408	-	-	0/4/4/4	-
10	EDO	E	911	-	-	1/1/1/1	-
4	MGD	G	2402	7	-	4/22/66/66	0/6/6/6
4	MGD	A	902	7	-	5/22/66/66	0/6/6/6
10	EDO	A	909	-	-	0/1/1/1	-
9	GOL	A	908	-	-	0/4/4/4	-
4	MGD	C	902	7	-	4/22/66/66	0/6/6/6
4	MGD	C	901	7	-	4/22/66/66	0/6/6/6
10	EDO	D	202	-	-	1/1/1/1	-
9	GOL	A	912	-	-	0/4/4/4	-
11	FES	D	201	2	-	-	0/1/1/1
9	GOL	C	907	-	-	0/4/4/4	-
9	GOL	G	2411	-	-	0/4/4/4	-
10	EDO	C	910	-	-	1/1/1/1	-
4	MGD	A	901	7	-	4/22/66/66	0/6/6/6
5	F3S	G	2404	3	-	-	0/3/3/3
12	PEG	H	202	-	-	4/4/4/4	-
5	F3S	E	903	1	-	-	0/3/3/3
11	FES	F	201	2	-	-	0/1/1/1
9	GOL	B	202	-	-	1/4/4/4	-
4	MGD	G	2403	7	-	5/22/66/66	0/6/6/6
9	GOL	G	2409	-	-	2/4/4/4	-
9	GOL	C	908	-	-	2/4/4/4	-
9	GOL	C	906	-	-	3/4/4/4	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	904	FC6	C23-FE2	-8.69	1.68	1.93
6	C	905	FC6	C21-FE2	-8.59	1.68	1.93
4	E	901	MGD	C23-C14	-8.13	1.47	1.53
6	E	905	FC6	C21-FE2	-7.25	1.72	1.93
6	A	904	FC6	C21-FE2	-6.49	1.74	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	MGD	PA-O3B	6.47	1.66	1.59
4	G	2402	MGD	C23-C14	-6.39	1.48	1.53
6	E	905	FC6	C23-FE2	-6.33	1.75	1.93
6	C	905	FC6	C23-FE2	-6.18	1.75	1.93
6	G	2405	FC6	C21-FE2	-5.97	1.76	1.93
6	G	2405	FC6	C23-FE2	-5.72	1.77	1.93
4	G	2402	MGD	PA-O3B	5.59	1.65	1.59
8	E	904	ART	O1-AS	5.10	1.86	1.69
4	A	901	MGD	C23-C14	-5.08	1.49	1.53
6	A	904	FC6	C22-FE2	-4.89	1.79	1.93
6	E	905	FC6	C22-FE2	-4.63	1.80	1.93
6	C	905	FC6	C22-FE2	-4.41	1.81	1.93
6	G	2405	FC6	C26-FE2	-4.16	1.81	1.93
6	A	904	FC6	C24-FE2	-4.13	1.81	1.93
4	C	902	MGD	C23-C14	-3.98	1.50	1.53
8	A	906	ART	O3-AS	3.90	1.82	1.69
8	G	2407	ART	O1-AS	3.83	1.82	1.69
6	E	905	FC6	C26-FE2	-3.37	1.84	1.93
6	G	2405	FC6	C22-FE2	-3.37	1.84	1.93
6	C	905	FC6	C24-FE2	-3.34	1.84	1.93
6	C	905	FC6	C26-FE2	-3.26	1.84	1.93
4	A	901	MGD	PA-O3B	3.20	1.62	1.59
8	G	2407	ART	O3-AS	3.16	1.80	1.69
4	C	901	MGD	C23-C14	-3.15	1.51	1.53
6	A	904	FC6	C26-N21	3.09	1.21	1.15
6	A	904	FC6	C26-FE2	-3.06	1.84	1.93
6	G	2405	FC6	C22-N22	2.91	1.21	1.15
4	C	902	MGD	C19-N20	-2.76	1.26	1.33
4	E	901	MGD	PA-O3B	2.61	1.62	1.59
4	C	902	MGD	PA-O3B	2.50	1.62	1.59
8	A	906	ART	O1-AS	2.49	1.77	1.69
6	A	904	FC6	C21-N25	2.46	1.20	1.15
6	G	2405	FC6	C11-FE2	-2.36	1.86	1.93
4	A	902	MGD	C23-N22	-2.34	1.41	1.45
6	E	905	FC6	C21-N25	2.33	1.20	1.15
6	C	905	FC6	C11-FE2	-2.32	1.87	1.93
4	E	902	MGD	PB-O3B	2.31	1.62	1.59
4	A	902	MGD	PB-O3B	2.31	1.62	1.59
6	E	905	FC6	C11-FE2	-2.31	1.87	1.93
4	G	2402	MGD	C23-N22	-2.29	1.41	1.45
6	E	905	FC6	C26-N21	2.28	1.20	1.15
4	A	901	MGD	PA-O2A	-2.23	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	905	FC6	C23-N23	2.21	1.20	1.15
6	G	2405	FC6	C24-FE2	-2.18	1.87	1.93
4	A	901	MGD	C21-N22	2.14	1.37	1.35
4	G	2403	MGD	PA-O2A	-2.14	1.45	1.55
6	A	904	FC6	C11-FE2	-2.10	1.87	1.93
6	C	905	FC6	C21-N25	-2.09	1.11	1.15

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	904	ART	O3-AS-O4	20.79	171.23	111.50
8	G	2407	ART	O3-AS-O1	19.60	169.74	107.31
8	A	906	ART	O3-AS-O1	18.55	166.40	107.31
8	E	904	ART	O1-AS-O4	14.19	152.27	111.50
8	E	904	ART	O3-AS-O4	-7.35	90.39	111.50
8	C	904	ART	O1-AS-O4	-6.83	91.86	111.50
4	C	902	MGD	C23-C14-N15	6.33	114.09	107.87
8	G	2407	ART	O3-AS-O2	-6.06	88.00	107.31
8	A	906	ART	O3-AS-O4	-6.06	94.10	111.50
8	G	2407	ART	O1-AS-O4	-6.01	94.22	111.50
8	C	904	ART	O3-AS-O1	-5.95	88.37	107.31
8	A	906	ART	O1-AS-O4	-5.92	94.49	111.50
8	G	2407	ART	O3-AS-O4	-5.73	95.04	111.50
8	C	904	ART	O2-AS-O4	-5.55	95.54	111.50
4	G	2403	MGD	C23-C14-N15	5.48	113.25	107.87
4	A	902	MGD	C23-C14-N15	5.46	113.23	107.87
8	A	906	ART	O3-AS-O2	-5.25	90.59	107.31
8	E	904	ART	O2-AS-O4	-4.78	97.78	111.50
8	C	904	ART	O3-AS-O2	-4.72	92.27	107.31
8	G	2407	ART	O2-AS-O1	-4.61	92.64	107.31
4	C	901	MGD	O11-C23-N22	-4.32	104.69	108.61
4	C	902	MGD	O11-C23-C14	4.14	111.73	108.96
4	E	901	MGD	C23-C14-N15	3.67	111.47	107.87
4	A	901	MGD	O11-C23-C14	3.65	111.40	108.96
4	E	901	MGD	O2B-PB-O3B	3.58	116.95	107.27
8	A	906	ART	O2-AS-O1	-3.50	96.16	107.31
4	C	902	MGD	C19-N20-C21	3.49	119.51	113.36
4	E	901	MGD	O11-C23-N22	-3.48	105.45	108.61
4	G	2403	MGD	O11-C23-N22	-3.46	105.46	108.61
4	C	902	MGD	O11-C23-N22	-3.46	105.47	108.61
4	E	902	MGD	C17-C16-N15	3.40	125.54	116.27
4	A	902	MGD	O11-C23-C14	3.39	111.23	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	902	MGD	C23-C14-N15	3.38	111.19	107.87
4	C	901	MGD	C4'-O4'-C1'	-3.24	102.31	109.47
4	E	901	MGD	C4'-O4'-C1'	-3.19	102.42	109.47
4	G	2403	MGD	C19-N20-C21	3.18	118.97	113.36
4	G	2402	MGD	O11-C23-C14	3.13	111.05	108.96
4	A	901	MGD	C4'-O4'-C1'	-3.10	102.62	109.47
4	E	902	MGD	O11-C23-N22	-3.02	105.86	108.61
4	G	2402	MGD	C4'-O4'-C1'	-3.02	102.81	109.47
4	E	901	MGD	O11-C23-C14	3.01	110.97	108.96
4	A	901	MGD	C23-C14-N15	3.00	110.81	107.87
8	E	904	ART	O3-AS-O1	-2.70	98.72	107.31
8	C	904	ART	O2-AS-O1	2.58	115.51	107.31
4	A	902	MGD	C19-N20-C21	2.54	117.83	113.36
4	C	902	MGD	C17-C16-N15	2.53	123.18	116.27
9	G	2408	GOL	O2-C2-C3	2.53	119.67	109.18
9	C	908	GOL	O1-C1-C2	2.51	121.66	110.38
4	E	902	MGD	O3A-C10-C11	-2.51	102.39	108.58
4	G	2402	MGD	O4'-C1'-C2'	-2.39	101.50	106.62
4	G	2403	MGD	C17-C16-N15	2.34	122.65	116.27
4	G	2402	MGD	O3B-PB-O1B	-2.24	103.95	110.70
4	E	902	MGD	O2A-PA-O1A	2.23	122.84	112.44
4	A	902	MGD	O2A-PA-O1A	2.22	122.79	112.44
4	G	2403	MGD	O2A-PA-O1A	2.18	122.57	112.44
4	E	901	MGD	C19-N20-C21	2.15	117.16	113.36
4	A	901	MGD	O4'-C1'-C2'	-2.15	102.01	106.62
4	G	2402	MGD	O2A-PA-O1A	2.12	122.30	112.44
4	E	902	MGD	C19-N20-C21	2.11	117.08	113.36
4	E	902	MGD	O4'-C4'-C3'	2.04	109.21	105.15
4	C	901	MGD	O11-C23-C14	2.02	110.31	108.96

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	MGD	PA-O3B-PB-O5'
4	A	901	MGD	C5'-O5'-PB-O1B
4	A	901	MGD	C5'-O5'-PB-O3B
4	A	902	MGD	PA-O3B-PB-O5'
4	A	902	MGD	C5'-O5'-PB-O1B
4	C	901	MGD	C5'-O5'-PB-O1B
4	C	901	MGD	C5'-O5'-PB-O3B
4	C	902	MGD	PA-O3B-PB-O5'

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Mol	Chain	Res	Type	Atoms
4	C	902	MGD	C5'-O5'-PB-O1B
4	E	901	MGD	PA-O3B-PB-O5'
4	E	901	MGD	C5'-O5'-PB-O1B
4	E	901	MGD	C5'-O5'-PB-O3B
4	E	902	MGD	PA-O3B-PB-O5'
4	E	902	MGD	C5'-O5'-PB-O1B
4	G	2402	MGD	C5'-O5'-PB-O1B
4	G	2402	MGD	C5'-O5'-PB-O3B
4	G	2403	MGD	PA-O3B-PB-O5'
4	G	2403	MGD	C5'-O5'-PB-O1B
9	C	906	GOL	C1-C2-C3-O3
9	C	908	GOL	O1-C1-C2-C3
9	E	908	GOL	O1-C1-C2-C3
9	E	910	GOL	O1-C1-C2-C3
9	G	2409	GOL	O1-C1-C2-C3
9	G	2410	GOL	C1-C2-C3-O3
9	G	2410	GOL	O2-C2-C3-O3
9	C	906	GOL	O2-C2-C3-O3
9	E	908	GOL	O1-C1-C2-O2
12	C	911	PEG	O2-C3-C4-O4
9	C	906	GOL	O1-C1-C2-C3
9	E	909	GOL	C1-C2-C3-O3
9	C	908	GOL	O1-C1-C2-O2
9	G	2409	GOL	O1-C1-C2-O2
4	C	902	MGD	O4'-C4'-C5'-O5'
4	C	902	MGD	C3'-C4'-C5'-O5'
10	A	911	EDO	O1-C1-C2-O2
9	E	910	GOL	O1-C1-C2-O2
4	A	902	MGD	O4'-C4'-C5'-O5'
4	E	902	MGD	O4'-C4'-C5'-O5'
12	C	911	PEG	O1-C1-C2-O2
4	G	2403	MGD	O4'-C4'-C5'-O5'
4	A	902	MGD	C3'-C4'-C5'-O5'
4	C	901	MGD	PA-O3B-PB-O5'
4	G	2402	MGD	PA-O3B-PB-O5'
9	E	909	GOL	O1-C1-C2-C3
12	H	202	PEG	C4-C3-O2-C2
12	H	202	PEG	C1-C2-O2-C3
10	A	910	EDO	O1-C1-C2-O2
4	E	901	MGD	PB-O3B-PA-O1A
12	H	202	PEG	O2-C3-C4-O4
10	E	911	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	C	913	EDO	O1-C1-C2-O2
4	E	902	MGD	C3'-C4'-C5'-O5'
9	B	202	GOL	O1-C1-C2-O2
10	C	910	EDO	O1-C1-C2-O2
10	C	912	EDO	O1-C1-C2-O2
10	D	202	EDO	O1-C1-C2-O2
9	E	909	GOL	O2-C2-C3-O3
4	E	902	MGD	PB-O3B-PA-O2A
12	H	202	PEG	O1-C1-C2-O2
4	G	2403	MGD	C3'-C4'-C5'-O5'
4	A	901	MGD	PB-O3B-PA-O2A
4	A	902	MGD	PB-O3B-PA-O2A
4	C	901	MGD	PB-O3B-PA-O2A
4	G	2402	MGD	PB-O3B-PA-O2A
4	G	2403	MGD	PB-O3B-PA-O2A

There are no ring outliers.

