



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:49 AM EDT

PDB ID : 6CZ8 / pdb_00006cz8
Title : The arsenate respiratory reductase (Arr) complex from Shewanella sp. ANA-3 bound to arsenate
Authors : Glasser, N.R.; Newman, D.K.
Deposited on : 2018-04-08
Resolution : 1.78 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

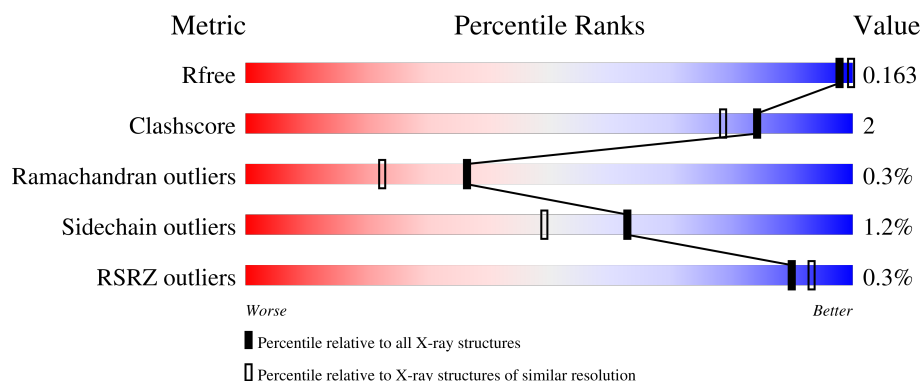
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	814	95% 5%
1	C	814	94% 5%
2	B	234	93% 7%
2	D	234	90% 10%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 35085 atoms, of which 16074 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 ArrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	807	Total	C	H	N	O	S	0	13	0
			12662	4094	6252	1108	1179	29			
1	A	814	Total	C	H	N	O	S	0	8	0
			12652	4098	6229	1108	1188	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	GLY	-	expression tag	UNP Q7WTU0
A	41	GLY	-	expression tag	UNP Q7WTU0

- Molecule 2 is a protein called 4Fe-4S ferredoxin, iron-sulfur binding domain protein.

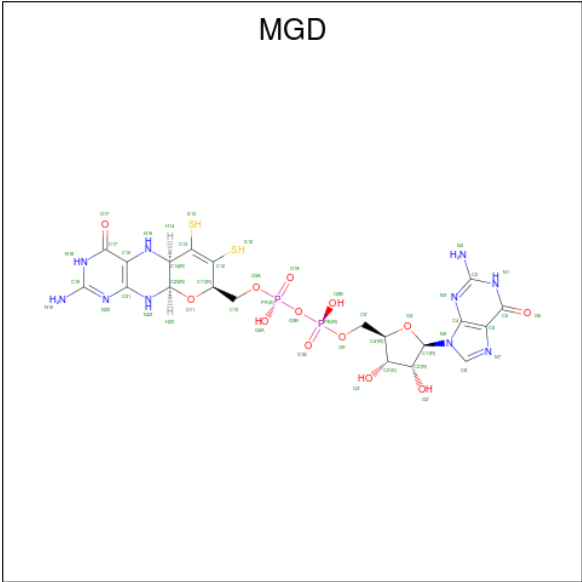
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	234	Total	C	H	N	O	S	0	3	0
			3452	1092	1682	318	337	23			
2	B	234	Total	C	H	N	O	S	0	9	0
			3609	1130	1783	327	345	24			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



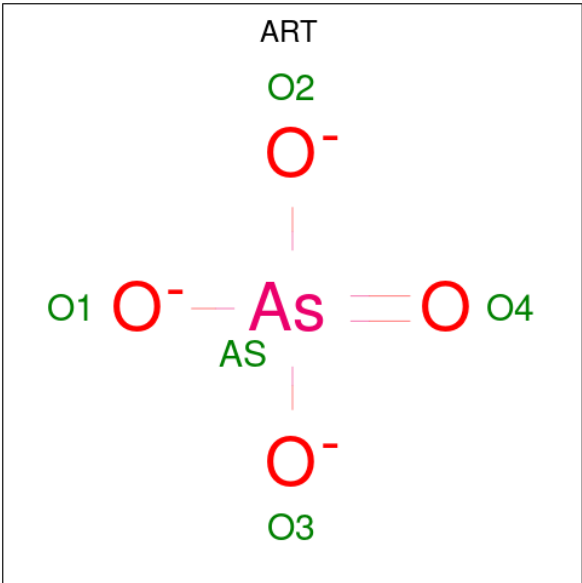
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3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

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	P	S	0	0
			69	20	22	10	13	2	2		
4	C	1	Total	C	H	N	O	P	S	0	0
			69	20	22	10	13	2	2		
4	A	1	Total	C	H	N	O	P	S	0	0
			67	20	20	10	13	2	2		
4	A	1	Total	C	H	N	O	P	S	0	0
			68	20	21	10	13	2	2		

- Molecule 5 is ARSENATE (CCD ID: ART) (formula: AsO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	As	O	0	1
			10	2	8		
5	A	1	Total	As	O	0	1
			10	2	8		

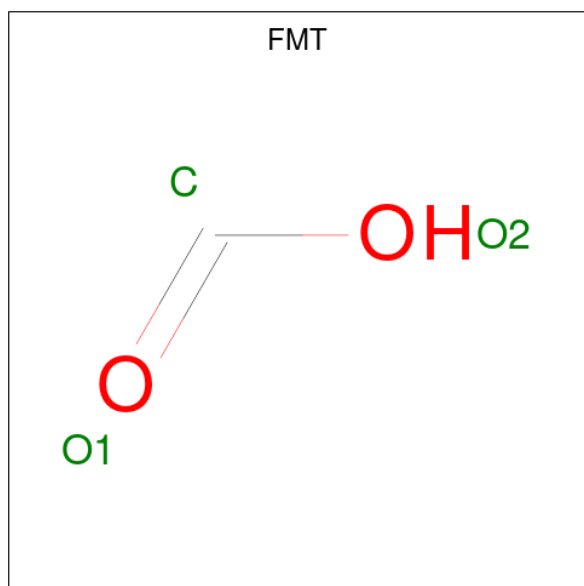
- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

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

- Molecule 8 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



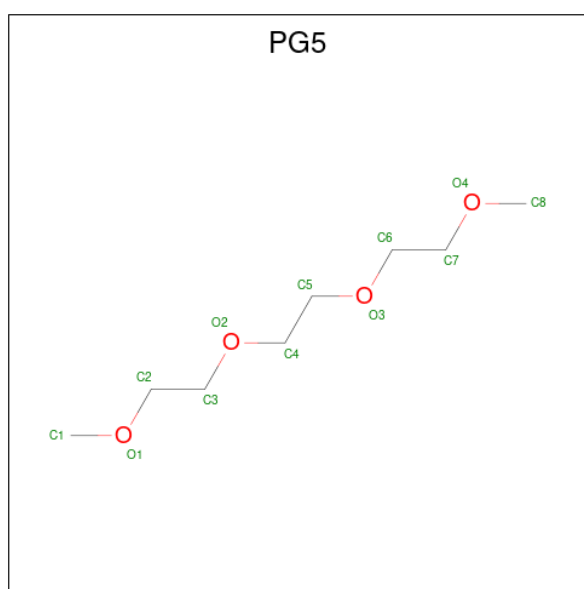
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			4	1	1	2		

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

- Molecule 9 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (CCD ID: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			30	8	18	4		
9	A	1	Total	C	H	O	0	0
			30	8	18	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	970	Total	O	0	0
			970	970		

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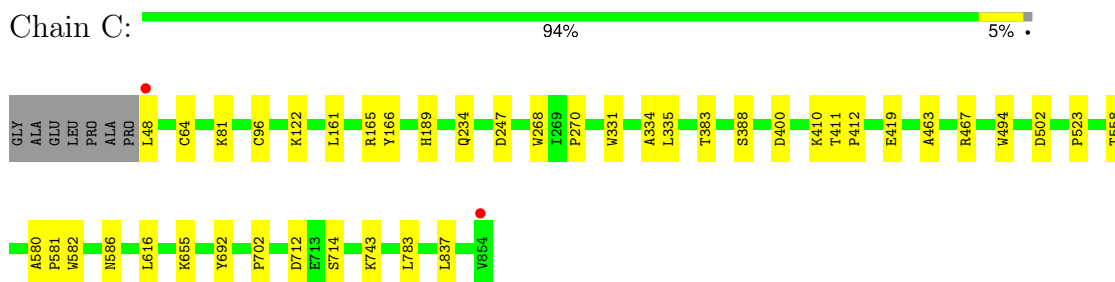
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	276	Total 276	O 276	0	0
10	A	733	Total 733	O 733	0	0
10	B	262	Total 262	O 262	0	0

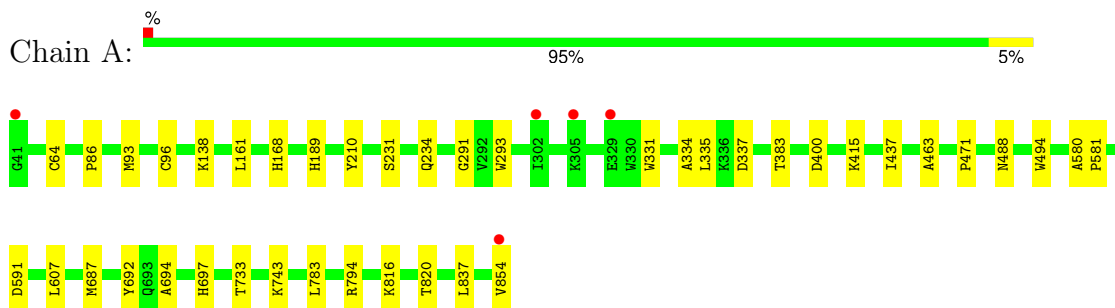
3 Residue-property plots

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

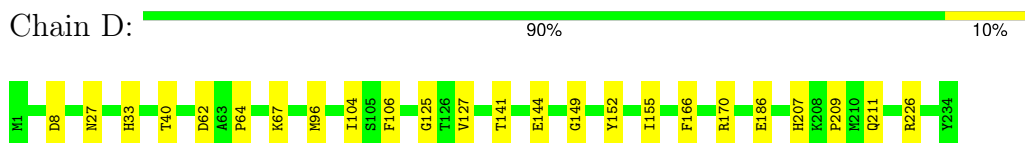
- Molecule 1: ArrA



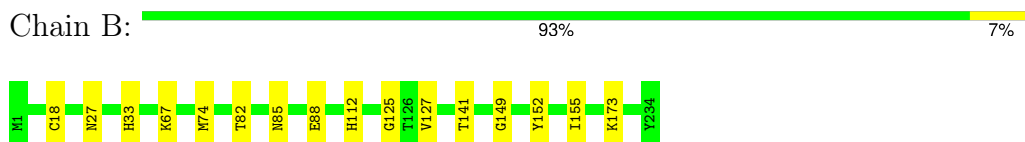
- Molecule 1: ArrA



- Molecule 2: 4Fe-4S ferredoxin, iron-sulfur binding domain protein



- Molecule 2: 4Fe-4S ferredoxin, iron-sulfur binding domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.16Å 86.34Å 148.22Å 90.00° 127.67° 90.00°	Depositor
Resolution (Å)	39.10 – 1.78 39.10 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.10-1.78) 99.8 (39.10-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.137 , 0.168 0.133 , 0.163	Depositor DCC
R_{free} test set	2776 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	35085	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: SF4, ART, MO, MGD, PG5, FMT, O

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	0.37	0/6621	0.49	0/8979
1	C	0.42	0/6621	0.54	0/8969
2	B	0.38	0/1892	0.52	0/2567
2	D	0.41	0/1818	0.55	0/2473
All	All	0.39	0/16952	0.52	0/22988

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6423	6229	6247	21	0
1	C	6410	6252	6274	25	0
2	B	1826	1783	1796	10	0
2	D	1770	1682	1691	20	0
3	A	8	0	0	0	0
3	B	32	0	0	2	0
3	C	8	0	0	0	0
3	D	32	0	0	1	0
4	A	94	41	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	94	44	43	1	0
5	A	10	0	0	0	0
5	C	10	0	0	2	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	3	0	0	1	0
7	C	3	0	0	0	0
8	A	9	3	3	0	0
8	C	9	3	3	0	0
8	D	3	1	1	0	0
9	A	12	18	18	1	0
9	C	12	18	18	0	0
10	A	733	0	0	3	0
10	B	262	0	0	2	0
10	C	970	0	0	5	1
10	D	276	0	0	6	0
All	All	19011	16074	16137	75	1

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 (75) 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)
3:B:301:SF4:S3	10:B:536:HOH:O	2.14	1.06
2:D:211:GLN:HG2	10:D:401:HOH:O	1.59	1.03
2:B:18:CYS:SG	10:B:536:HOH:O	2.34	0.84
1:C:166:TYR:OH	5:C:904[B]:ART:O3	2.04	0.75
2:B:85[B]:ASN:ND2	2:B:88:GLU:OE1	2.21	0.73
1:A:337:ASP:OD2	10:A:1002:HOH:O	2.06	0.72
1:C:48:LEU:N	10:C:1005:HOH:O	2.24	0.69
1:C:502[B]:ASP:OD1	10:C:1001:HOH:O	2.14	0.64
2:D:211:GLN:NE2	10:D:401:HOH:O	1.92	0.64
2:D:186:GLU:CD	10:D:405:HOH:O	2.41	0.63
1:A:64:CYS:HB2	4:A:902:MGD:H14	1.81	0.63
1:A:697:HIS:ND1	10:A:1005:HOH:O	2.31	0.63
2:B:74[B]:MET:HG2	3:B:304:SF4:S1	2.40	0.62
1:A:138:LYS:NZ	10:A:1004:HOH:O	2.28	0.61
1:C:64:CYS:HB2	4:C:902:MGD:H14	1.85	0.59
2:D:40:THR:HG23	10:D:517:HOH:O	2.02	0.58
1:C:122:LYS:NZ	10:C:1008:HOH:O	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27[B]:ASN:ND2	2:B:155:ILE:HD13	2.20	0.56
1:C:502[B]:ASP:OD2	10:C:1002:HOH:O	2.18	0.55
2:D:8:ASP:OD1	2:D:226[B]:ARG:HD3	2.07	0.55
1:A:816:LYS:HB3	1:A:820[B]:THR:HG22	1.89	0.54
1:C:412:PRO:HG2	1:C:616:LEU:HD23	1.90	0.54
2:D:207:HIS:C	10:D:402:HOH:O	2.52	0.53
2:B:149:GLY:HA2	2:B:152:TYR:O	2.09	0.53
1:C:463:ALA:O	1:C:467:ARG:HB2	2.09	0.53
1:A:210:TYR:OH	7:A:906[B]:O:O	2.23	0.53
1:C:331:TRP:HA	1:C:335:LEU:HB3	1.91	0.52
1:A:331:TRP:HA	1:A:335:LEU:HB3	1.94	0.50
2:D:27[B]:ASN:ND2	2:D:155:ILE:CD1	2.74	0.50
1:A:783:LEU:C	1:A:783:LEU:HD12	2.39	0.48
1:C:463:ALA:HB2	1:C:494:TRP:CE2	2.49	0.48
2:D:62[A]:ASP:OD1	2:D:67:LYS:NZ	2.44	0.47
2:D:27[B]:ASN:ND2	2:D:144:GLU:HB2	2.30	0.47
1:A:580:ALA:HB3	1:A:581:PRO:HD3	1.96	0.47
2:D:96:MET:HG2	2:D:104:ILE:HG22	1.96	0.46
2:B:27[B]:ASN:ND2	2:B:155:ILE:CD1	2.79	0.46
1:C:165:ARG:NH1	5:C:904[A]:ART:O3	2.41	0.46
1:A:463:ALA:HB2	1:A:494:TRP:CE2	2.50	0.46
2:D:207:HIS:O	2:D:209:PRO:HD3	2.15	0.46
1:A:161:LEU:HD13	1:A:161:LEU:C	2.41	0.46
1:C:161:LEU:C	1:C:161:LEU:HD13	2.40	0.46
1:A:189:HIS:C	1:A:189:HIS:CD2	2.94	0.45
2:B:27[B]:ASN:ND2	2:B:112:HIS:NE2	2.64	0.45
1:C:247:ASP:OD2	2:D:226[B]:ARG:NH2	2.50	0.44
1:C:523:PRO:HB2	1:C:558:THR:HG22	1.98	0.44
1:C:712:ASP:OD1	1:C:714:SER:OG	2.33	0.44
1:C:268:TRP:CZ2	1:C:270:PRO:HB3	2.52	0.44
2:D:27[B]:ASN:ND2	2:D:155:ILE:HD13	2.33	0.43
2:D:149:GLY:HA2	2:D:152:TYR:O	2.18	0.43
2:B:74[B]:MET:CE	2:B:82:THR:HG22	2.48	0.43
1:A:86:PRO:HG3	1:A:93:MET:HE2	2.00	0.43
2:D:96:MET:SD	2:D:106:PHE:HB2	2.57	0.43
1:C:783:LEU:C	1:C:783:LEU:HD12	2.42	0.43
1:C:580:ALA:HB3	1:C:581:PRO:HD3	2.01	0.43
2:D:27[B]:ASN:HD21	2:D:144:GLU:HB2	1.84	0.43
1:A:794:ARG:HH21	9:A:911:PG5:C5	2.32	0.43
2:D:27[B]:ASN:HD21	2:D:144:GLU:CB	2.31	0.43
1:C:419[A]:GLU:H	1:C:419[A]:GLU:CD	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:64:PRO:HD2	3:D:303:SF4:S1	2.59	0.42
1:C:655:LYS:HE2	10:C:1429:HOH:O	2.19	0.42
1:C:582:TRP:CE2	1:C:586:ASN:OD1	2.73	0.42
1:C:692:TYR:CE1	1:C:837:LEU:HG	2.55	0.42
1:A:231:SER:HA	4:A:902:MGD:N20	2.35	0.42
1:A:687[B]:MET:HE2	1:A:694:ALA:HB3	2.02	0.41
2:B:173:LYS:O	2:B:173:LYS:HG3	2.20	0.41
1:C:388:SER:HA	1:C:702:PRO:HB3	2.02	0.41
1:A:692:TYR:CE1	1:A:837:LEU:HG	2.55	0.41
1:C:189:HIS:CD2	1:C:189:HIS:C	2.98	0.41
1:A:591:ASP:HA	1:A:607:LEU:CD1	2.51	0.41
1:A:437:ILE:HD12	1:A:471:PRO:HD2	2.03	0.41
1:C:81[B]:LYS:NZ	2:D:170:ARG:NH1	2.68	0.41
1:A:291:GLY:HA2	1:A:293:TRP:CZ3	2.56	0.41
1:A:168:HIS:CE1	1:A:415:LYS:HE3	2.56	0.40
2:D:211:GLN:CG	10:D:401:HOH:O	2.31	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1009:HOH:O	10:C:1620:HOH:O[4_555]	1.91	0.29

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	820/814 (101%)	790 (96%)	29 (4%)	1 (0%)	48	33
1	C	818/814 (100%)	788 (96%)	29 (4%)	1 (0%)	48	33
2	B	241/234 (103%)	236 (98%)	3 (1%)	2 (1%)	16	6
2	D	235/234 (100%)	230 (98%)	3 (1%)	2 (1%)	14	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2114/2096 (101%)	2044 (97%)	64 (3%)	6 (0%)	36	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	334	ALA
1	A	334	ALA
2	D	125	GLY
2	D	127	VAL
2	B	127	VAL
2	B	125	GLY

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	669/672 (100%)	661 (99%)	8 (1%)	63	49
1	C	671/672 (100%)	664 (99%)	7 (1%)	68	55
2	B	208/201 (104%)	205 (99%)	3 (1%)	59	44
2	D	195/201 (97%)	192 (98%)	3 (2%)	57	41
All	All	1743/1746 (100%)	1722 (99%)	21 (1%)	63	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	96	CYS
1	C	234	GLN
1	C	383	THR
1	C	400	ASP
1	C	410	LYS
1	C	411	THR
1	C	743	LYS
2	D	33	HIS
2	D	141	THR

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Mol	Chain	Res	Type
2	D	166	PHE
1	A	96	CYS
1	A	234	GLN
1	A	383	THR
1	A	400	ASP
1	A	488	ASN
1	A	733	THR
1	A	743	LYS
1	A	854	VAL
2	B	33	HIS
2	B	67	LYS
2	B	141	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	549	GLN
1	C	673	GLN
2	D	97	ASN
2	D	124	ASN
2	D	207	HIS
1	A	87	ASN
1	A	154	ASN
1	A	240	GLN
1	A	588	GLN

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 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FMT	D	305	-	2,2,2	0.63	0	1,1,1	0.62	0
3	SF4	C	901	1	0,12,12	-	-	-		
3	SF4	D	301	2	0,12,12	-	-	-		
4	MGD	A	902	6	47,52,52	4.49	28 (59%)	58,81,81	3.09	24 (41%)
4	MGD	C	903	6	47,52,52	4.36	27 (57%)	58,81,81	2.97	24 (41%)
8	FMT	A	910	-	2,2,2	0.67	0	1,1,1	0.32	0
3	SF4	B	303	2	0,12,12	-	-	-		
8	FMT	C	909	-	2,2,2	0.75	0	1,1,1	0.30	0
4	MGD	A	903	6	47,52,52	4.61	26 (55%)	58,81,81	3.26	27 (46%)
3	SF4	B	302	2	0,12,12	-	-	-		
3	SF4	D	302	2	0,12,12	-	-	-		
5	ART	C	904[B]	-	3,4,4	2.88	3 (100%)	6,6,6	1.13	0
3	SF4	B	304	2	0,12,12	-	-	-		
8	FMT	A	908	-	2,2,2	0.70	0	1,1,1	0.42	0
8	FMT	C	910	-	2,2,2	0.54	0	1,1,1	0.63	0
5	ART	A	904[B]	-	3,4,4	2.80	3 (100%)	6,6,6	0.79	0
5	ART	C	904[A]	-	3,4,4	2.88	3 (100%)	6,6,6	0.83	0
3	SF4	A	901	1	0,12,12	-	-	-		
3	SF4	B	301	2,10	0,12,12	-	-	-		
8	FMT	C	908	-	2,2,2	1.00	0	1,1,1	0.50	0
5	ART	A	904[A]	-	3,4,4	2.61	3 (100%)	6,6,6	0.46	0
3	SF4	D	304	2	0,12,12	-	-	-		
9	PG5	C	911	-	11,11,11	0.51	0	10,10,10	0.20	0
3	SF4	D	303	2	0,12,12	-	-	-		
8	FMT	A	909	-	2,2,2	0.81	0	1,1,1	0.52	0
4	MGD	C	902	6	47,52,52	4.20	30 (63%)	58,81,81	3.03	20 (34%)
9	PG5	A	911	-	11,11,11	0.50	0	10,10,10	0.36	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
3	SF4	B	303	2	-	-	0/6/5/5
9	PG5	C	911	-	-	6/9/9/9	-
3	SF4	D	304	2	-	-	0/6/5/5
4	MGD	A	903	6	-	0/22/66/66	0/6/6/6
3	SF4	B	302	2	-	-	0/6/5/5
3	SF4	D	302	2	-	-	0/6/5/5
3	SF4	D	303	2	-	-	0/6/5/5
4	MGD	C	903	6	-	2/22/66/66	0/6/6/6
3	SF4	A	901	1	-	-	0/6/5/5
3	SF4	B	301	2,10	-	-	0/6/5/5
3	SF4	B	304	2	-	-	0/6/5/5
4	MGD	C	902	6	-	3/22/66/66	0/6/6/6
3	SF4	C	901	1	-	-	0/6/5/5
9	PG5	A	911	-	-	5/9/9/9	-
3	SF4	D	301	2	-	-	0/6/5/5
4	MGD	A	902	6	-	4/22/66/66	0/6/6/6