23 monomers are involved in 37 short contacts:

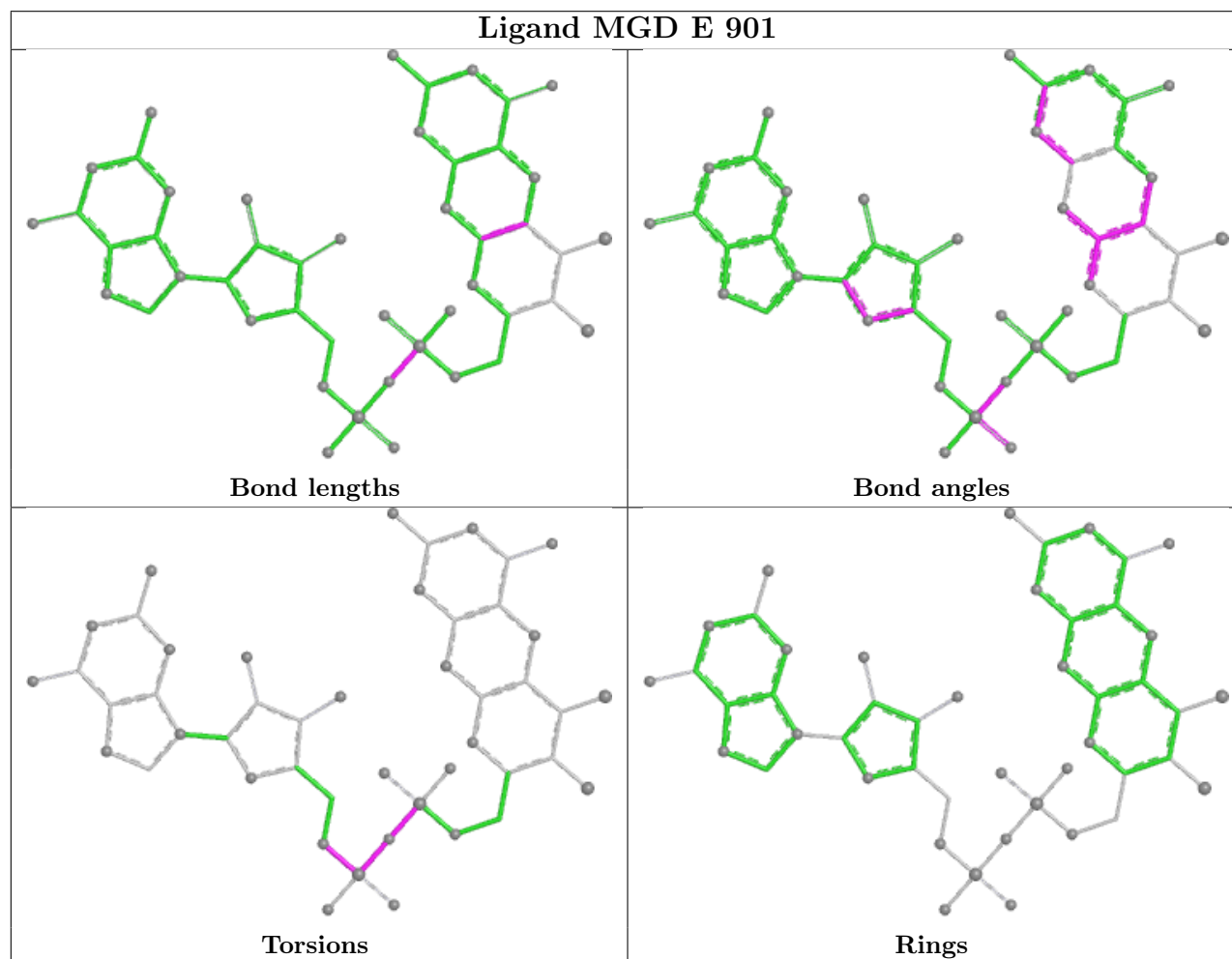
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	909	GOL	4	0
10	A	910	EDO	1	0
6	C	905	FC6	1	0
9	E	907	GOL	3	0
6	A	904	FC6	1	0
10	A	911	EDO	1	0
12	C	911	PEG	2	0
10	C	913	EDO	2	0
10	G	2401	EDO	2	0
4	E	902	MGD	2	0
9	E	910	GOL	1	0
6	E	905	FC6	1	0
9	G	2408	GOL	1	0
4	A	902	MGD	1	0
4	C	902	MGD	1	0
8	E	904	ART	1	0
9	A	908	GOL	1	0
10	D	202	EDO	1	0
9	A	912	GOL	3	0
12	H	202	PEG	3	0
9	B	202	GOL	1	0
4	G	2403	MGD	1	0

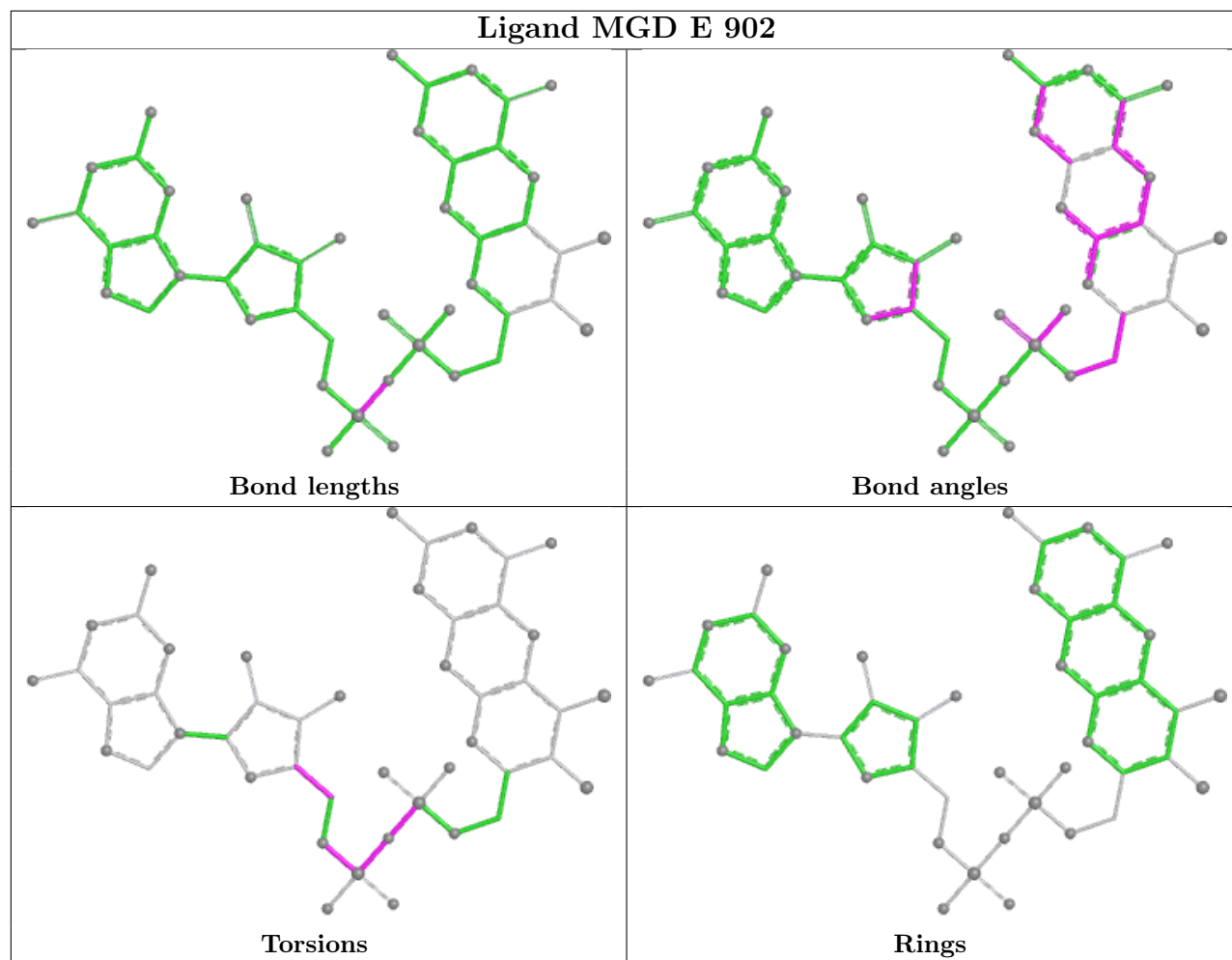
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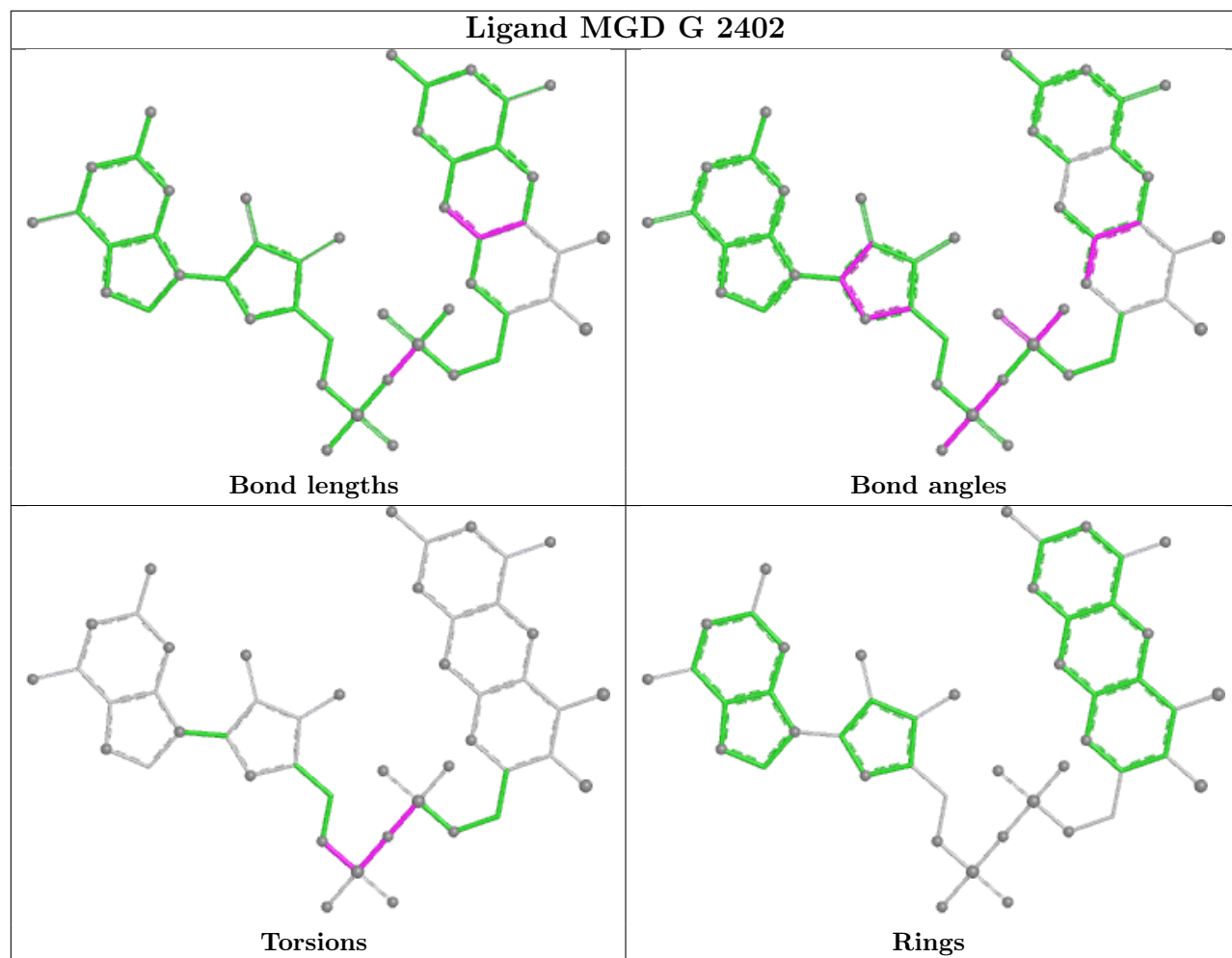
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	906	GOL	3	0