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	MGD	C16-C21	12.97	1.60	1.38
4	A	903	MGD	C16-C21	11.99	1.59	1.38
4	C	903	MGD	C16-C21	11.71	1.58	1.38
4	A	903	MGD	C14-N15	11.48	1.59	1.46
4	C	902	MGD	C16-C21	11.45	1.58	1.38
4	C	902	MGD	C23-C14	-11.15	1.44	1.53
4	C	903	MGD	C14-N15	10.84	1.58	1.46
4	A	903	MGD	O11-C23	-10.71	1.27	1.43
4	C	903	MGD	O11-C23	-10.44	1.28	1.43
4	A	902	MGD	C23-C14	-9.19	1.46	1.53
4	A	902	MGD	O11-C11	8.53	1.60	1.43
4	A	903	MGD	C3'-C4'	-8.52	1.31	1.53
4	C	902	MGD	O11-C11	8.50	1.59	1.43
4	C	903	MGD	O11-C11	8.42	1.59	1.43
4	A	903	MGD	C23-N22	8.39	1.59	1.45
4	A	903	MGD	O11-C11	8.34	1.59	1.43
4	C	902	MGD	C3'-C4'	-8.18	1.32	1.53
4	C	903	MGD	C3'-C4'	-8.18	1.32	1.53
4	A	902	MGD	C3'-C4'	-8.15	1.32	1.53
4	A	902	MGD	C14-N15	7.95	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	MGD	O4'-C4'	7.76	1.62	1.45
4	A	902	MGD	O4'-C4'	7.60	1.61	1.45
4	C	903	MGD	O4'-C4'	7.18	1.61	1.45
4	C	902	MGD	O4'-C4'	6.95	1.60	1.45
4	C	903	MGD	C23-N22	6.84	1.56	1.45
4	A	902	MGD	PA-O3B	6.66	1.66	1.59
4	A	902	MGD	C23-N22	6.30	1.55	1.45
4	A	902	MGD	C19-N18	6.12	1.52	1.37
4	A	902	MGD	C19-N20	5.97	1.47	1.33
4	A	903	MGD	C19-N20	5.96	1.47	1.33
4	A	902	MGD	C4-N3	5.90	1.47	1.34
4	A	903	MGD	PA-O3B	5.76	1.65	1.59
4	C	903	MGD	C19-N20	5.73	1.47	1.33
4	C	902	MGD	C14-N15	5.68	1.52	1.46
4	A	903	MGD	C19-N18	5.61	1.51	1.37
4	C	902	MGD	C4-N3	5.56	1.47	1.34
4	C	902	MGD	PA-O3B	5.56	1.65	1.59
4	C	902	MGD	C23-N22	5.54	1.54	1.45
4	C	902	MGD	C19-N20	5.32	1.46	1.33
4	C	902	MGD	C21-N20	5.30	1.44	1.36
4	C	903	MGD	C19-N18	5.26	1.50	1.37
4	C	903	MGD	C4-N3	5.21	1.46	1.34
4	A	903	MGD	C2-N2	4.90	1.45	1.34
4	C	903	MGD	C2-N2	4.75	1.45	1.34
4	A	903	MGD	C4-N3	4.73	1.45	1.34
4	C	903	MGD	PA-O3B	4.73	1.64	1.59
4	A	902	MGD	PB-O3B	4.72	1.64	1.59
4	C	902	MGD	C19-N18	4.68	1.49	1.37
4	A	903	MGD	C19-N19	4.66	1.45	1.34
4	A	903	MGD	C21-N22	4.61	1.40	1.35
4	A	902	MGD	C21-N20	4.52	1.43	1.36
4	A	902	MGD	C2-N2	4.51	1.44	1.34
4	A	902	MGD	C21-N22	4.45	1.40	1.35
4	C	903	MGD	C21-N20	4.36	1.42	1.36
4	A	903	MGD	C2-N3	4.33	1.43	1.33
4	A	903	MGD	C21-N20	4.25	1.42	1.36
4	A	902	MGD	C19-N19	4.24	1.44	1.34
4	A	902	MGD	C2-N3	4.10	1.43	1.33
4	C	902	MGD	C2-N2	4.04	1.43	1.34
4	C	902	MGD	C2-N3	4.03	1.43	1.33
4	C	902	MGD	C4-N9	-4.02	1.27	1.38
4	C	902	MGD	C19-N19	4.00	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	903	MGD	C17-N18	3.85	1.46	1.38
4	A	903	MGD	PB-O3B	3.76	1.63	1.59
4	C	902	MGD	C17-N18	3.75	1.45	1.38
4	A	902	MGD	C17-N18	3.72	1.45	1.38
4	C	903	MGD	C19-N19	3.68	1.42	1.34
4	A	902	MGD	O3'-C3'	3.64	1.52	1.43
4	A	902	MGD	O17-C17	-3.63	1.16	1.23
5	C	904[B]	ART	O1-AS	3.55	1.81	1.69
4	C	903	MGD	C21-N22	3.52	1.39	1.35
4	C	903	MGD	C2-N3	3.50	1.41	1.33
4	C	902	MGD	PB-O3B	3.49	1.63	1.59
4	C	903	MGD	PB-O3B	3.38	1.63	1.59
4	A	903	MGD	C6-N1	3.38	1.45	1.38
4	A	902	MGD	C4-N9	-3.32	1.29	1.38
4	A	903	MGD	C4-N9	-3.30	1.29	1.38
4	A	903	MGD	C17-N18	3.29	1.45	1.38
4	A	903	MGD	O17-C17	-3.26	1.17	1.23
4	A	902	MGD	C6-N1	3.23	1.44	1.38
4	C	903	MGD	C4-N9	-3.17	1.30	1.38
4	C	902	MGD	O3'-C3'	3.17	1.50	1.43
4	A	902	MGD	O6-C6	-3.14	1.17	1.23
4	C	902	MGD	C21-N22	3.12	1.38	1.35
5	C	904[A]	ART	O2-AS	3.11	1.80	1.69
4	A	902	MGD	O2'-C2'	-3.04	1.35	1.43
5	A	904[B]	ART	O1-AS	3.01	1.79	1.69
4	C	903	MGD	C6-N1	2.97	1.44	1.38
5	A	904[B]	ART	O2-AS	2.96	1.79	1.69
5	C	904[A]	ART	O1-AS	2.84	1.79	1.69
4	C	903	MGD	O17-C17	-2.83	1.18	1.23
4	C	903	MGD	C16-C17	2.80	1.50	1.41
4	C	903	MGD	C5-C6	2.73	1.54	1.44
5	A	904[A]	ART	O3-AS	2.67	1.78	1.69
5	C	904[A]	ART	O3-AS	2.66	1.78	1.69
4	A	902	MGD	C5-C6	2.65	1.54	1.44
4	A	903	MGD	C5-C6	2.63	1.54	1.44
5	A	904[A]	ART	O1-AS	2.58	1.78	1.69
5	A	904[A]	ART	O2-AS	2.58	1.78	1.69
4	C	902	MGD	C8-N7	2.53	1.39	1.32
5	C	904[B]	ART	O3-AS	2.52	1.78	1.69
4	A	902	MGD	O4'-C1'	-2.51	1.36	1.42
4	C	902	MGD	O6-C6	-2.50	1.18	1.23
4	C	902	MGD	O17-C17	-2.49	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904[B]	ART	O2-AS	2.45	1.77	1.69
4	A	903	MGD	O4'-C1'	-2.43	1.36	1.42
4	A	903	MGD	C16-C17	2.43	1.49	1.41
4	C	902	MGD	C5-C6	2.42	1.53	1.44
4	A	902	MGD	C16-C17	2.39	1.49	1.41
5	A	904[B]	ART	O3-AS	2.39	1.77	1.69
4	C	903	MGD	C8-N7	2.29	1.39	1.32
4	C	902	MGD	C6-N1	2.28	1.43	1.38
4	C	903	MGD	C16-N15	2.27	1.43	1.37
4	A	903	MGD	O3'-C3'	2.25	1.48	1.43
4	C	902	MGD	C2-N1	2.25	1.43	1.37
4	A	902	MGD	C8-N7	2.20	1.38	1.32
4	C	902	MGD	C8-N9	-2.17	1.32	1.37
4	C	902	MGD	C16-C17	2.15	1.48	1.41
4	C	903	MGD	C2-N1	2.12	1.42	1.37
4	C	903	MGD	O6-C6	-2.11	1.19	1.23
4	A	903	MGD	C8-N7	2.10	1.38	1.32
4	C	902	MGD	O2'-C2'	-2.04	1.37	1.43
4	C	902	MGD	O11-C23	-2.02	1.40	1.43

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	MGD	O11-C23-C14	13.18	117.75	108.96
4	C	902	MGD	O11-C23-N22	-12.86	96.94	108.61
4	A	902	MGD	O11-C23-N22	-12.59	97.18	108.61
4	C	903	MGD	O11-C23-C14	11.22	116.45	108.96
4	C	903	MGD	O11-C23-N22	9.21	116.96	108.61
4	A	903	MGD	O11-C23-N22	8.70	116.50	108.61
4	A	902	MGD	C23-C14-N15	8.49	116.21	107.87
4	A	903	MGD	C23-C14-N15	6.87	114.61	107.87
4	A	902	MGD	C1'-N9-C8	-6.34	108.73	126.73
4	C	902	MGD	C1'-N9-C8	-6.28	108.90	126.73
4	C	902	MGD	C23-C14-N15	6.26	114.02	107.87
4	C	902	MGD	C2'-C1'-N9	6.21	130.54	113.25
4	A	903	MGD	C2'-C1'-N9	6.20	130.51	113.25
4	A	903	MGD	C1'-N9-C8	-6.16	109.22	126.73
4	C	903	MGD	C1'-N9-C8	-5.83	110.18	126.73
4	A	902	MGD	C2'-C1'-N9	5.53	128.65	113.25
4	C	902	MGD	C2'-C3'-C4'	5.44	113.12	102.61
4	C	903	MGD	C2'-C1'-N9	5.02	127.23	113.25
4	A	902	MGD	O11-C23-C14	4.81	112.17	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	MGD	C1'-N9-C4	4.77	140.59	126.49
4	C	902	MGD	N9-C8-N7	-4.65	104.78	113.40
4	C	903	MGD	C23-C14-N15	4.59	112.38	107.87
4	C	903	MGD	C6-C5-N7	4.57	138.60	130.29
4	C	902	MGD	N2-C2-N1	4.54	126.33	116.76
4	A	902	MGD	C6-C5-N7	4.53	138.53	130.29
4	A	903	MGD	C6-C5-N7	4.47	138.43	130.29
4	A	903	MGD	C19-N20-C21	4.43	121.19	113.36
4	A	902	MGD	C1'-N9-C4	4.37	139.39	126.49
4	C	902	MGD	C6-C5-N7	4.33	138.17	130.29
4	A	902	MGD	N9-C8-N7	-4.29	105.44	113.40
4	C	903	MGD	C1'-N9-C4	4.24	139.00	126.49
4	C	902	MGD	C1'-N9-C4	4.23	138.98	126.49
4	A	903	MGD	N2-C2-N1	4.21	125.64	116.76
4	A	902	MGD	C19-N20-C21	4.12	120.63	113.36
4	A	902	MGD	C2'-C3'-C4'	4.02	110.38	102.61
4	A	902	MGD	N2-C2-N1	3.91	125.02	116.76
4	C	903	MGD	C19-N20-C21	3.89	120.23	113.36
4	A	903	MGD	O4'-C1'-N9	-3.82	99.71	108.36
4	A	903	MGD	C2-N3-C4	3.81	118.87	112.30
4	C	903	MGD	O4'-C1'-N9	-3.81	99.73	108.36
4	A	903	MGD	N9-C8-N7	-3.78	106.39	113.40
4	C	903	MGD	N2-C2-N1	3.75	124.67	116.76
4	C	903	MGD	N9-C8-N7	-3.66	106.61	113.40
4	C	902	MGD	C19-N20-C21	3.60	119.70	113.36
4	C	902	MGD	O11-C23-C14	3.42	111.24	108.96
4	C	902	MGD	C8-N9-C4	3.20	112.03	106.03
4	C	903	MGD	C2-N3-C4	3.19	117.79	112.30
4	A	902	MGD	C6-C5-C4	-3.12	114.13	118.83
4	A	902	MGD	C8-N9-C4	3.09	111.82	106.03
4	C	902	MGD	N2-C2-N3	-3.08	113.67	119.67
4	A	902	MGD	C2-N3-C4	3.01	117.49	112.30
4	A	903	MGD	C17-C16-N15	2.84	124.00	116.27
4	C	903	MGD	C17-C16-N15	2.82	123.97	116.27
4	C	903	MGD	C6-C5-C4	-2.79	114.63	118.83
4	C	902	MGD	O4'-C1'-N9	-2.77	102.07	108.36
4	C	903	MGD	O2B-PB-O3B	2.74	114.69	107.27
4	C	903	MGD	C4'-O4'-C1'	-2.74	103.43	109.47
4	C	902	MGD	C4-C5-N7	-2.73	106.34	110.67
4	A	903	MGD	C4-C5-N7	-2.68	106.43	110.67
4	A	902	MGD	O4'-C1'-N9	-2.67	102.30	108.36
4	C	902	MGD	N18-C19-N20	-2.66	118.46	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	MGD	N1-C2-N3	-2.63	118.51	123.32
4	C	902	MGD	C2-N3-C4	2.60	116.78	112.30
4	A	903	MGD	N19-C19-N18	2.60	122.24	116.76
4	A	902	MGD	C16-C17-N18	2.57	119.20	112.13
4	A	902	MGD	C4'-O4'-C1'	-2.49	103.98	109.47
4	A	903	MGD	C6-C5-C4	-2.47	115.11	118.83
4	C	903	MGD	C4-C5-N7	-2.46	106.77	110.67
4	A	903	MGD	C4'-O4'-C1'	-2.39	104.18	109.47
4	A	903	MGD	O2'-C2'-C1'	-2.39	101.88	110.10
4	A	902	MGD	N1-C2-N3	-2.37	118.99	123.32
4	C	902	MGD	N19-C19-N18	2.35	121.72	116.76
4	A	903	MGD	C16-C17-N18	2.34	118.55	112.13
4	C	903	MGD	O3'-C3'-C2'	-2.31	104.41	111.82
4	A	902	MGD	O3B-PA-O1A	-2.29	103.81	110.70
4	C	903	MGD	C8-N9-C4	2.29	110.32	106.03
4	A	902	MGD	C5-C6-N1	2.25	118.99	113.25
4	A	902	MGD	O17-C17-C16	-2.25	121.83	127.26
4	A	902	MGD	N19-C19-N18	2.25	121.51	116.76
4	A	903	MGD	O2B-PB-O3B	2.24	113.33	107.27
4	A	903	MGD	O3B-PB-O1B	-2.23	103.98	110.70
4	C	902	MGD	C6-C5-C4	-2.22	115.49	118.83
4	A	903	MGD	O3B-PA-O1A	-2.20	104.07	110.70
4	C	903	MGD	N1-C2-N3	-2.18	119.32	123.32
4	A	903	MGD	C5-C4-N9	2.18	109.55	105.66
4	C	903	MGD	N19-C19-N18	2.16	121.33	116.76
4	A	903	MGD	N18-C19-N20	-2.15	119.39	123.32
4	C	902	MGD	C5-C6-N1	2.14	118.70	113.25
4	A	902	MGD	C4-C5-N7	-2.10	107.33	110.67
4	C	903	MGD	O2'-C2'-C1'	-2.10	102.86	110.10
4	A	903	MGD	C8-N9-C4	2.09	109.95	106.03
4	C	903	MGD	C5-C4-N9	2.06	109.35	105.66
4	A	903	MGD	C5-C6-N1	2.02	118.40	113.25
4	C	903	MGD	O2A-PA-O3B	2.01	112.70	107.27
4	A	902	MGD	C19-N18-C17	-2.01	121.47	125.11

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	902	MGD	PB-O3B-PA-O3A
4	A	902	MGD	PB-O3B-PA-O3A
9	C	911	PG5	O1-C2-C3-O2

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Mol	Chain	Res	Type	Atoms
9	A	911	PG5	O3-C6-C7-O4
9	C	911	PG5	O3-C6-C7-O4
9	C	911	PG5	C4-C5-O3-C6
4	C	903	MGD	C3'-C4'-C5'-O5'
9	C	911	PG5	C6-C7-O4-C8
9	A	911	PG5	O2-C4-C5-O3
9	C	911	PG5	C2-C3-O2-C4
4	C	903	MGD	O4'-C4'-C5'-O5'
4	A	902	MGD	O4'-C4'-C5'-O5'
9	A	911	PG5	C3-C2-O1-C1
4	C	902	MGD	PB-O3B-PA-O1A
4	A	902	MGD	PB-O3B-PA-O1A
9	C	911	PG5	O2-C4-C5-O3
9	A	911	PG5	C2-C3-O2-C4
9	A	911	PG5	O1-C2-C3-O2
4	C	902	MGD	PB-O3B-PA-O2A
4	A	902	MGD	PB-O3B-PA-O2A

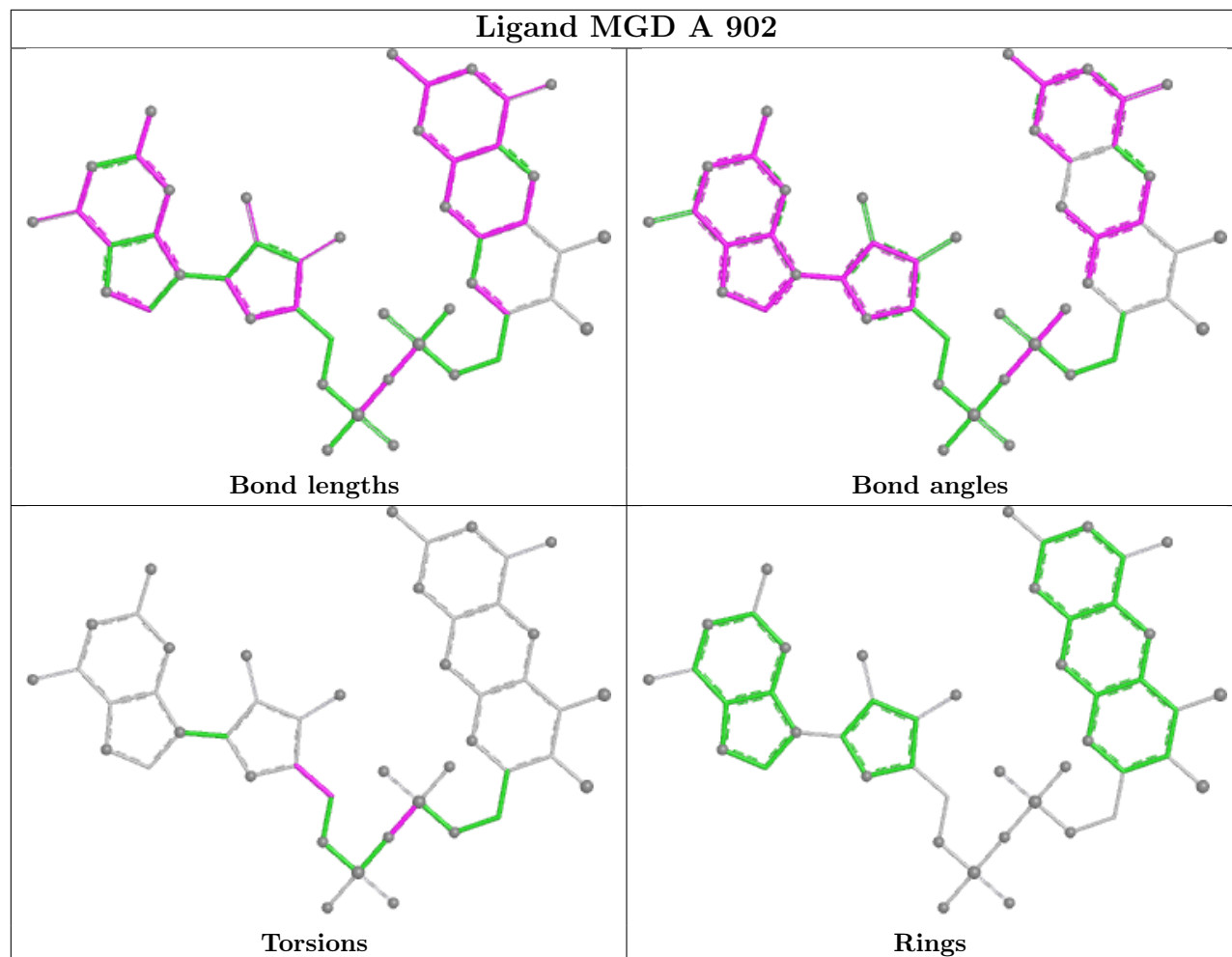
There are no ring outliers.

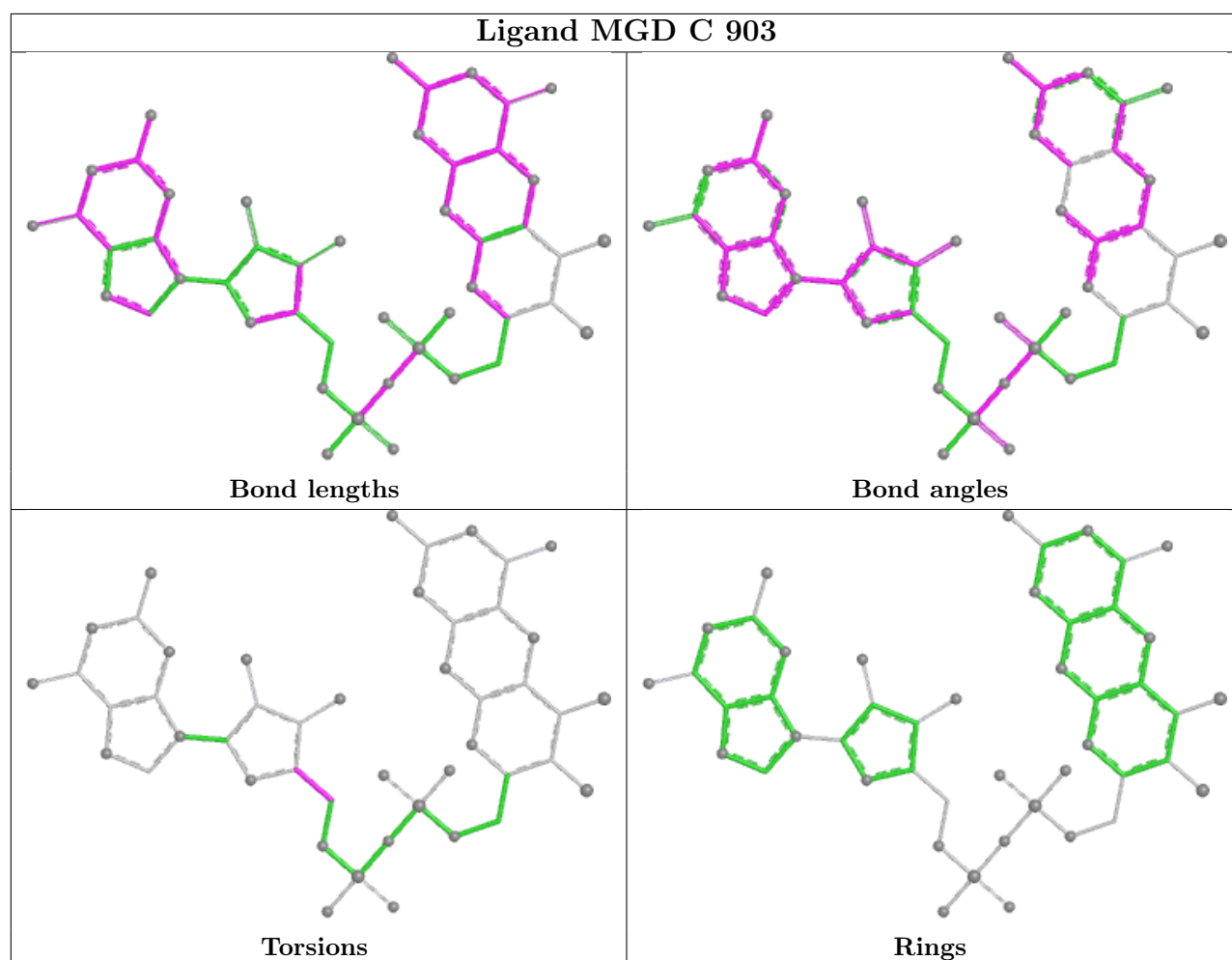
8 monomers are involved in 9 short contacts:

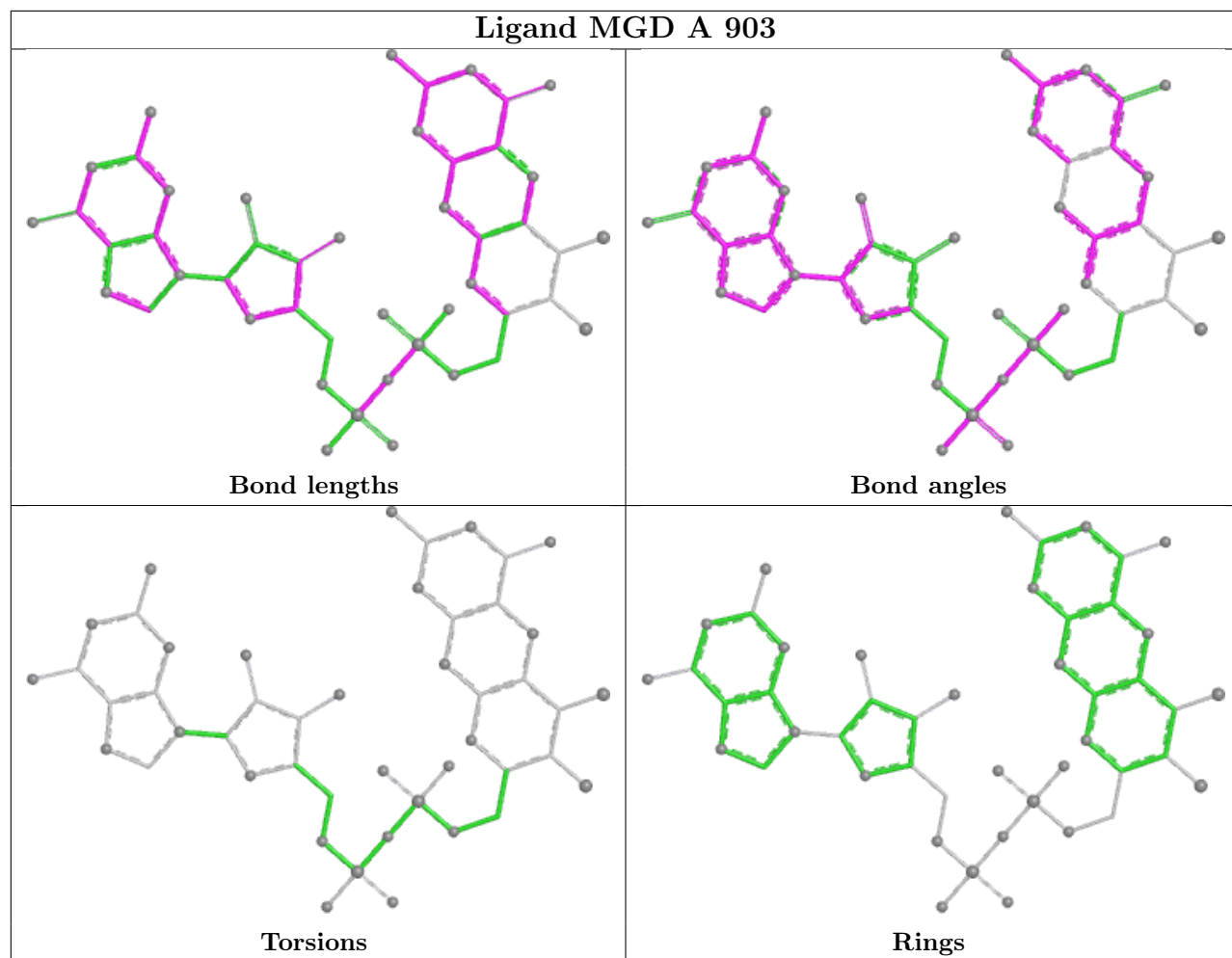
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	MGD	2	0
5	C	904[B]	ART	1	0
3	B	304	SF4	1	0
5	C	904[A]	ART	1	0
3	B	301	SF4	1	0
3	D	303	SF4	1	0
4	C	902	MGD	1	0
9	A	911	PG5	1	0