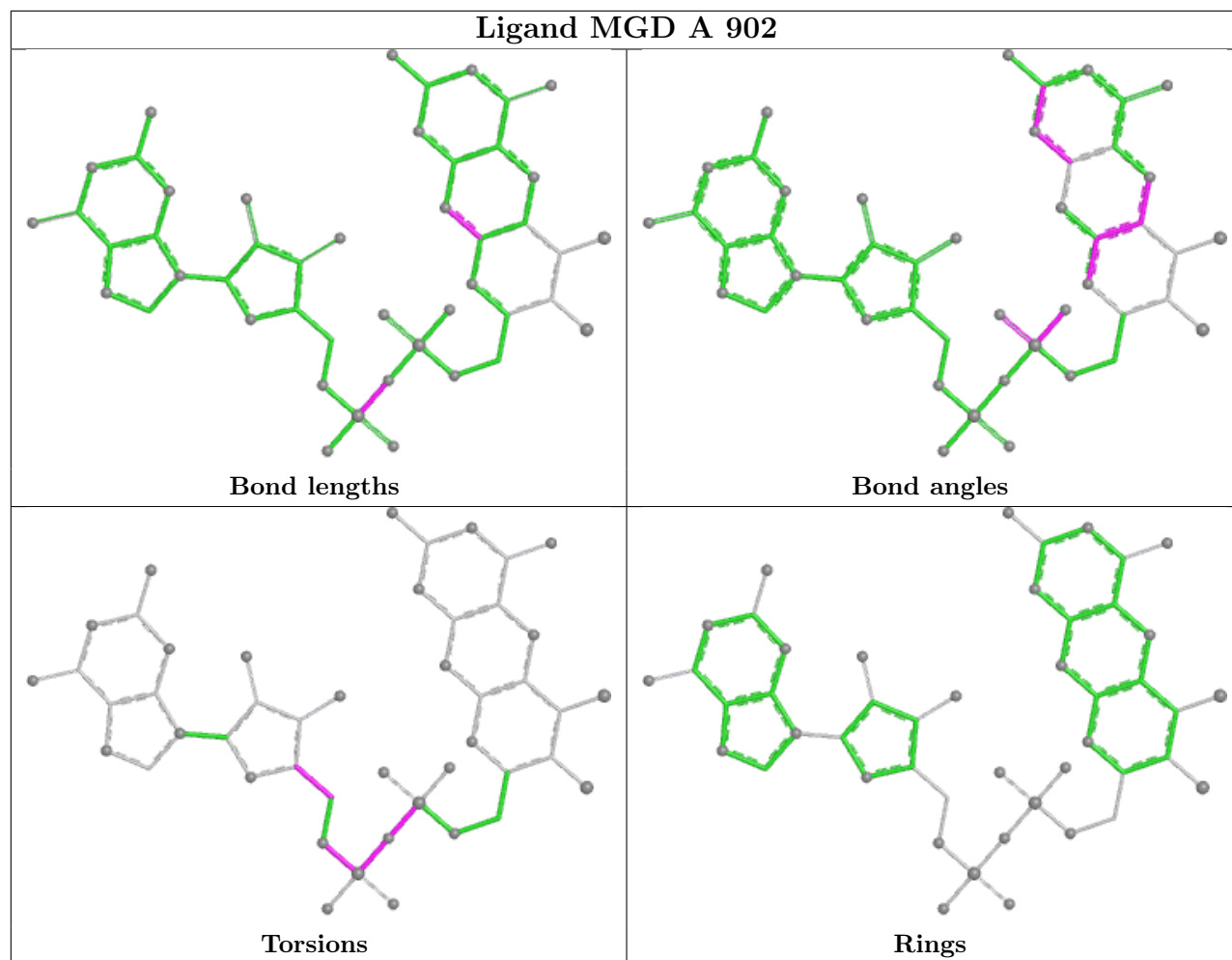
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