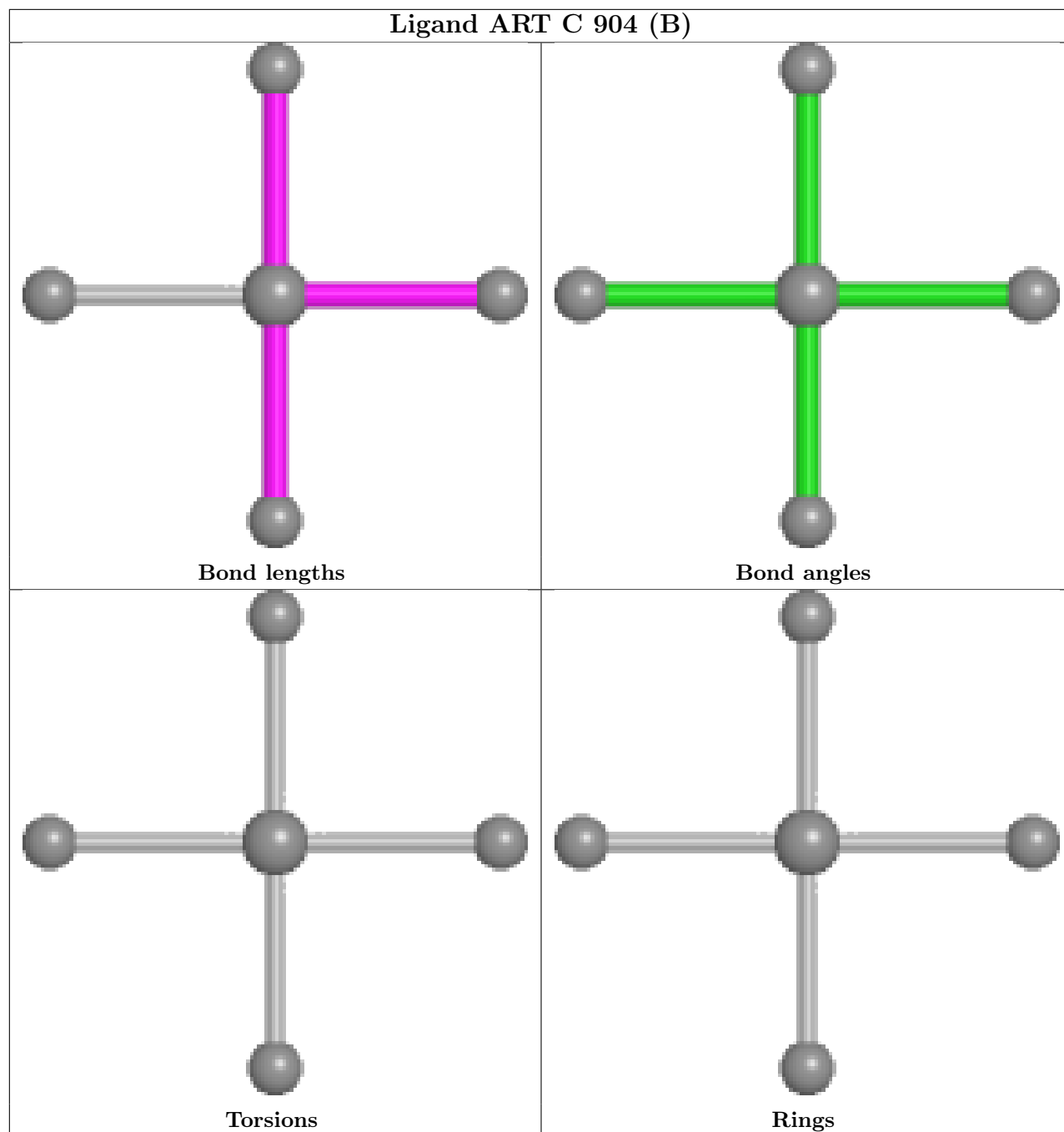
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

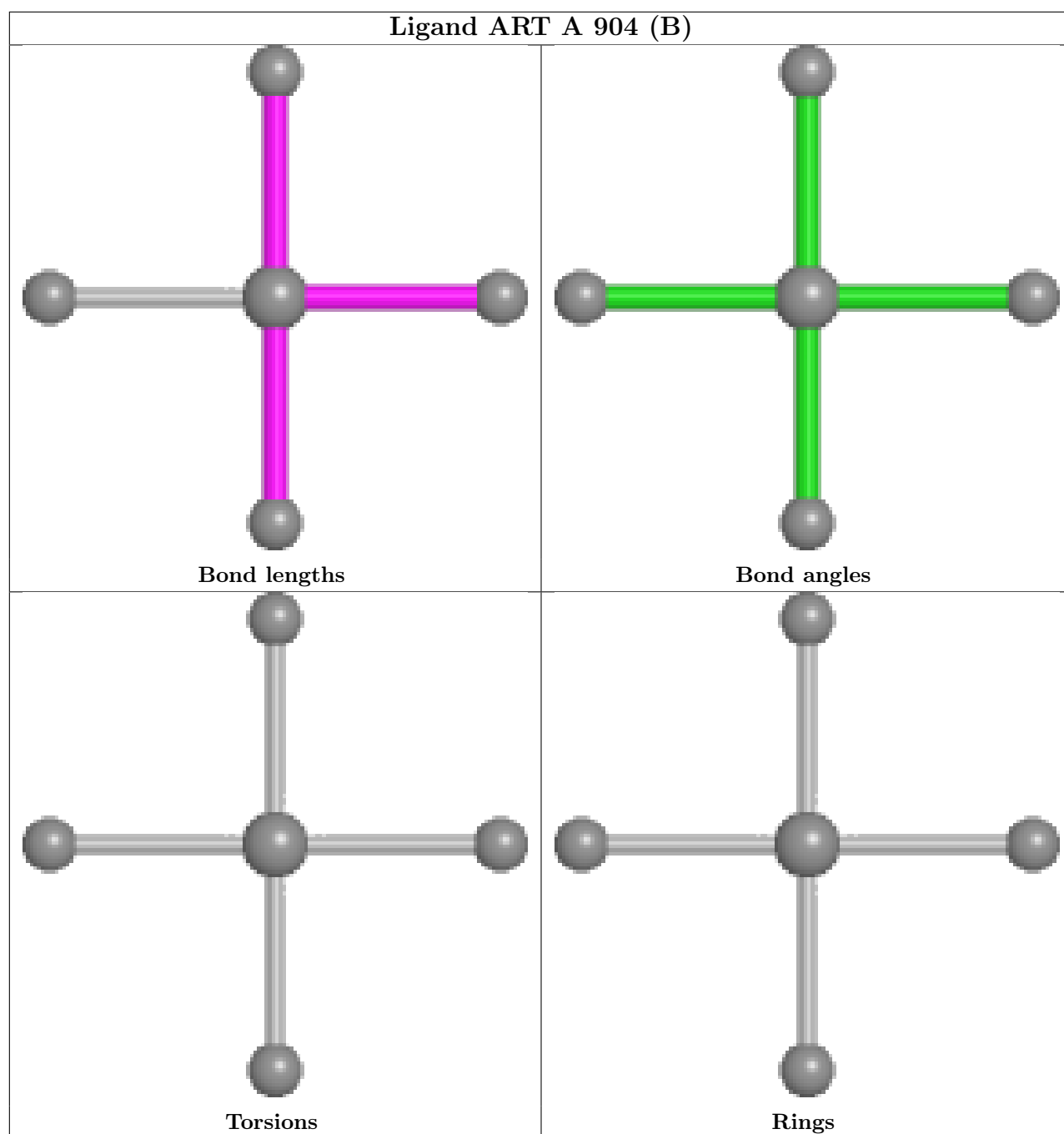
equivalents in the CSD to analyse the geometry.

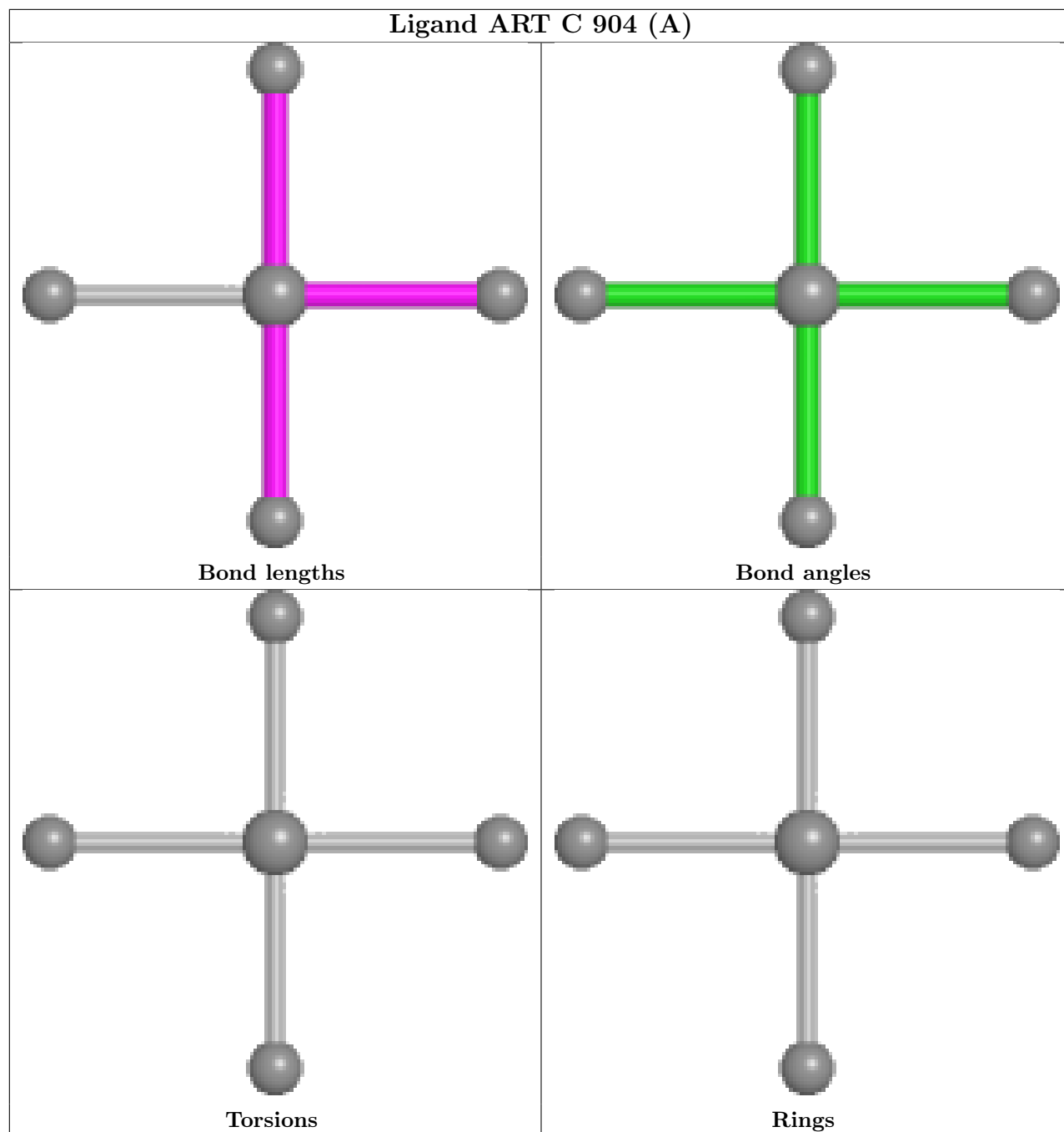


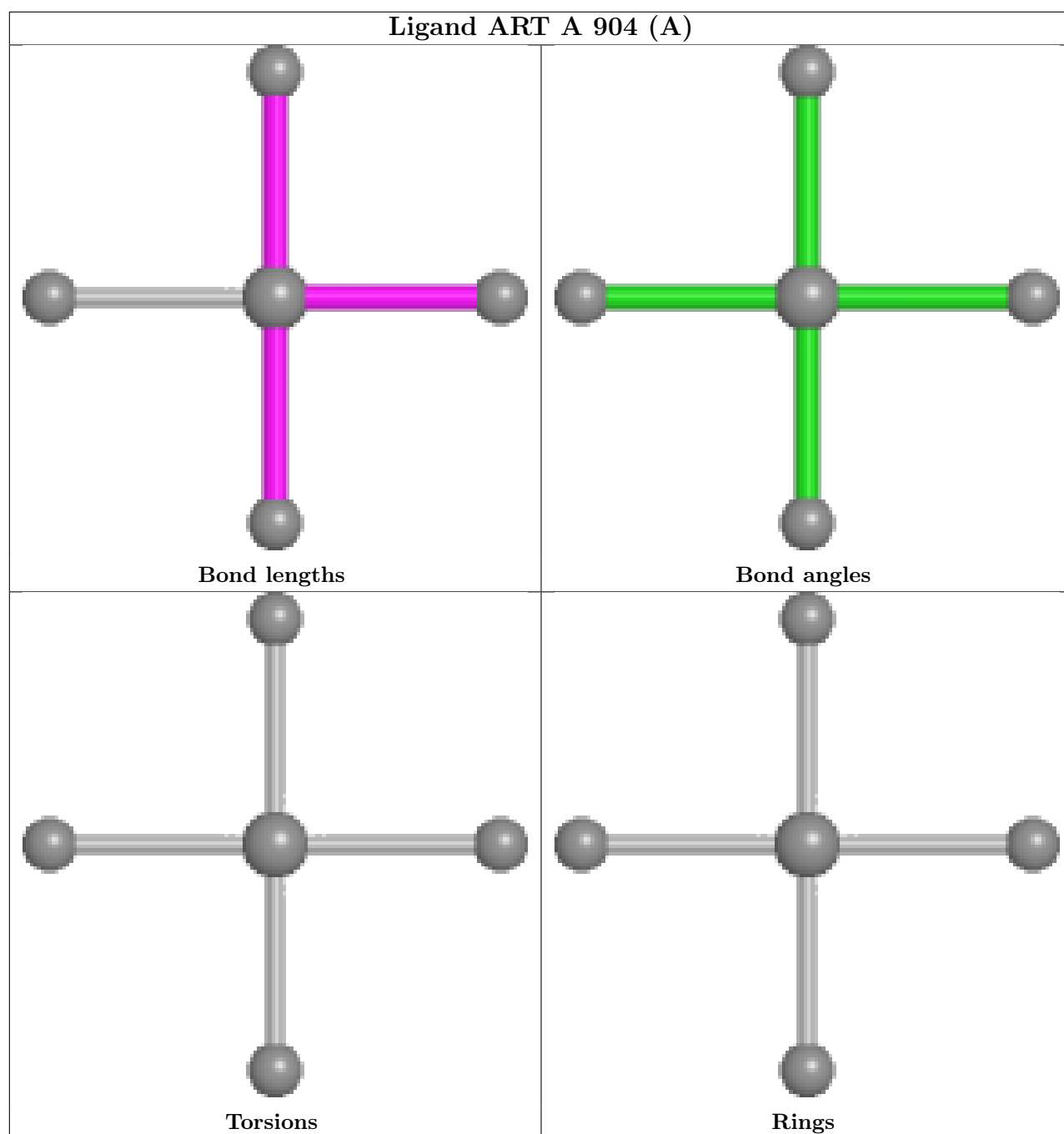


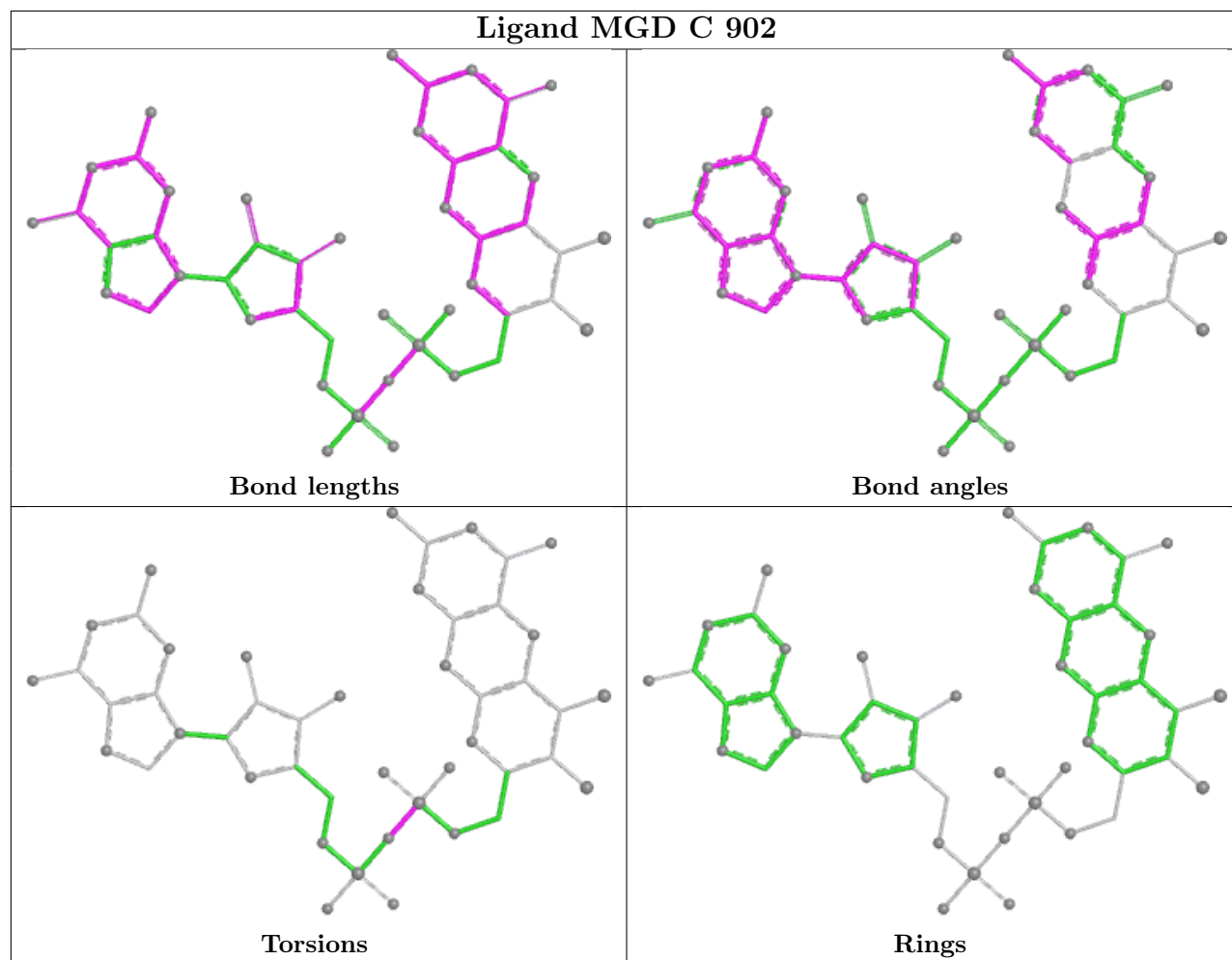












5.7 Other polymers [i](#)

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	814/814 (100%)	-0.52	5 (0%) 85 89	19, 35, 64, 117	8 (0%)
1	C	807/814 (99%)	-0.88	2 (0%) 91 93	12, 26, 45, 99	13 (1%)
2	B	234/234 (100%)	-0.64	0 100 100	15, 30, 55, 79	9 (3%)
2	D	234/234 (100%)	-0.63	0 100 100	15, 28, 51, 78	3 (1%)
All	All	2089/2096 (99%)	-0.68	7 (0%) 90 93	12, 30, 56, 117	33 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	3.6
1	C	854	VAL	3.6
1	A	329[A]	GLU	2.8
1	A	41	GLY	2.6
1	A	305	LYS	2.6
1	A	854	VAL	2.4
1	A	302	ILE	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 ⓘ

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

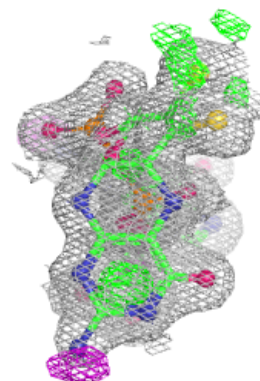
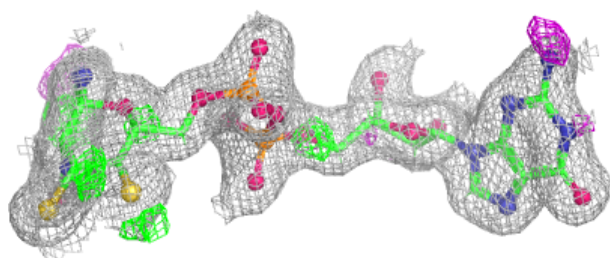
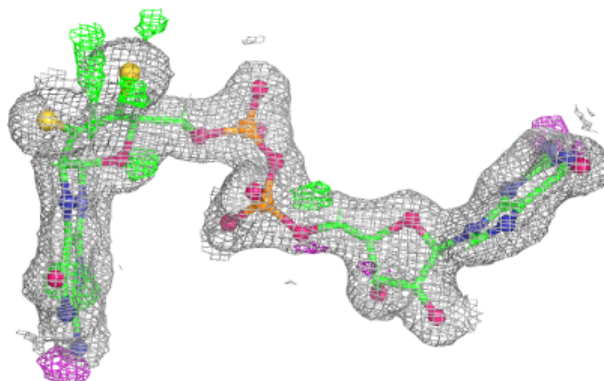
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PG5	A	911	12/12	0.68	0.17	53,76,93,93	0
9	PG5	C	911	12/12	0.77	0.19	58,81,108,128	0
8	FMT	A	909	3/3	0.91	0.13	39,39,41,50	0
8	FMT	A	910	3/3	0.92	0.19	35,45,66,80	0
7	O	A	912[A]	1/1	0.93	0.08	30,30,30,30	1
8	FMT	C	910	3/3	0.93	0.11	33,35,38,39	0
8	FMT	D	305	3/3	0.94	0.09	22,23,26,32	0
7	O	C	906[B]	1/1	0.95	0.09	33,33,33,33	1
7	O	C	912[A]	1/1	0.96	0.07	36,36,36,36	1
7	O	A	906[B]	1/1	0.97	0.06	32,32,32,32	1
4	MGD	A	902	47/47	0.97	0.06	20,25,33,33	0
8	FMT	C	909	3/3	0.97	0.06	29,30,35,36	0
7	O	A	907[B]	1/1	0.98	0.05	28,28,28,28	1
4	MGD	C	903	47/47	0.98	0.05	17,19,23,27	0
8	FMT	C	908	3/3	0.98	0.04	18,20,21,21	0
4	MGD	C	902	47/47	0.98	0.05	16,20,25,28	0
4	MGD	A	903	47/47	0.98	0.06	22,25,31,33	0
3	SF4	B	301	8/8	0.99	0.04	24,24,25,26	0
7	O	C	907[B]	1/1	0.99	0.03	17,17,17,17	1
3	SF4	B	304	8/8	0.99	0.02	29,30,31,32	0
8	FMT	A	908	3/3	0.99	0.04	20,21,24,24	0
5	ART	C	904[A]	5/5	0.99	0.05	14,18,21,24	5
5	ART	C	904[B]	5/5	0.99	0.05	24,28,42,82	5
5	ART	A	904[A]	5/5	0.99	0.05	23,26,29,33	5
5	ART	A	904[B]	5/5	0.99	0.05	29,31,56,84	5
3	SF4	B	302	8/8	1.00	0.01	19,20,20,20	0
3	SF4	B	303	8/8	1.00	0.01	22,23,24,24	0
3	SF4	D	301	8/8	1.00	0.02	21,21,23,23	0
6	MO	C	905	1/1	1.00	0.02	21,21,21,21	0
6	MO	A	905	1/1	1.00	0.02	26,26,26,26	0
3	SF4	D	302	8/8	1.00	0.02	19,20,20,21	0
3	SF4	D	303	8/8	1.00	0.02	22,23,23,23	0
3	SF4	D	304	8/8	1.00	0.01	22,22,23,23	0
3	SF4	A	901	8/8	1.00	0.02	20,20,20,21	0
3	SF4	C	901	8/8	1.00	0.01	17,17,17,17	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

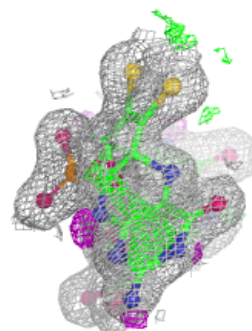
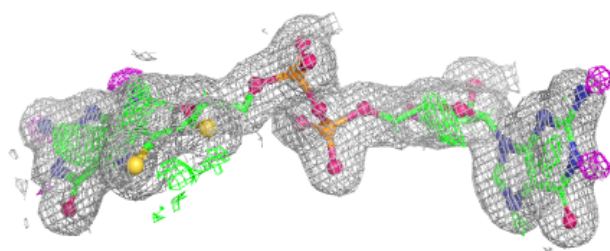
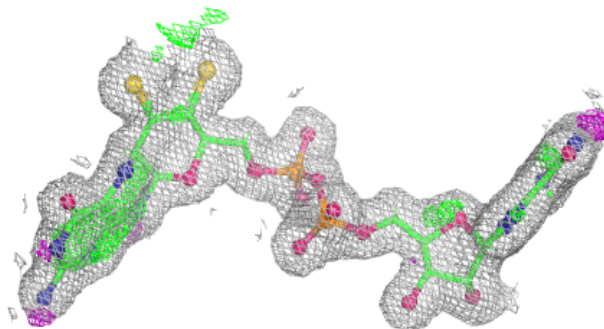
Electron density around MGD A 902:

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

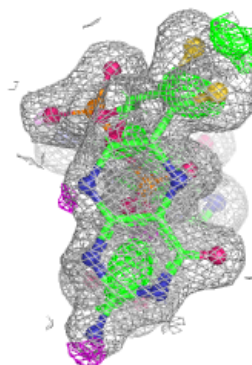
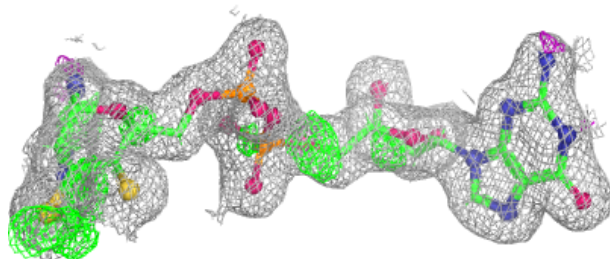
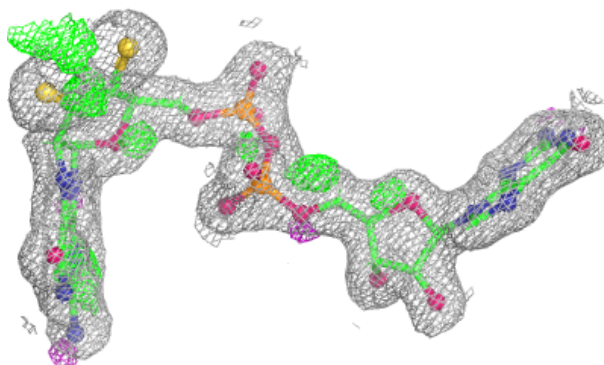


Electron density around MGD C 903:

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

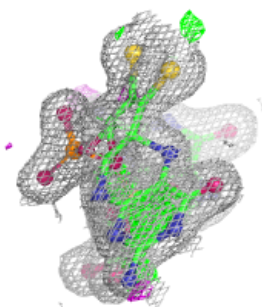
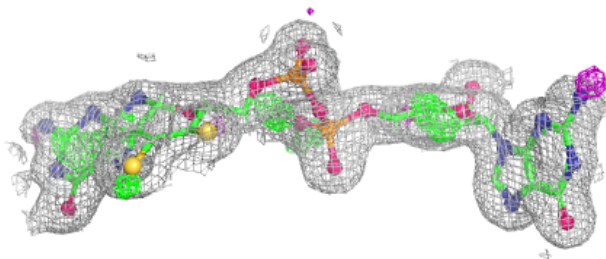
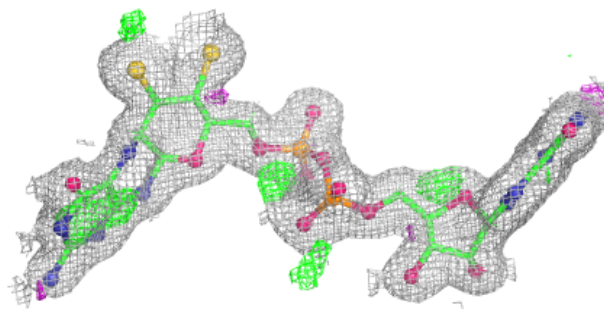
**Electron density around MGD C 902:**

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



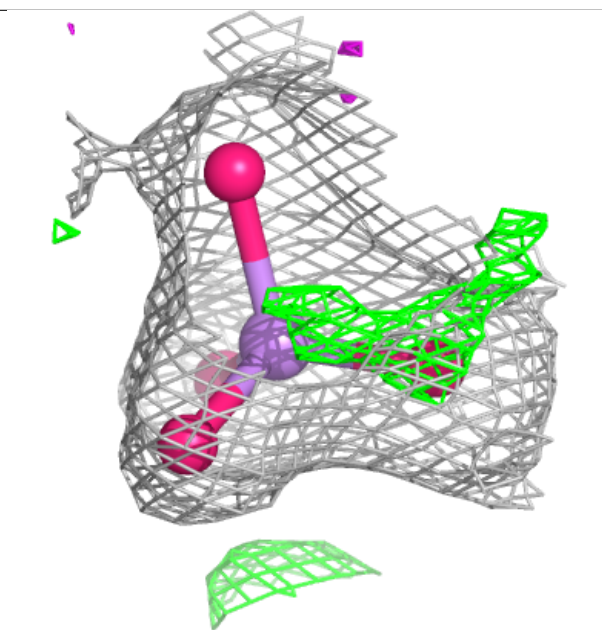
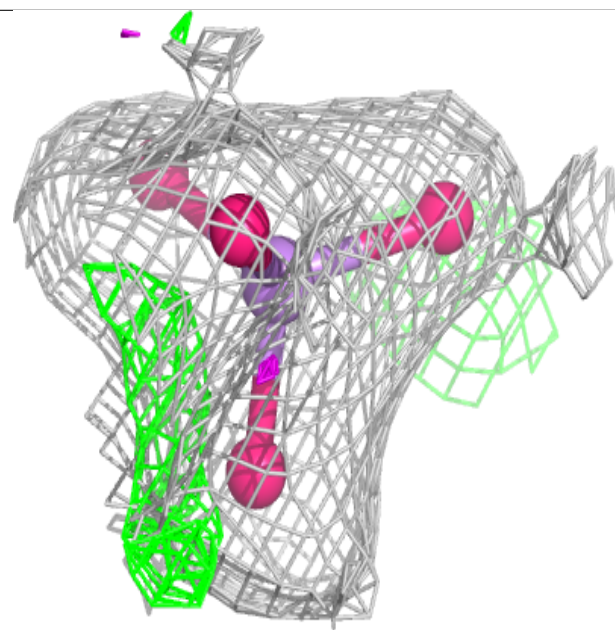
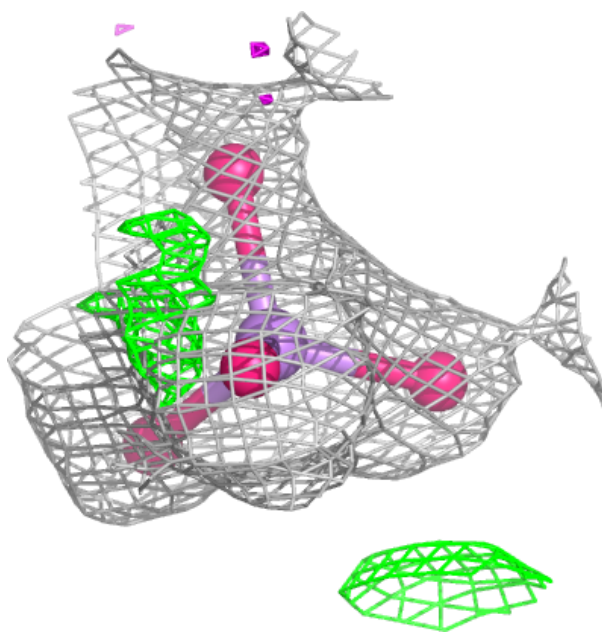
Electron density around MGD A 903:

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



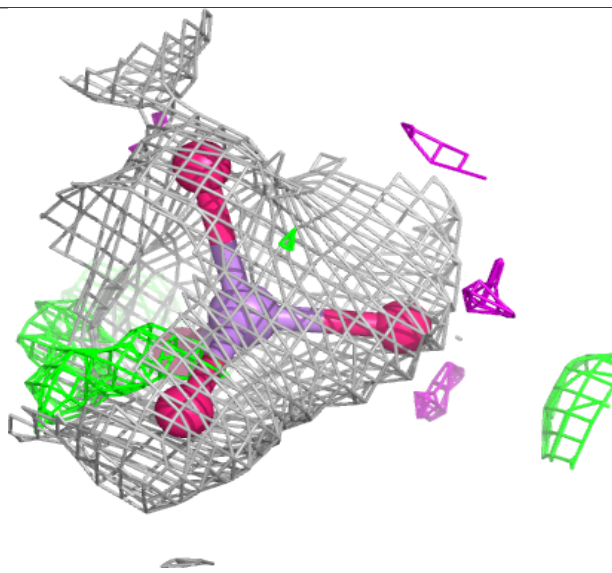
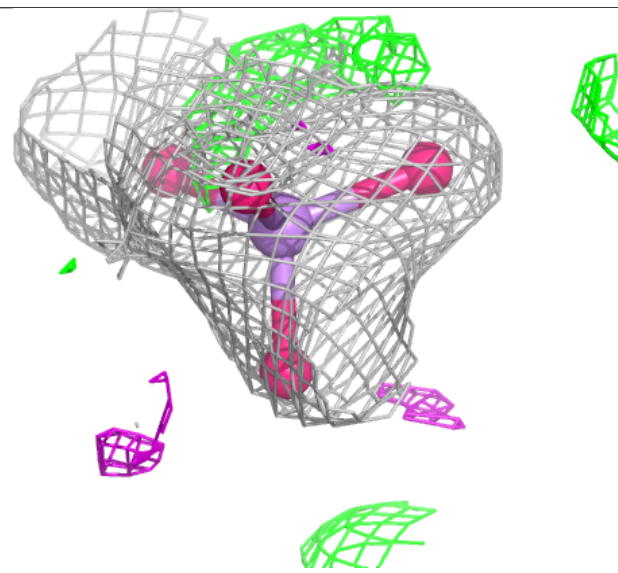
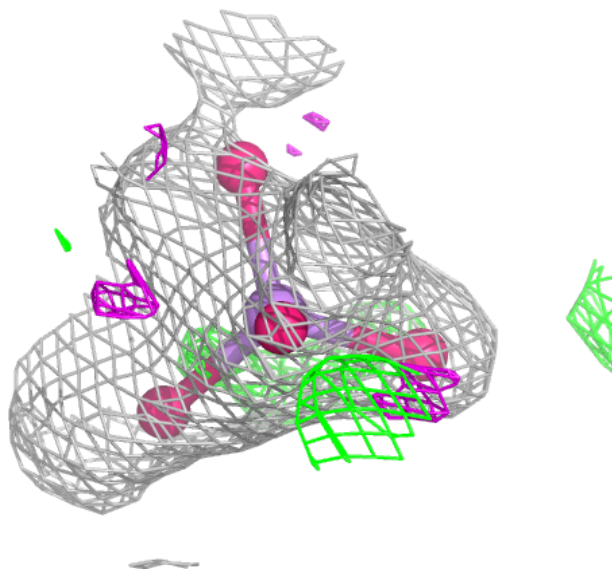
Electron density around ART C 904 (A):

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



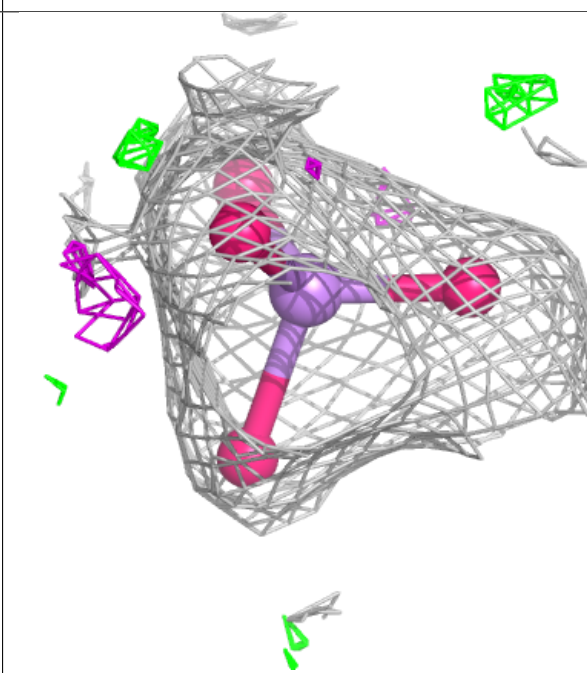
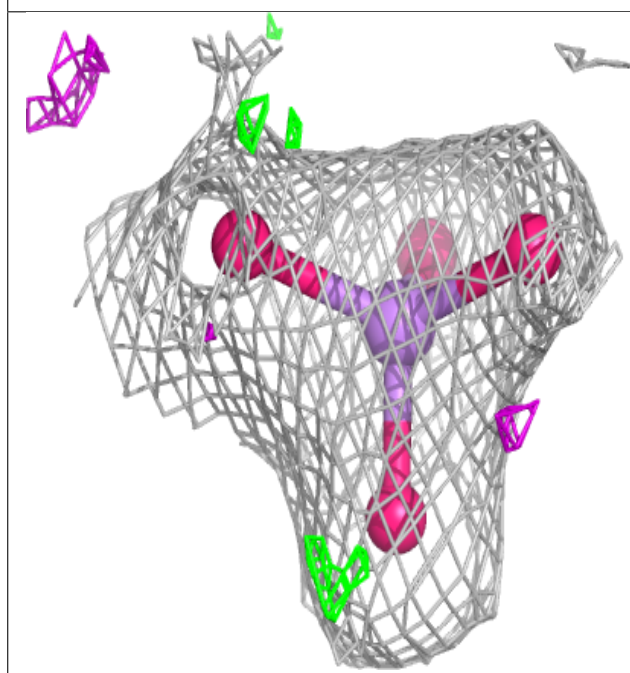
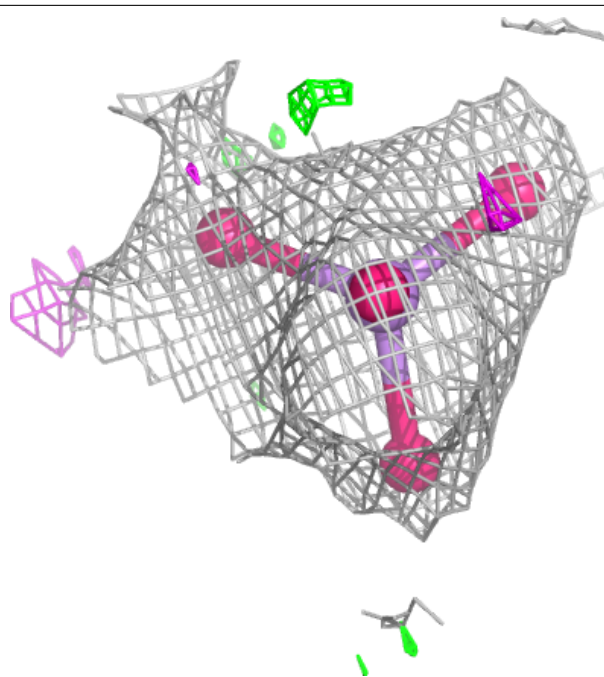
Electron density around ART C 904 (B):