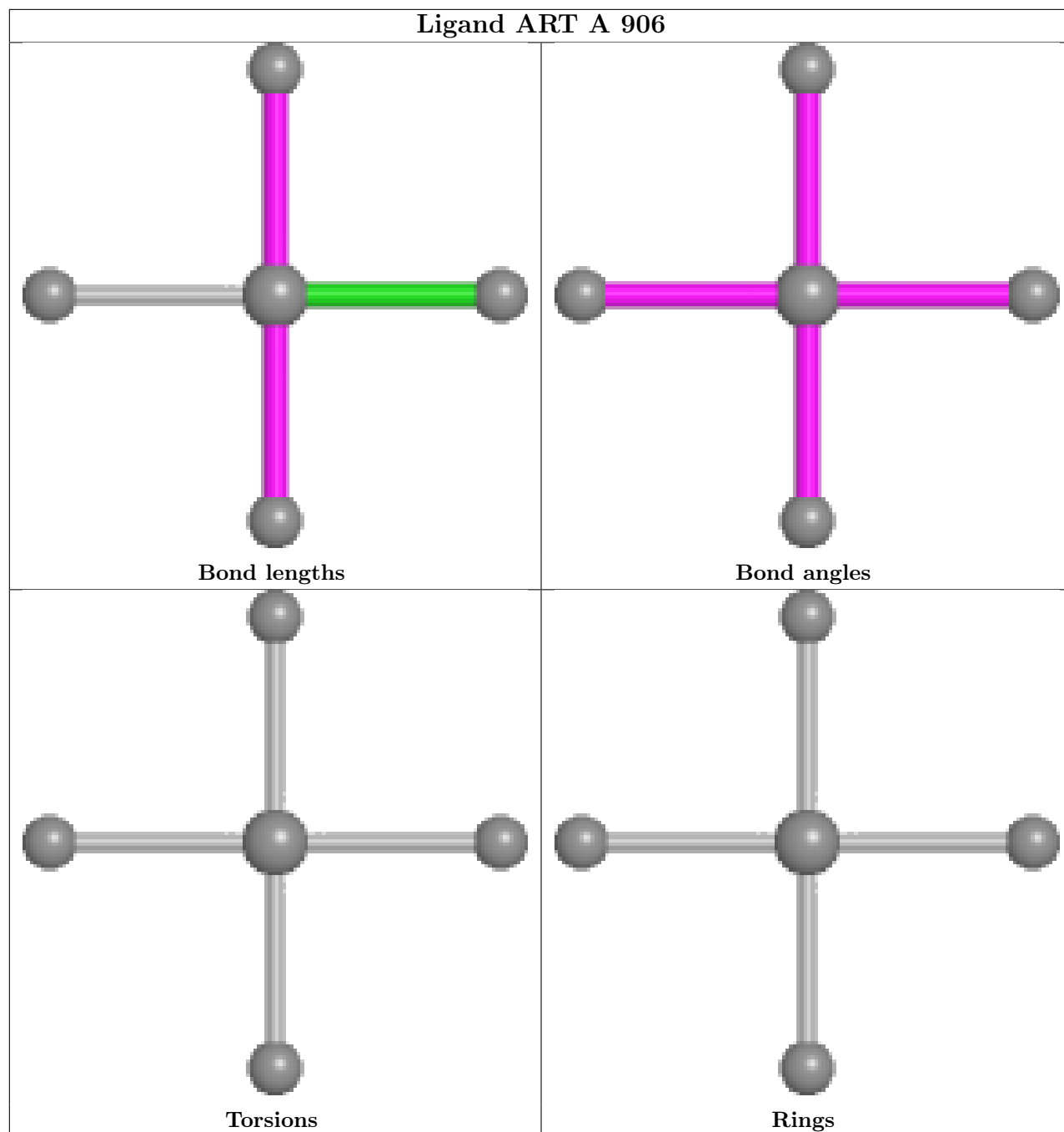


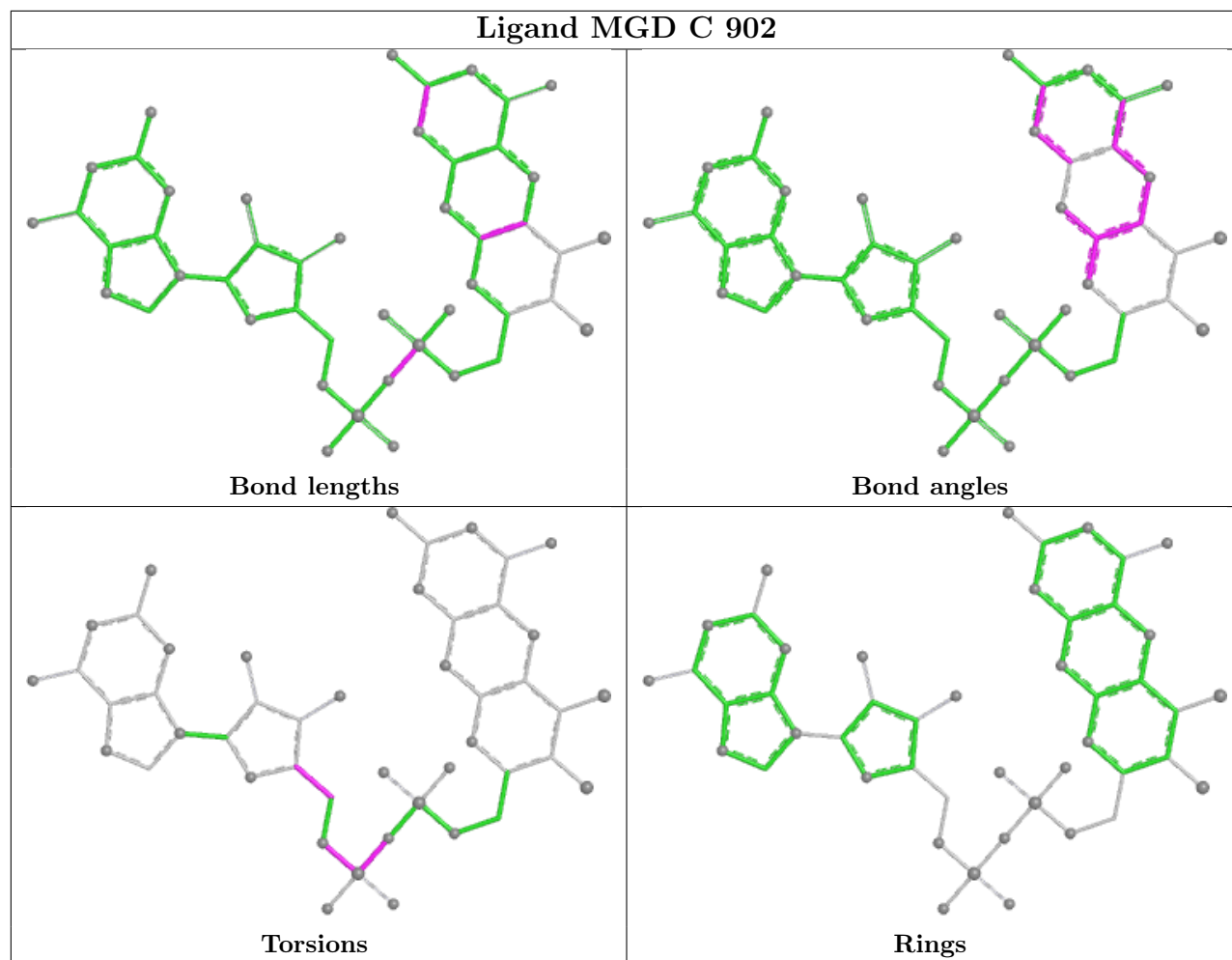


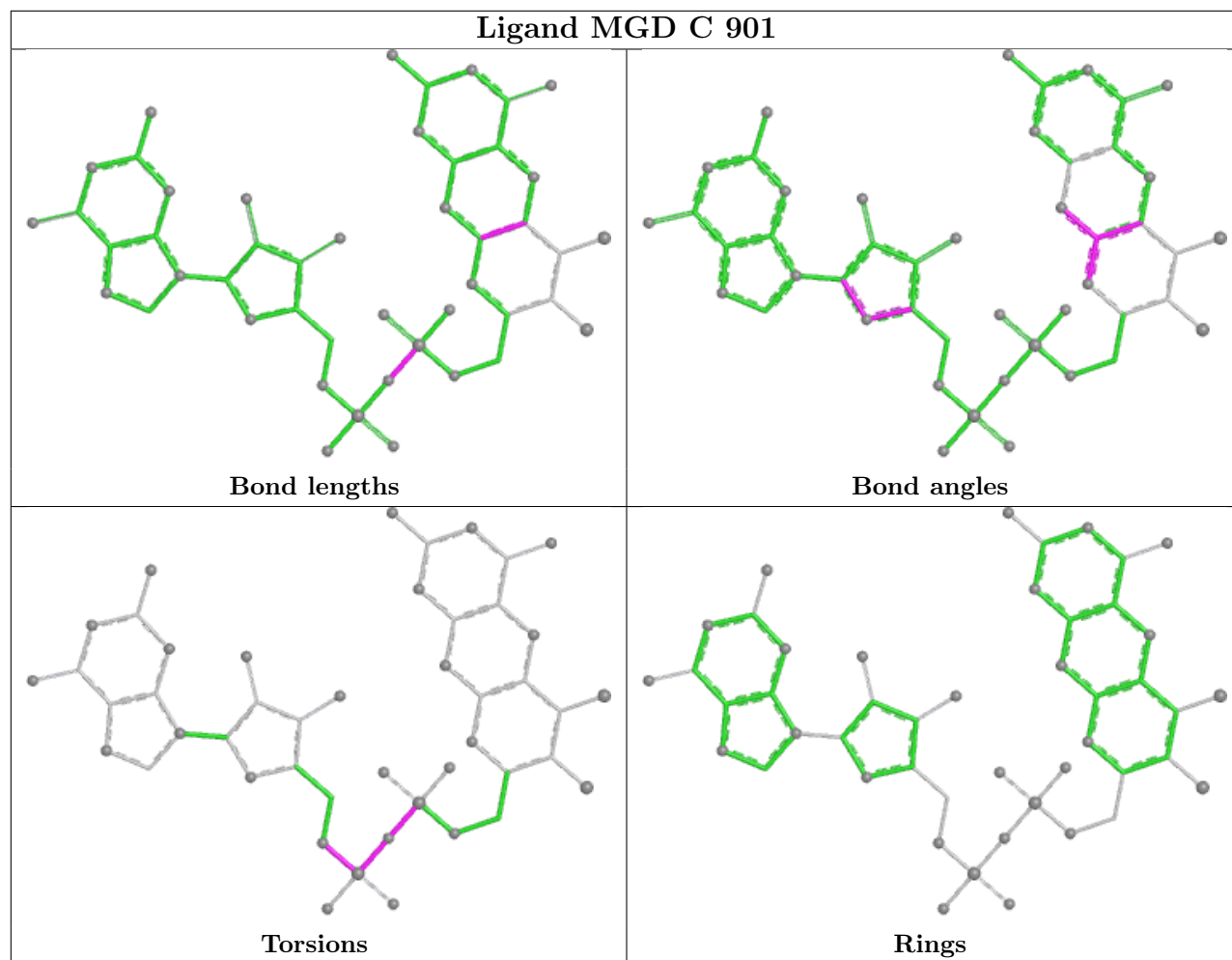
Ligand MGD G 2402

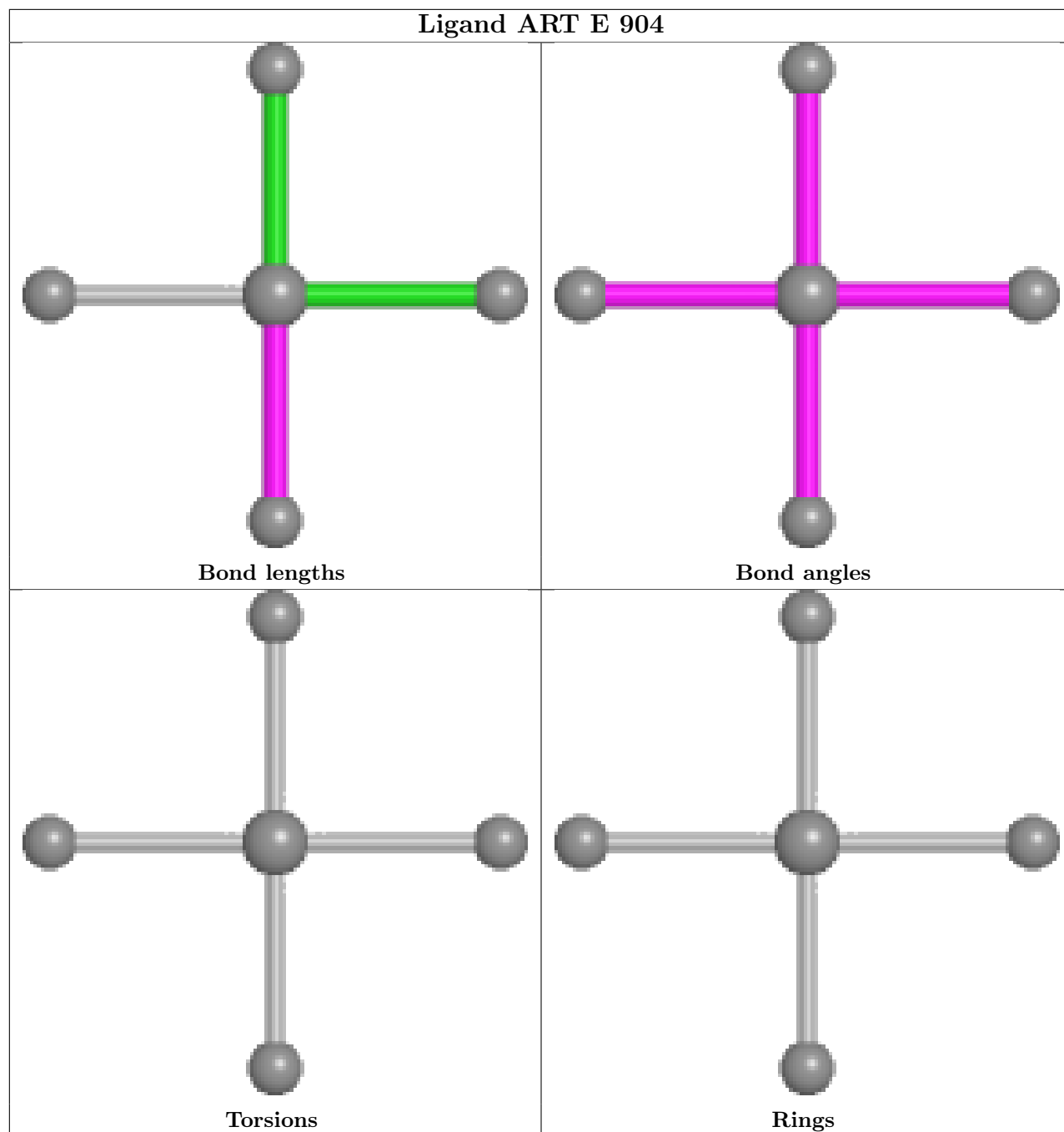


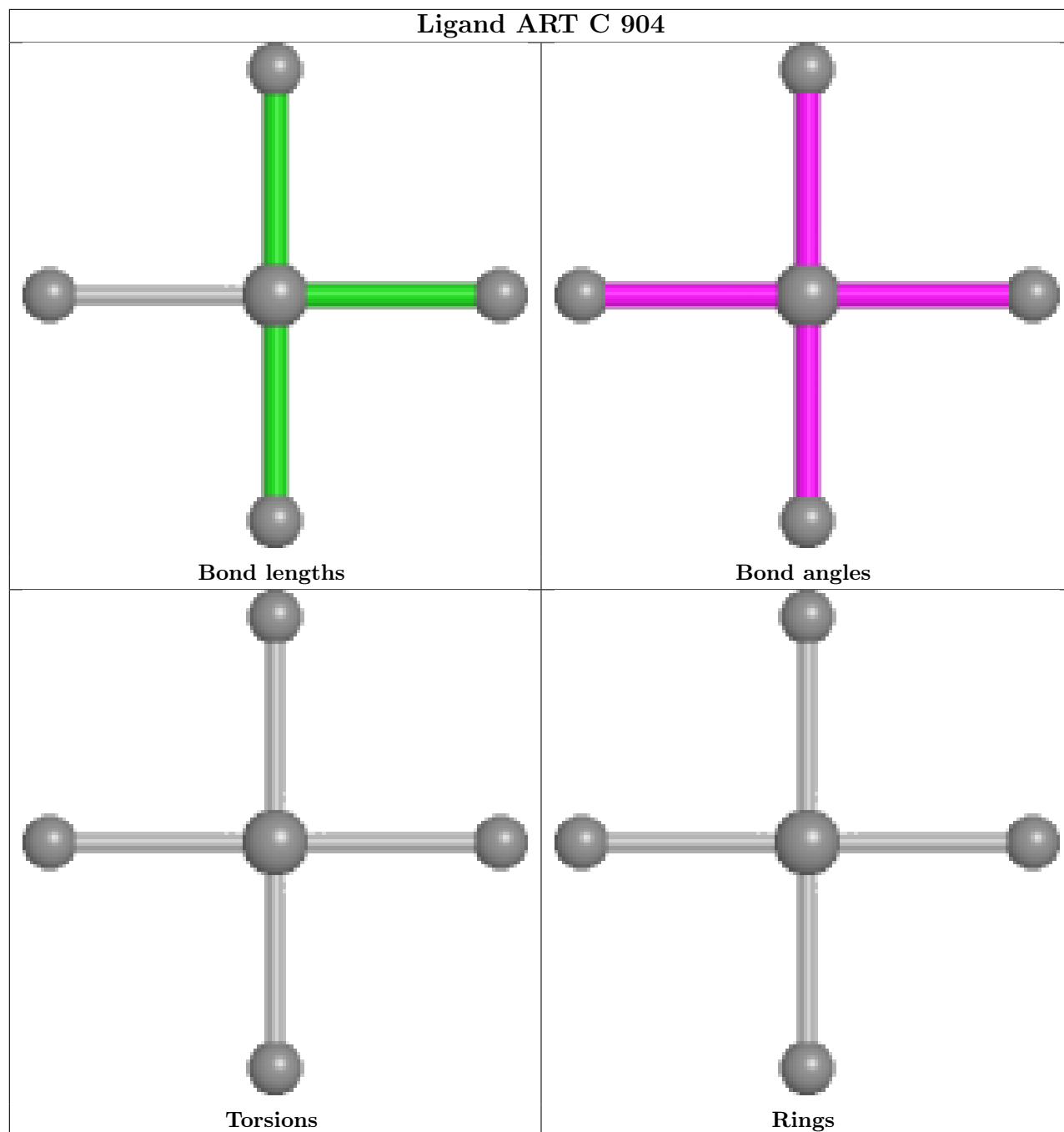


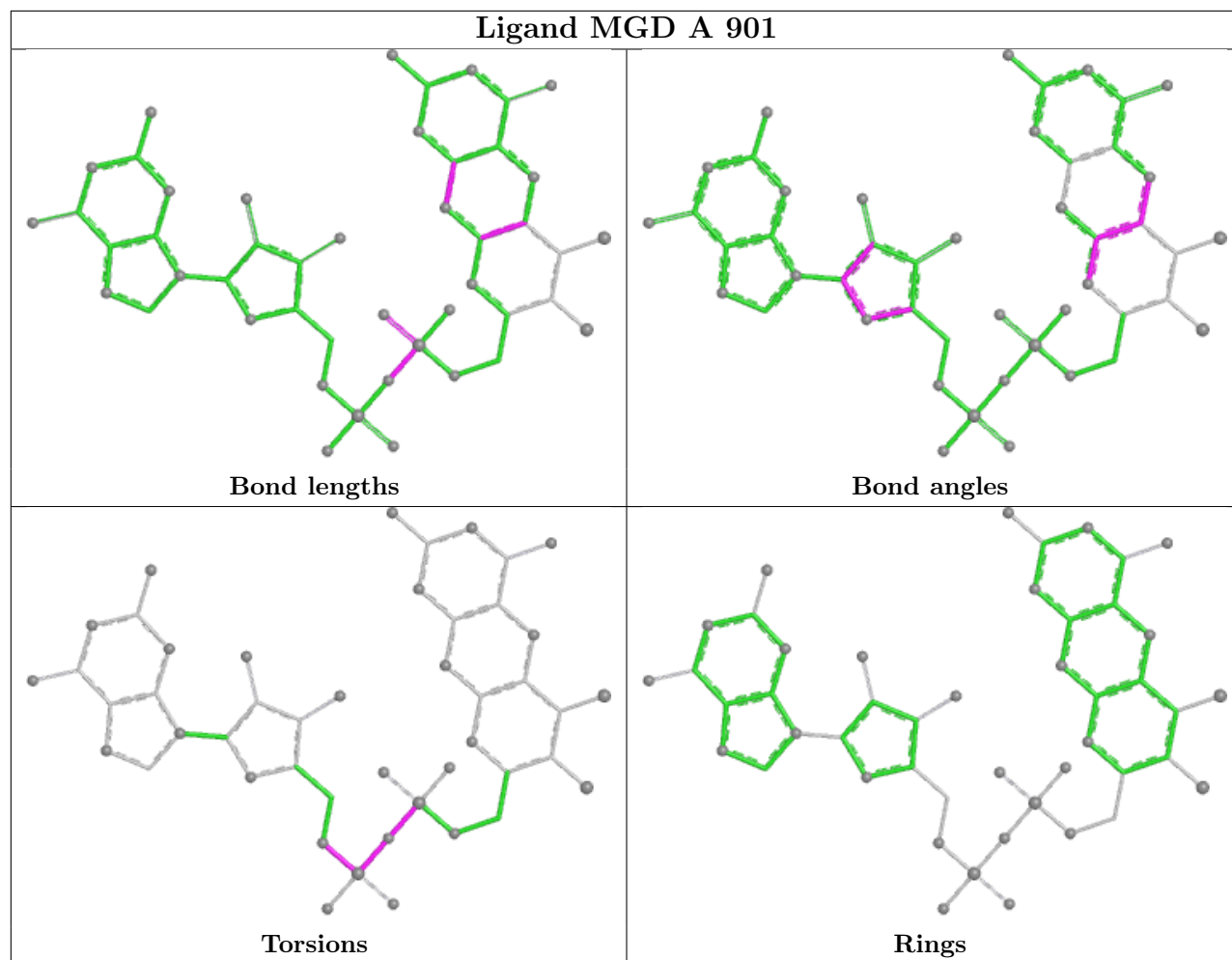


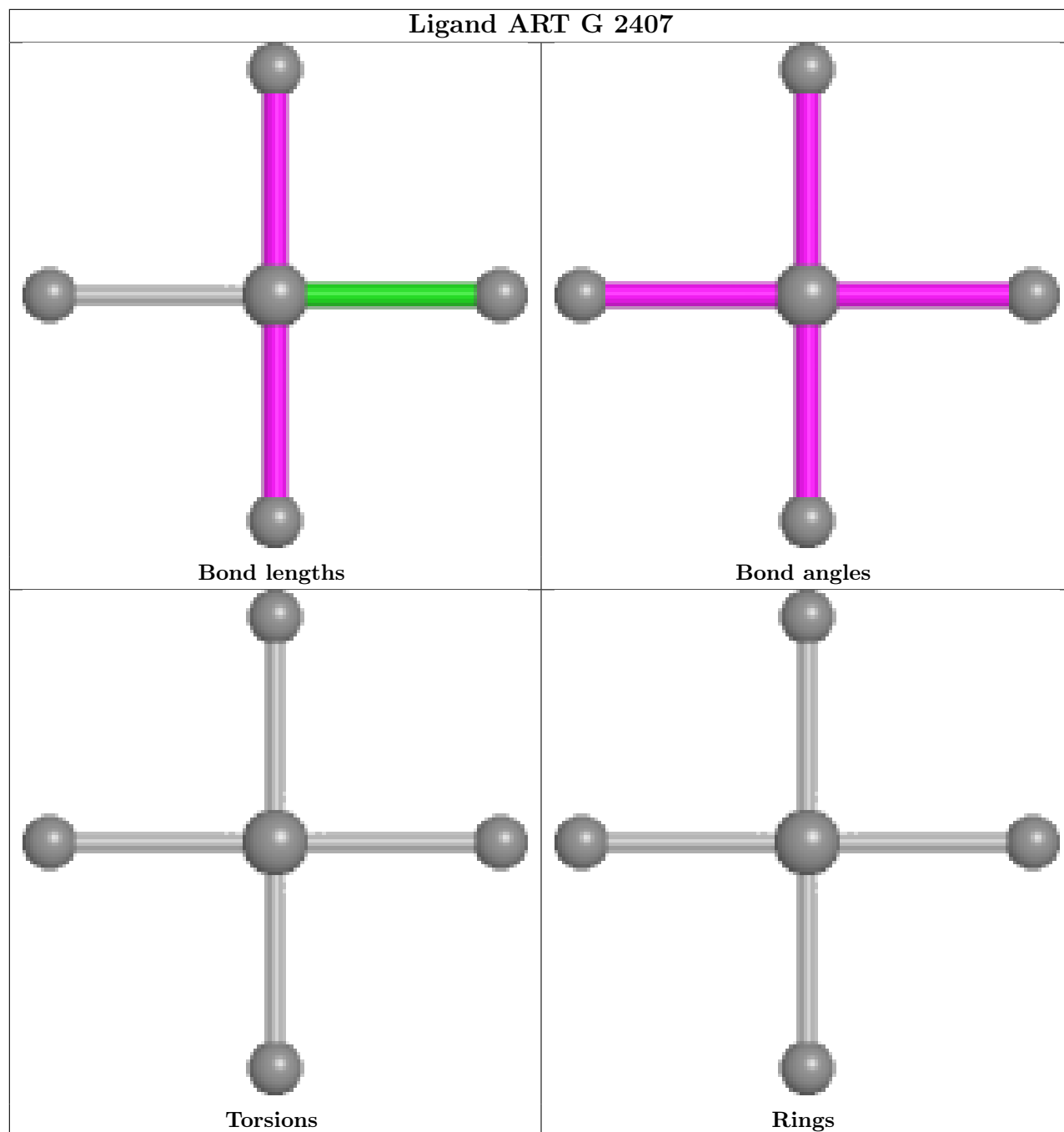


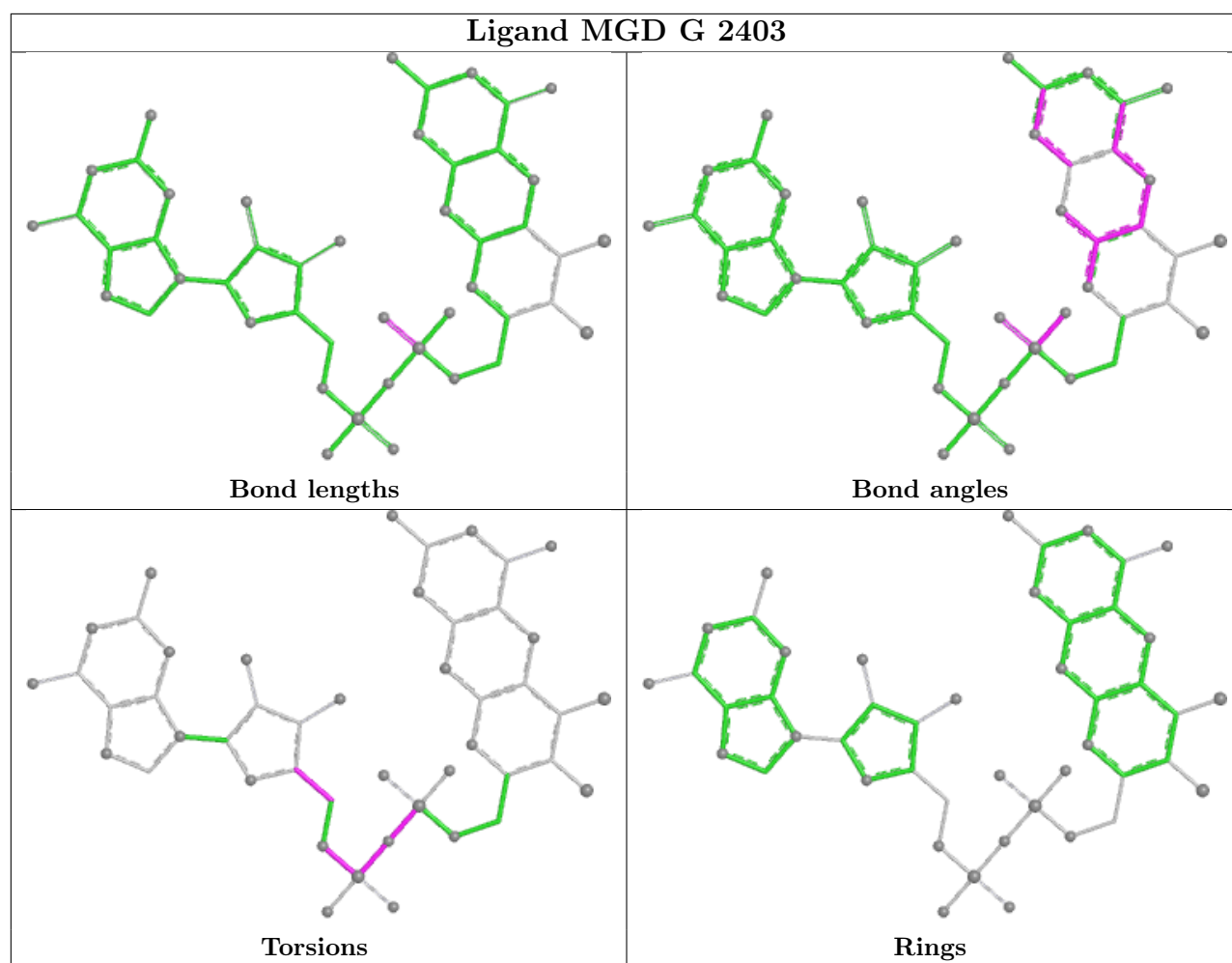












5.7 Other polymers [i](#)

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	822/823 (99%)	-0.30	12 (1%) 72 76	3, 12, 26, 46	21 (2%)
1	C	823/823 (100%)	-0.09	9 (1%) 78 82	4, 14, 28, 61	23 (2%)
1	E	822/823 (99%)	-0.16	7 (0%) 81 85	5, 13, 26, 59	28 (3%)
2	B	134/134 (100%)	-0.03	4 (2%) 52 56	6, 14, 28, 47	4 (2%)
2	D	133/134 (99%)	-0.08	5 (3%) 44 47	6, 14, 26, 49	8 (6%)
2	F	134/134 (100%)	0.06	4 (2%) 52 56	6, 14, 29, 49	6 (4%)
2	H	133/134 (99%)	-0.07	4 (3%) 52 56	6, 14, 27, 42	6 (4%)
3	G	821/823 (99%)	-0.17	5 (0%) 85 89	4, 14, 27, 51	21 (2%)
All	All	3822/3828 (99%)	-0.16	50 (1%) 75 79	3, 13, 27, 61	117 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	PRO	8.4
2	F	0	LEU	6.7
2	B	0	LEU	6.6
2	F	44	PRO	6.0
2	D	44[A]	PRO	5.5
1	E	4	ASN	4.7
2	H	44	PRO	4.6
1	A	4	ASN	4.4
2	B	44	PRO	3.9
3	G	5	ASP	3.6
1	C	4	ASN	3.6
1	C	5	ASP	3.3
1	A	5	ASP	3.2
1	A	299[A]	LEU	3.1
1	A	435	ASP	3.0
1	A	582	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	580[A]	LYS	2.8
1	A	825	ALA	2.7
1	E	435	ASP	2.7
1	C	333	LYS	2.6
3	G	582	GLY	2.6
1	C	584	ALA	2.6
2	D	1	ARG	2.6
2	D	4	LEU	2.5
2	F	45	GLY	2.4
1	A	7[A]	ILE	2.4
1	E	493	GLU	2.3
1	E	6	ARG	2.3
2	H	45	GLY	2.3
2	B	72	SER	2.3
1	A	581	ASP	2.2
1	E	5	ASP	2.2
1	A	695	ARG	2.2
1	A	585	GLU	2.2