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



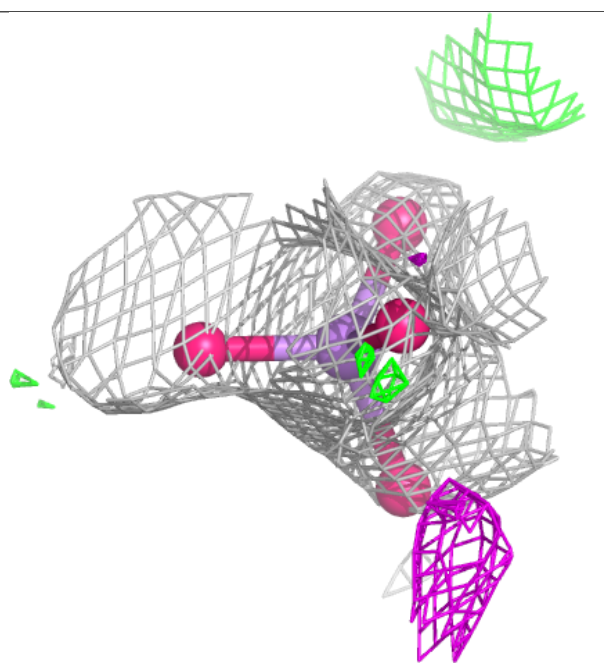
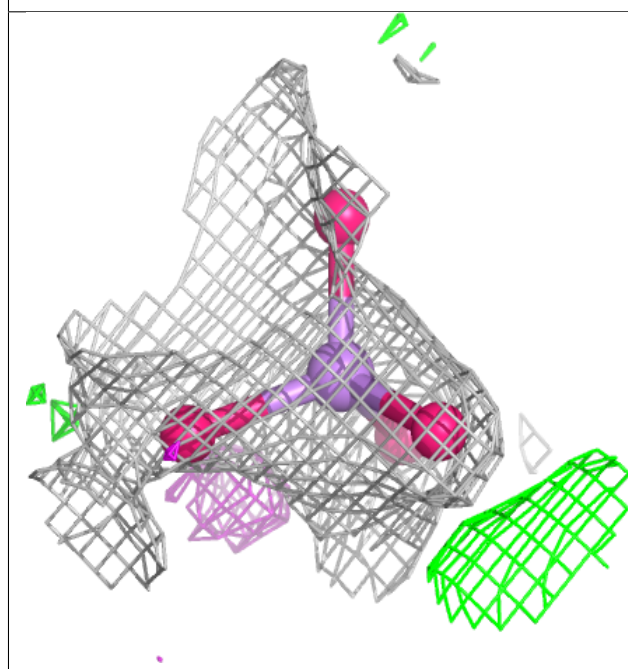
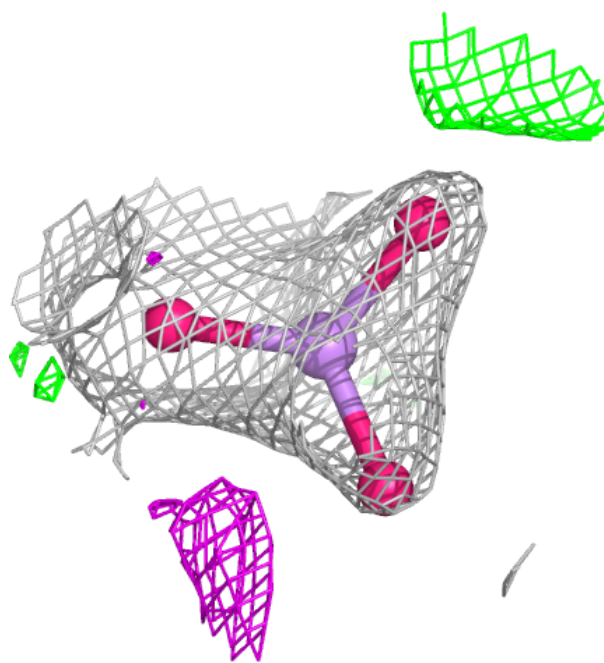
Electron density around ART A 904 (A):

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



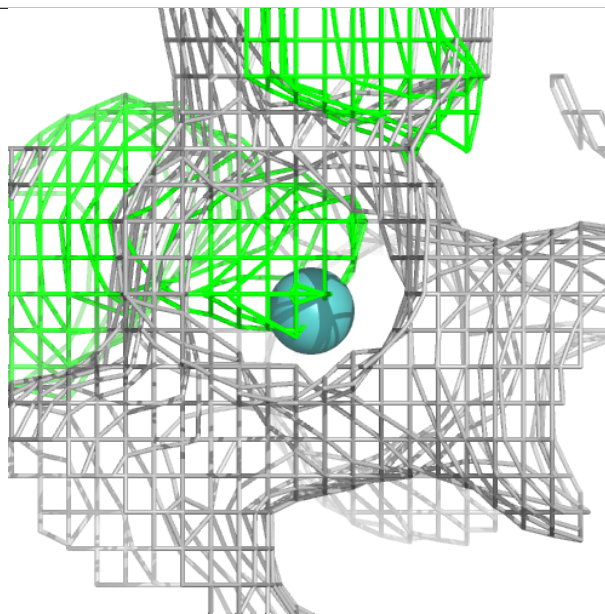
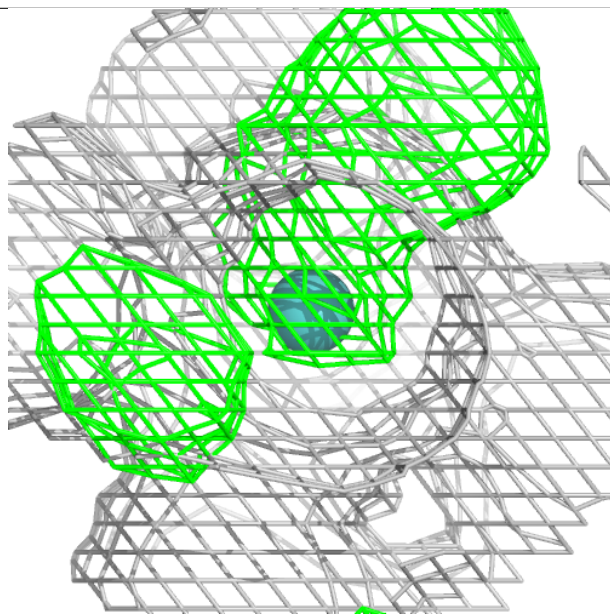
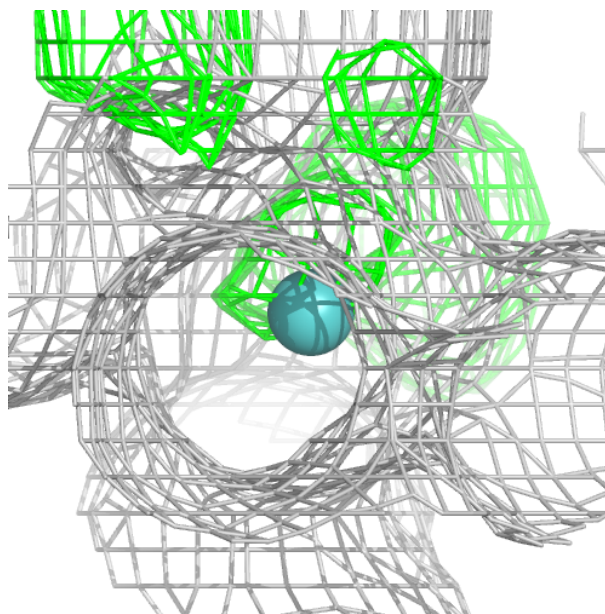
Electron density around ART A 904 (B):

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



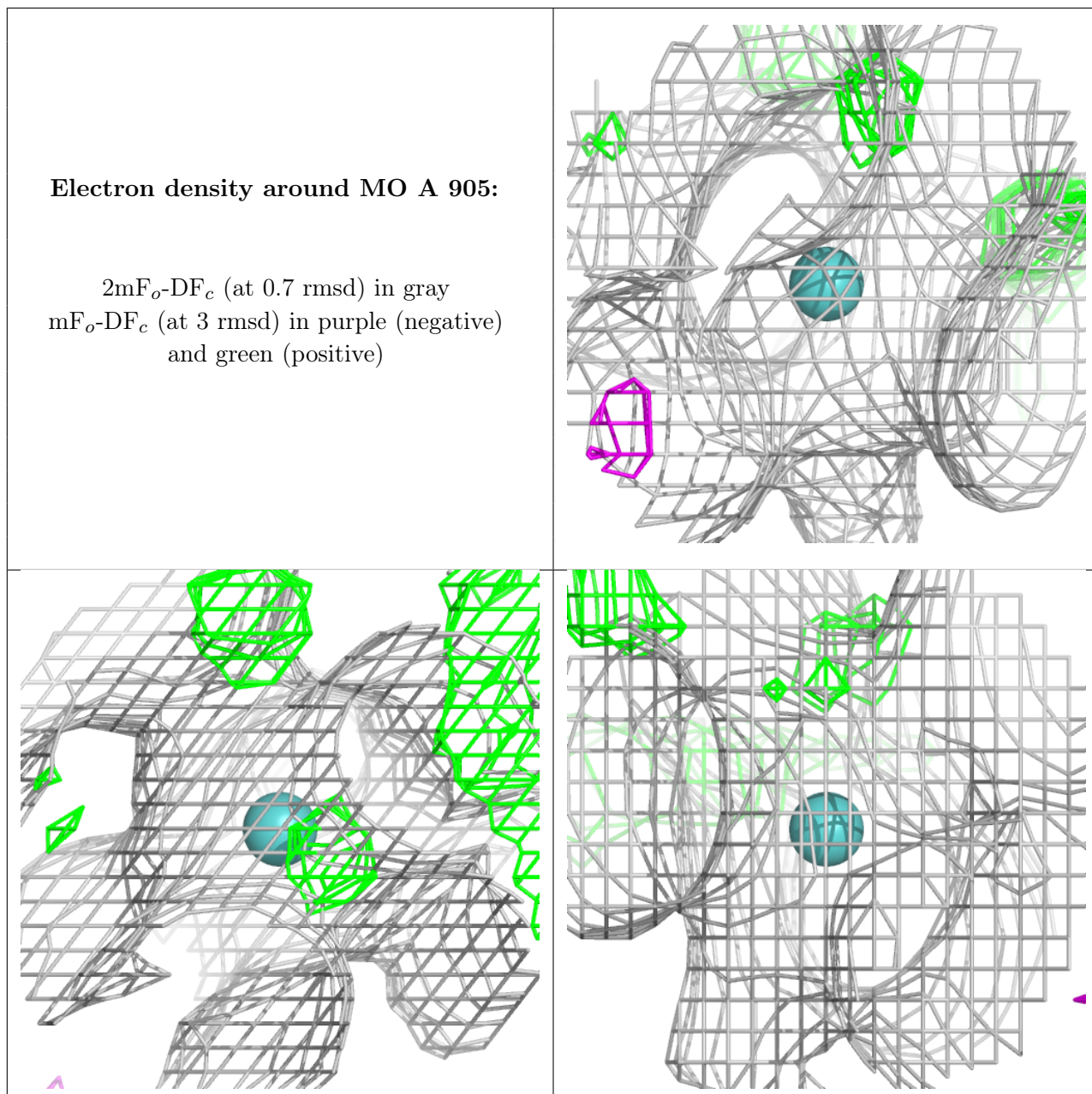
Electron density around MO C 905:

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



Electron density around MO 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.