1	C	437	LYS	2.2
3	G	435	ASP	2.2
1	A	146[A]	LEU	2.2
2	B	45	GLY	2.2
2	D	2	THR	2.1
1	C	613	GLY	2.1
1	E	811	GLU	2.1
1	C	583	LYS	2.1
1	E	437	LYS	2.1
2	H	1	ARG	2.1
3	G	434	GLY	2.1
3	G	581	ASP	2.1
2	D	18	LYS	2.0
2	F	1	ARG	2.0
2	H	41	SER	2.0
1	C	435	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
10	EDO	A	909	4/4	0.67	0.21	33,39,39,44	0
10	EDO	C	912	4/4	0.77	0.21	38,49,52,55	0
9	GOL	G	2410	6/6	0.78	0.16	27,37,46,47	0
9	GOL	B	202	6/6	0.79	0.18	48,50,54,55	0
10	EDO	C	910	4/4	0.80	0.17	39,42,42,42	0
10	EDO	A	911	4/4	0.80	0.20	32,34,38,40	0
10	EDO	D	202	4/4	0.81	0.16	42,42,42,44	0
10	EDO	E	911	4/4	0.81	0.19	31,39,40,40	0
9	GOL	E	910	6/6	0.82	0.17	28,40,47,49	0
12	PEG	H	202	7/7	0.84	0.16	32,37,42,43	0
12	PEG	C	911	7/7	0.85	0.18	35,53,64,64	0
9	GOL	G	2408	6/6	0.85	0.16	20,27,28,46	0
9	GOL	E	909	6/6	0.86	0.14	38,42,46,50	0
9	GOL	G	2411	6/6	0.86	0.18	20,36,37,39	0
10	EDO	G	2401	4/4	0.89	0.13	33,33,37,38	0
10	EDO	A	910	4/4	0.90	0.13	21,27,38,38	0
9	GOL	C	906	6/6	0.91	0.13	20,31,34,37	0
9	GOL	A	907	6/6	0.91	0.10	20,23,24,24	0
10	EDO	C	913	4/4	0.92	0.11	21,23,24,44	0
9	GOL	A	912	6/6	0.93	0.11	16,25,28,32	0
9	GOL	C	907	6/6	0.93	0.09	19,23,25,25	0
9	GOL	E	907	6/6	0.94	0.10	19,33,37,38	0
9	GOL	E	908	6/6	0.94	0.09	22,25,30,33	0
9	GOL	C	908	6/6	0.94	0.10	14,21,29,34	0
9	GOL	G	2409	6/6	0.95	0.09	12,20,31,33	0
9	GOL	A	908	6/6	0.95	0.10	13,17,26,33	0
4	MGD	E	902	47/47	0.98	0.04	8,10,11,13	0
4	MGD	G	2403	47/47	0.98	0.04	8,10,12,12	0
6	FC6	A	904	13/13	0.98	0.07	13,19,26,26	1
6	FC6	C	905	13/13	0.98	0.07	15,20,30,31	1
6	FC6	E	905	13/13	0.98	0.08	14,22,28,29	1
6	FC6	G	2405	13/13	0.98	0.08	13,20,27,30	1

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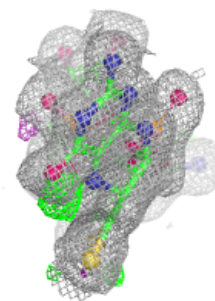
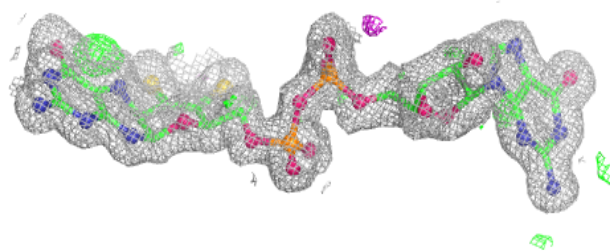
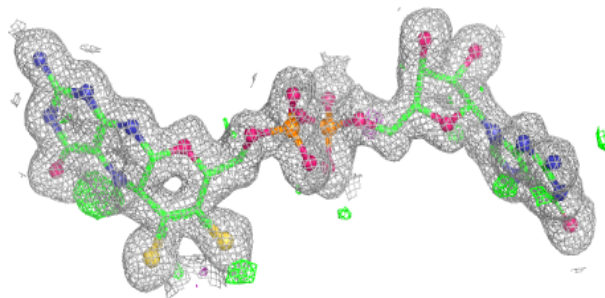
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MGD	C	902	47/47	0.98	0.04	8,10,12,12	0
4	MGD	E	901	47/47	0.98	0.04	7,9,10,11	0
4	MGD	G	2402	47/47	0.99	0.04	7,9,11,11	0
4	MGD	A	901	47/47	0.99	0.04	6,8,9,9	0
4	MGD	A	902	47/47	0.99	0.04	7,9,10,11	0
4	MGD	C	901	47/47	0.99	0.04	7,9,10,11	0
5	F3S	E	903	7/7	1.00	0.02	8,8,9,9	0
5	F3S	G	2404	7/7	1.00	0.01	8,8,9,9	0
7	4MO	A	905	1/1	1.00	0.01	8,8,8,8	0
7	4MO	C	909	1/1	1.00	0.01	11,11,11,11	0
7	4MO	E	906	1/1	1.00	0.01	8,8,8,8	0
7	4MO	G	2406	1/1	1.00	0.01	11,11,11,11	0
8	ART	A	906	5/5	1.00	0.04	9,11,13,13	2
8	ART	C	904	5/5	1.00	0.05	10,12,17,18	1
8	ART	E	904	5/5	1.00	0.05	7,12,16,18	1
8	ART	G	2407	5/5	1.00	0.04	8,12,16,18	1
11	FES	B	201	4/4	1.00	0.02	10,11,11,12	0
11	FES	D	201	4/4	1.00	0.02	10,11,12,13	0
11	FES	F	201	4/4	1.00	0.03	10,11,12,13	0
11	FES	H	201	4/4	1.00	0.02	11,11,11,13	0
5	F3S	A	903	7/7	1.00	0.01	8,8,8,8	0
5	F3S	C	903	7/7	1.00	0.02	9,9,9,9	0

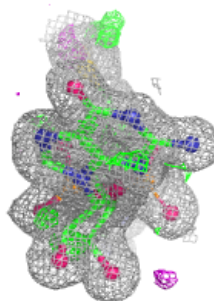
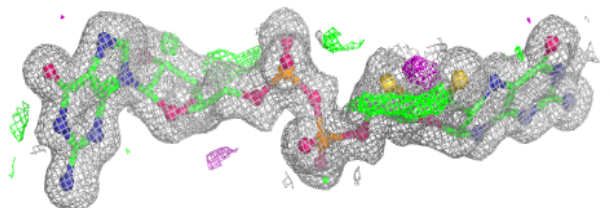
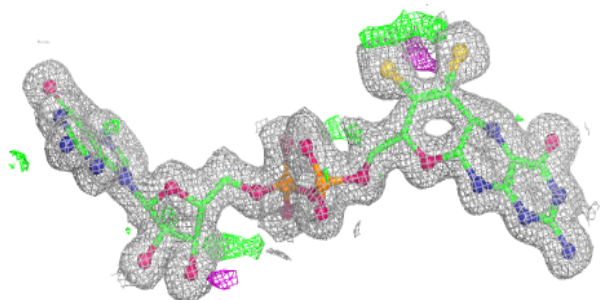
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD E 902:

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

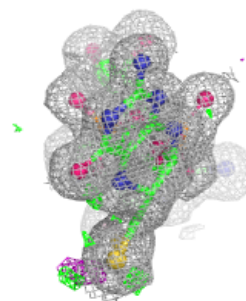
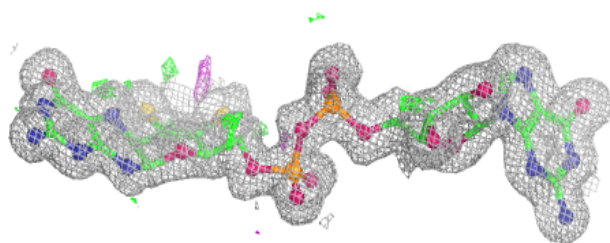
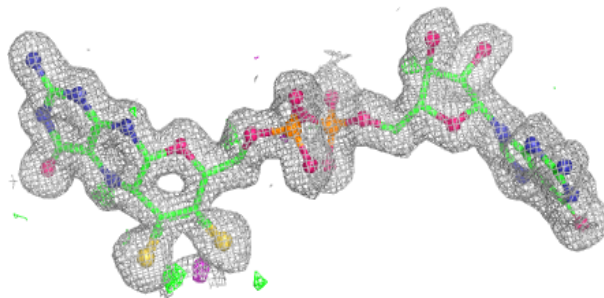
**Electron density around MGD G 2403:**

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

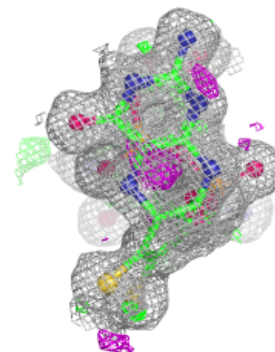
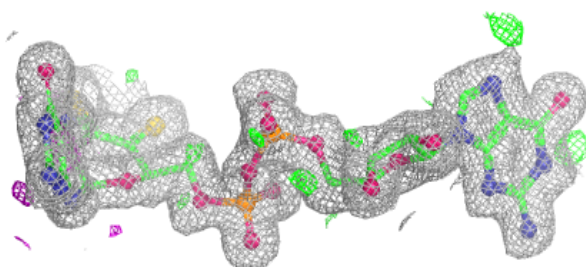
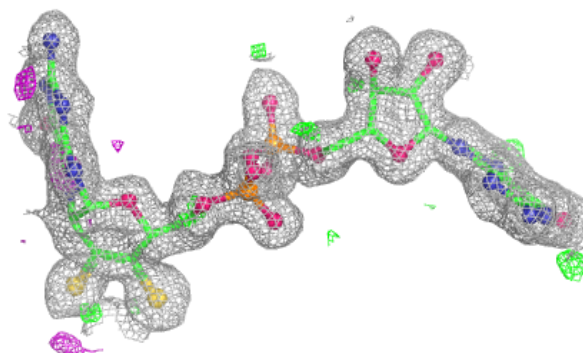


Electron density around MGD C 902:

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

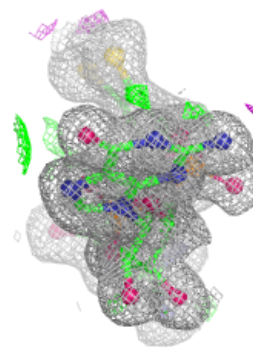
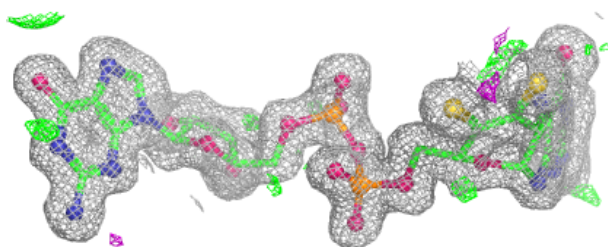
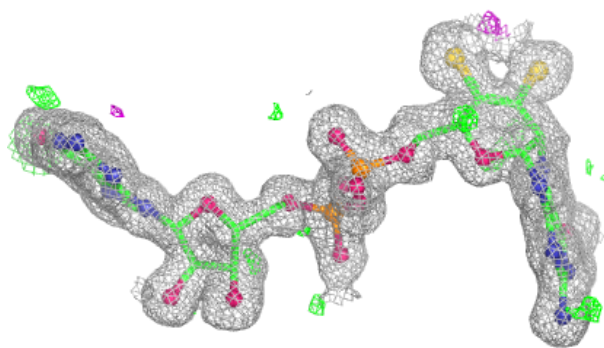
**Electron density around MGD E 901:**

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

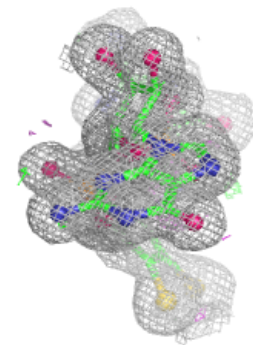
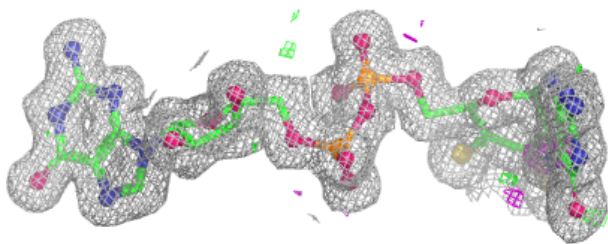
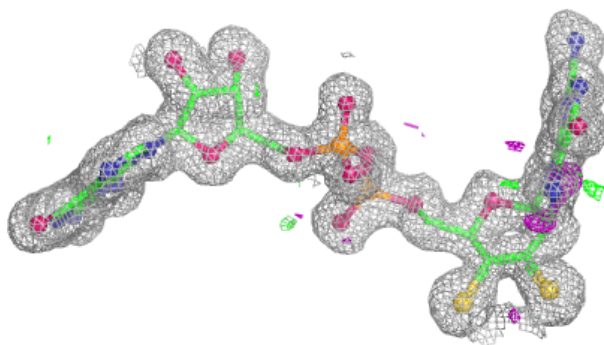


Electron density around MGD G 2402:

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

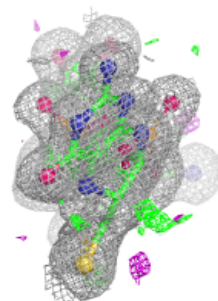
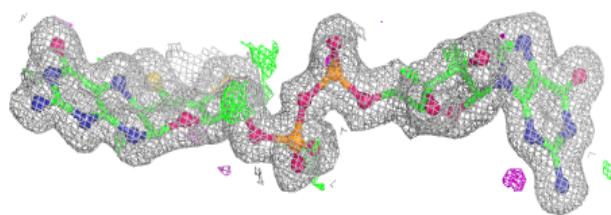
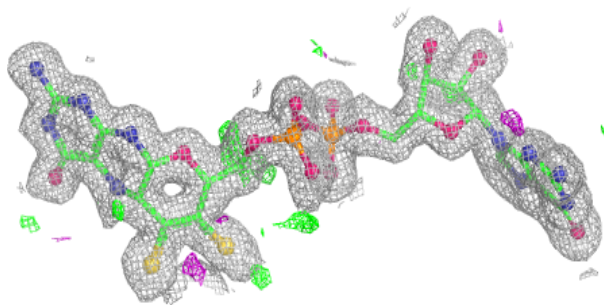
**Electron density around MGD A 901:**

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

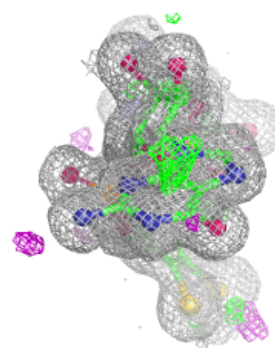
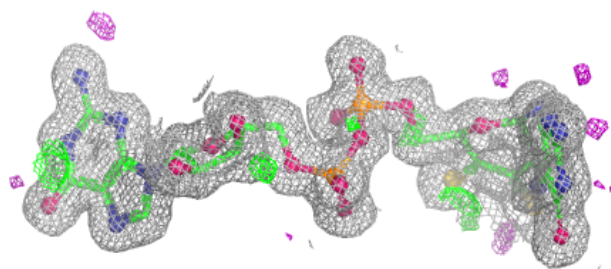
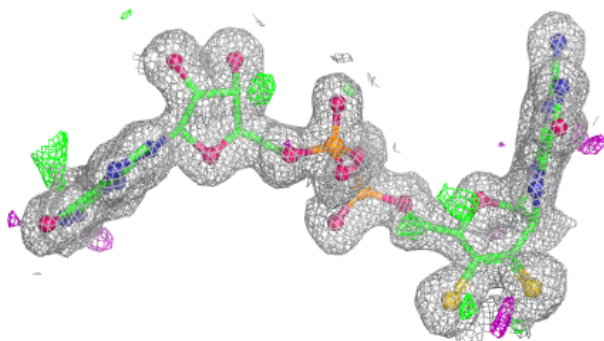


Electron density around MGD A 902:

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

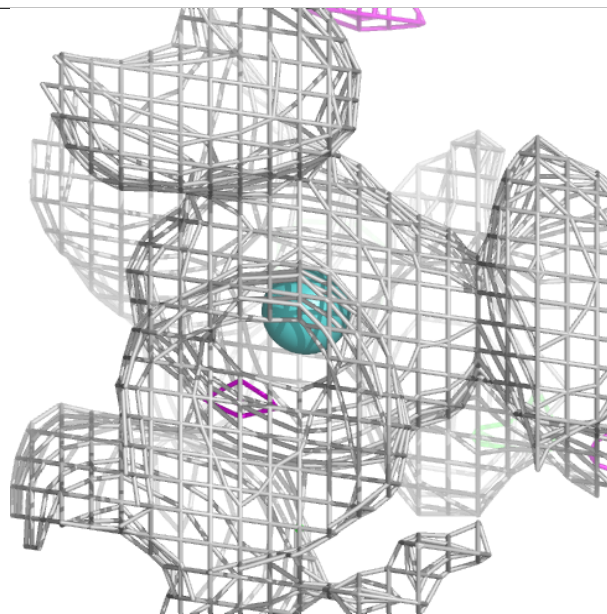
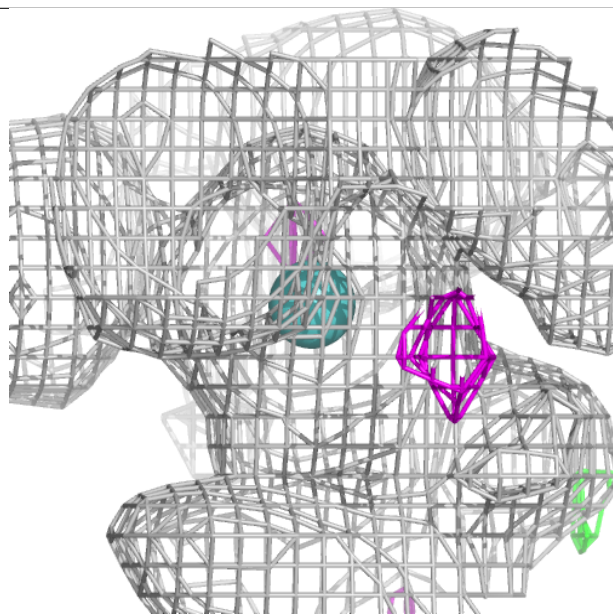
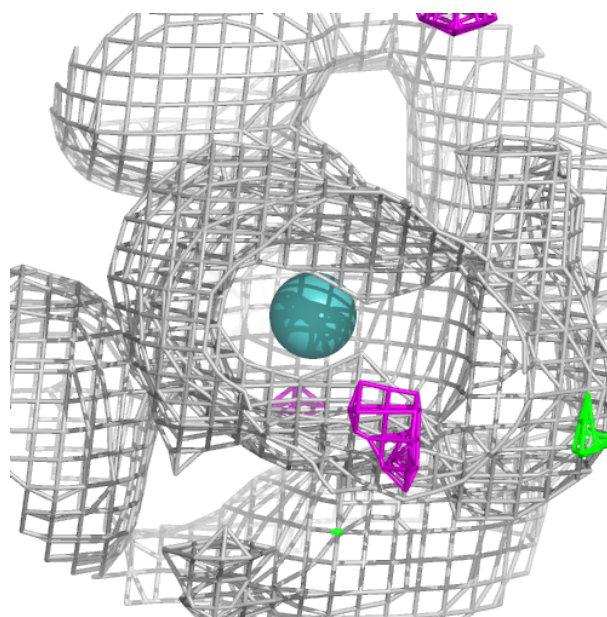
**Electron density around MGD C 901:**

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



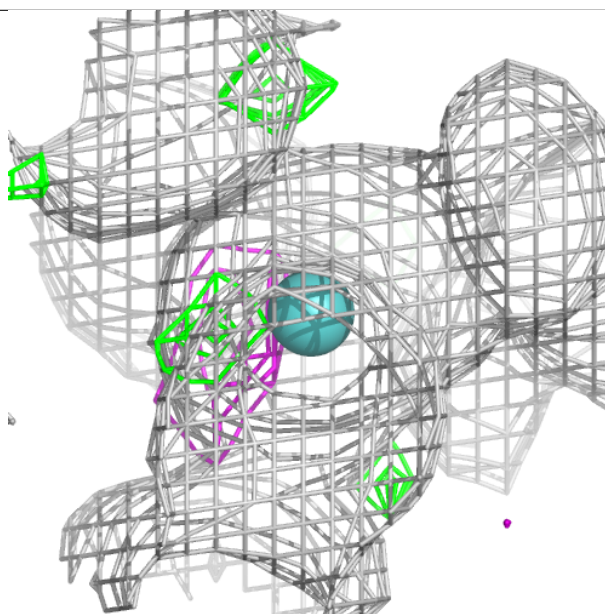
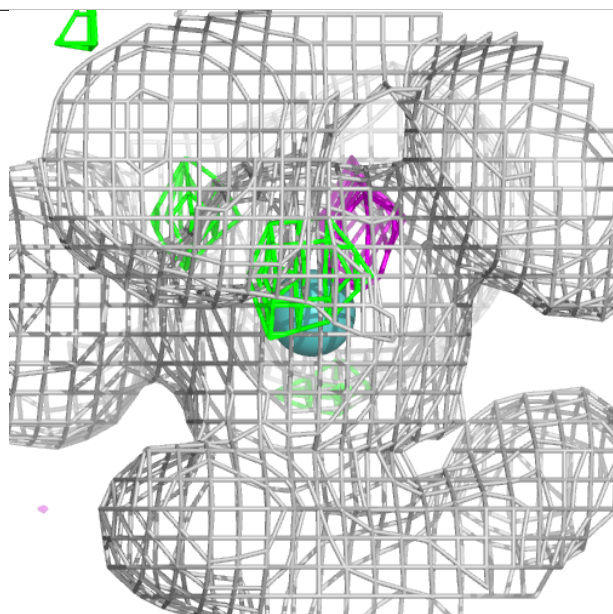
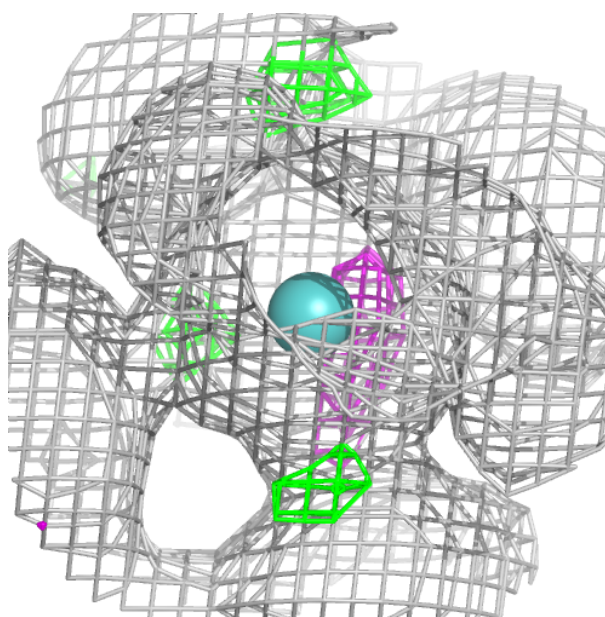
Electron density around 4MO A 905:

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



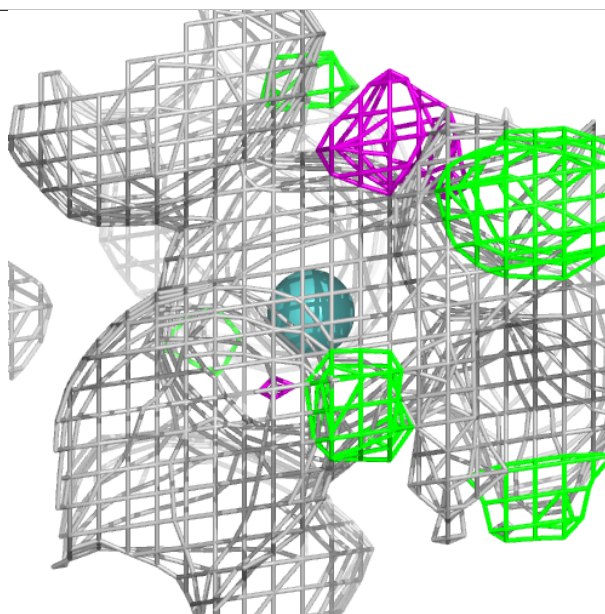
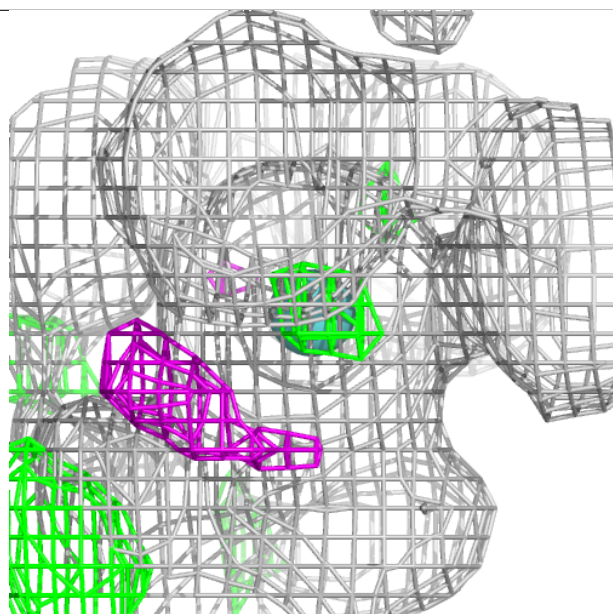
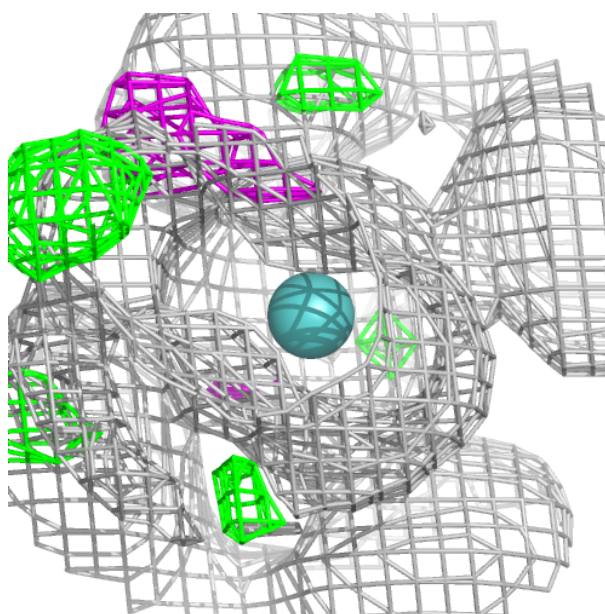
Electron density around 4MO C 909:

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



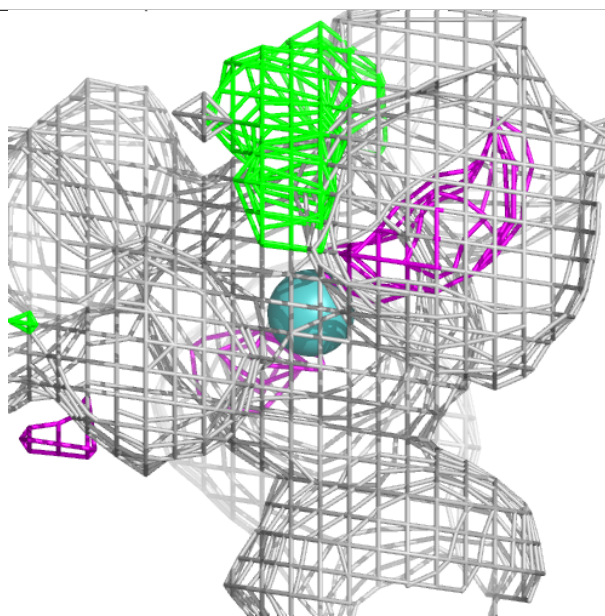
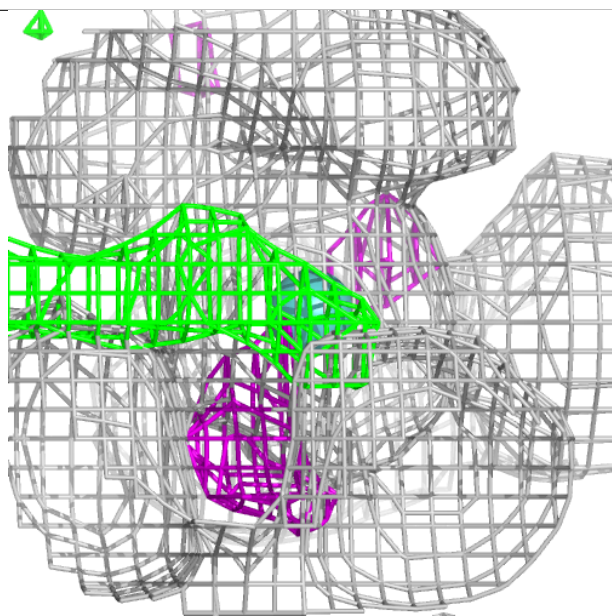
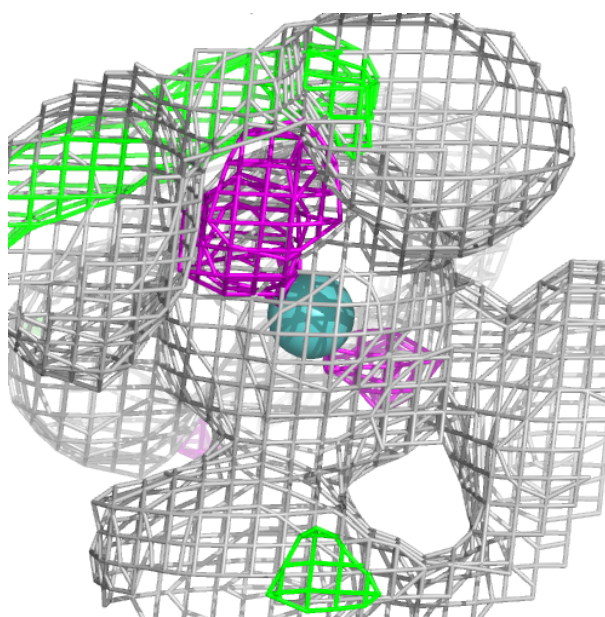
Electron density around 4MO E 906:

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



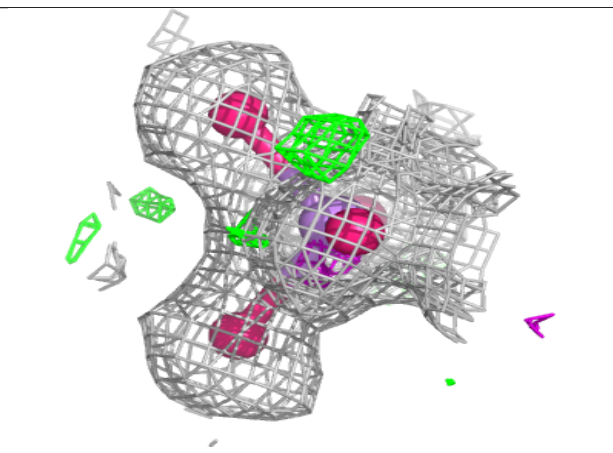
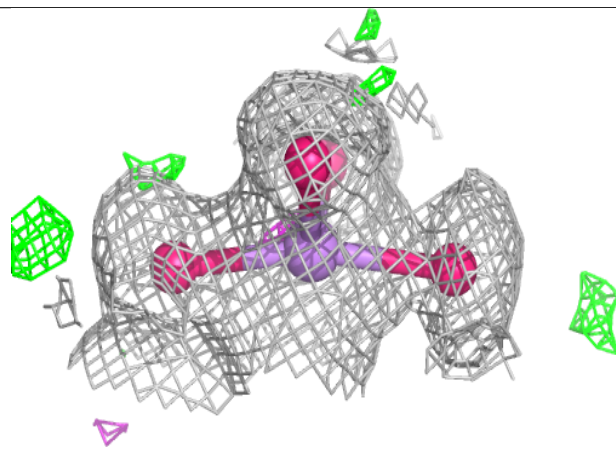
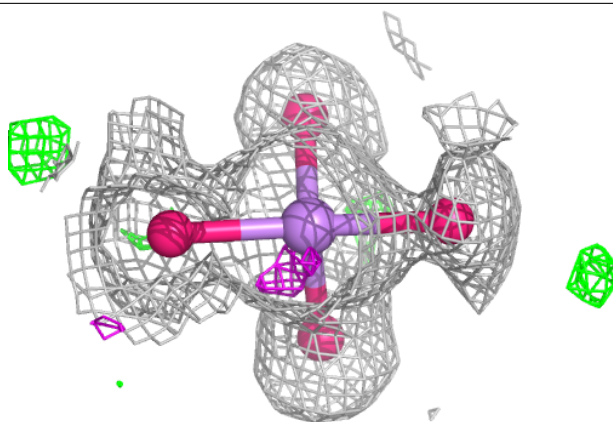
Electron density around 4MO G 2406:

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



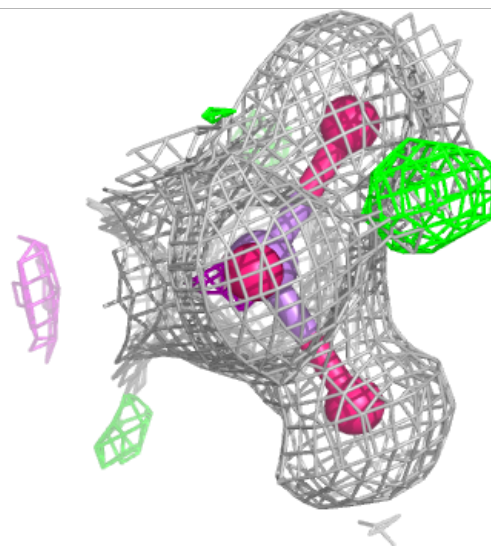
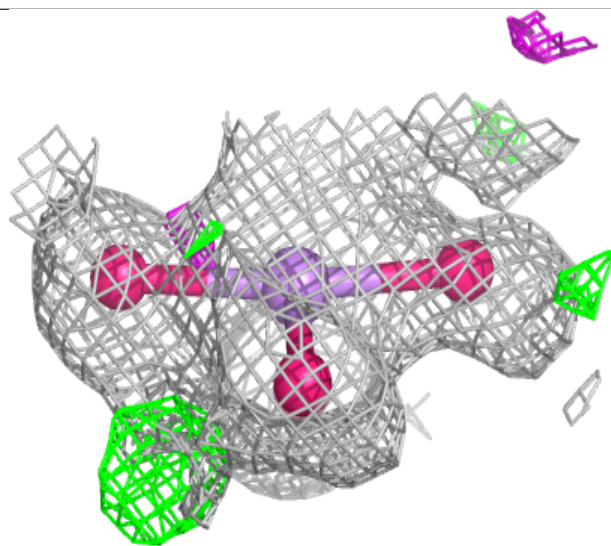
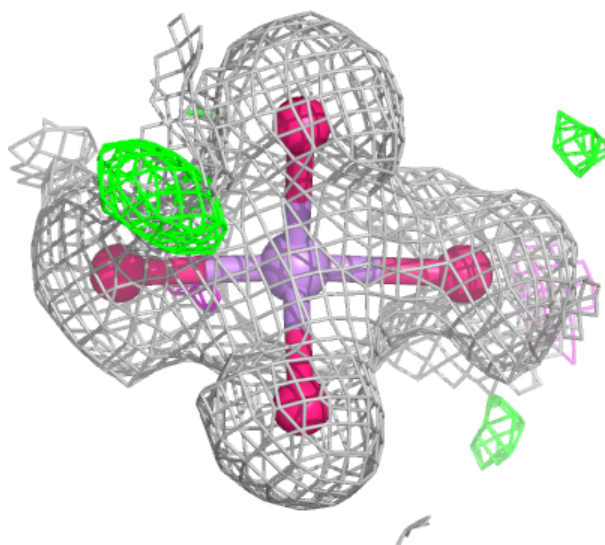
Electron density around ART A 906:

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



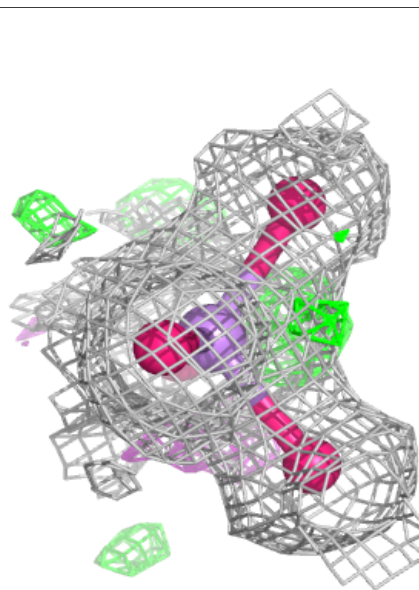
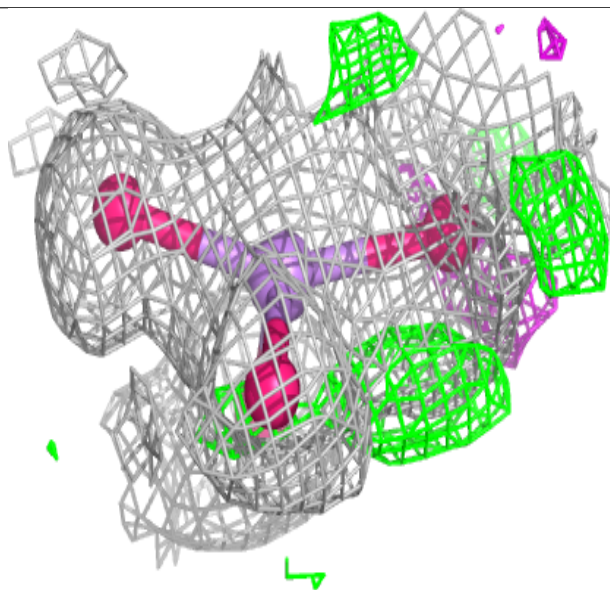
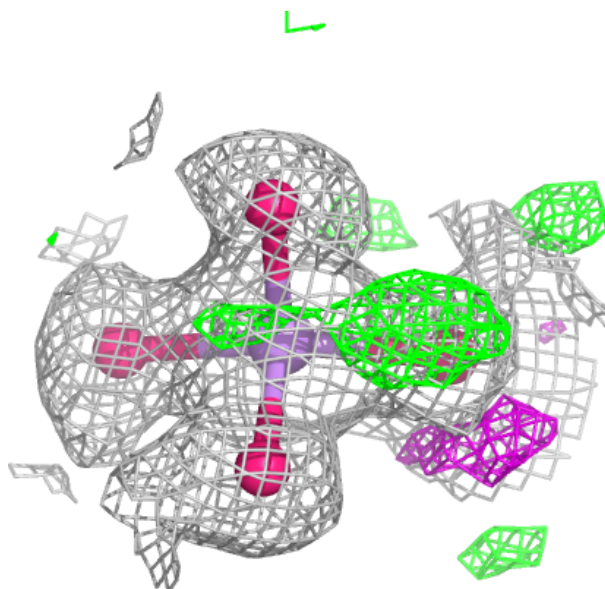
Electron density around ART C 904:

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



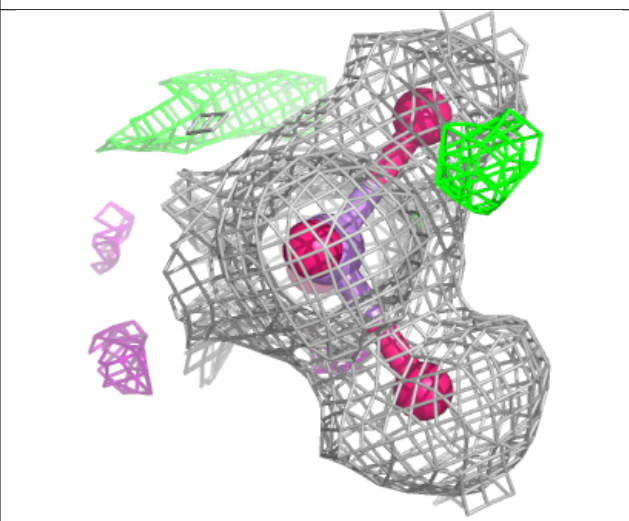
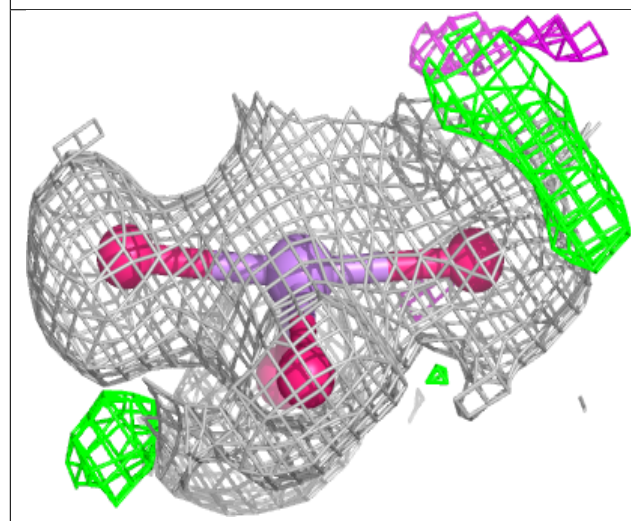
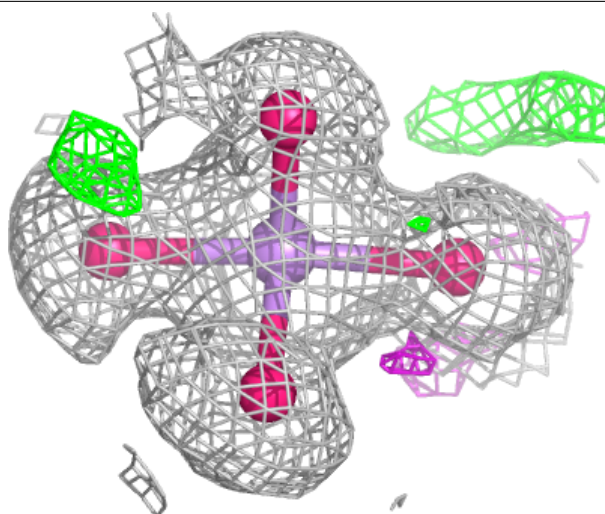
Electron density around ART E 904:

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



Electron density around ART G 2407:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.