Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 07:59 AM EST

PDB ID	:	6CZ8
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:

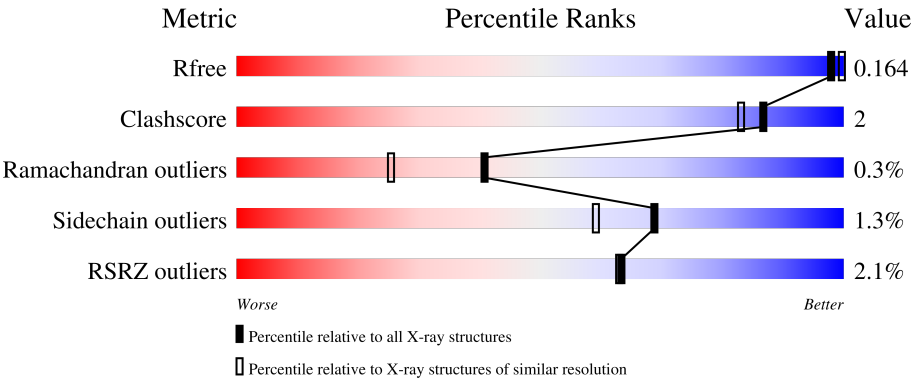
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 <=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	3% 95% 5%
1	C	814	2% 94% 5%
2	B	234	93% 7%
2	D	234	2% 91% 9%

2 Entry composition (i)

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			

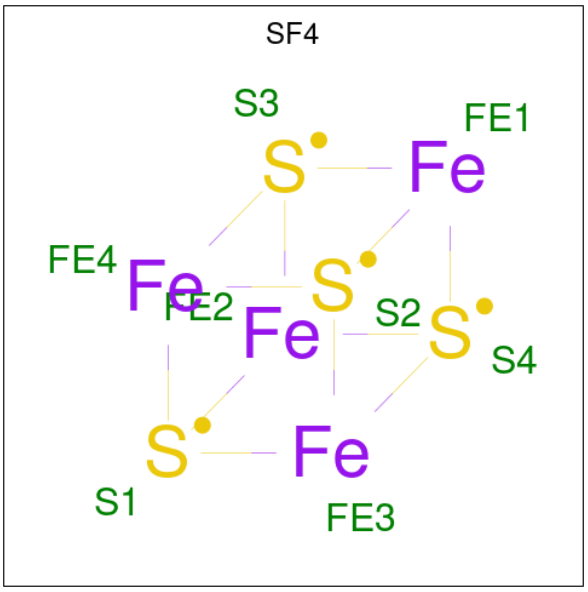
There are 2 discrepancies between the modelled and reference sequences:

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.

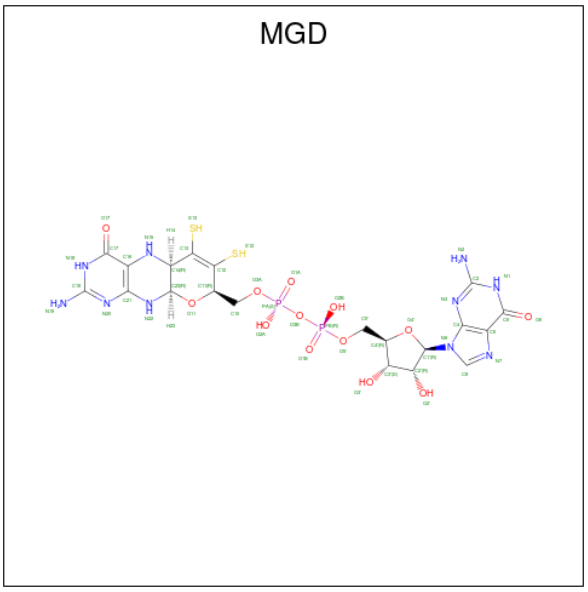
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	234	Total	C	H	N	O	S	0	3	0
			3452	1092	1682	318	337	23			
2	B	234	Total	C	H	N	O	S	0	9	0
			3609	1130	1783	327	345	24			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



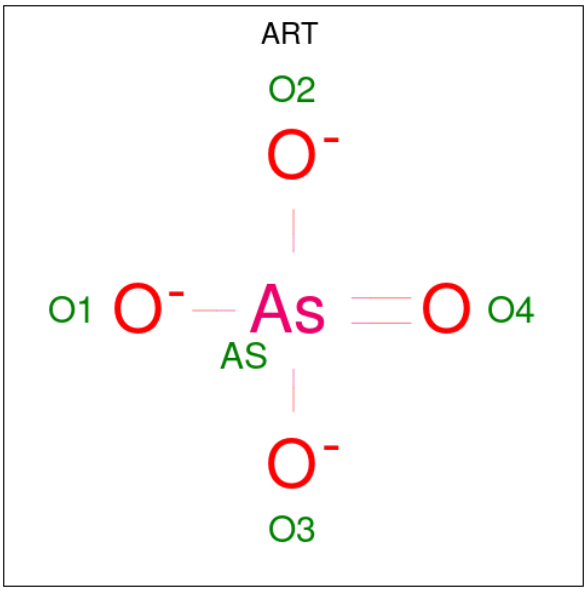
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S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

- 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 (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (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 (three-letter code: ART) (formula: AsO_4) (labeled as "Ligand of Interest" by depositor).



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

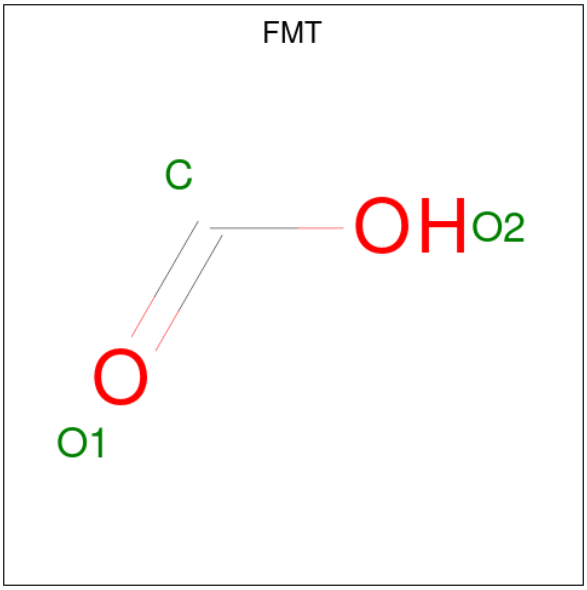
- Molecule 6 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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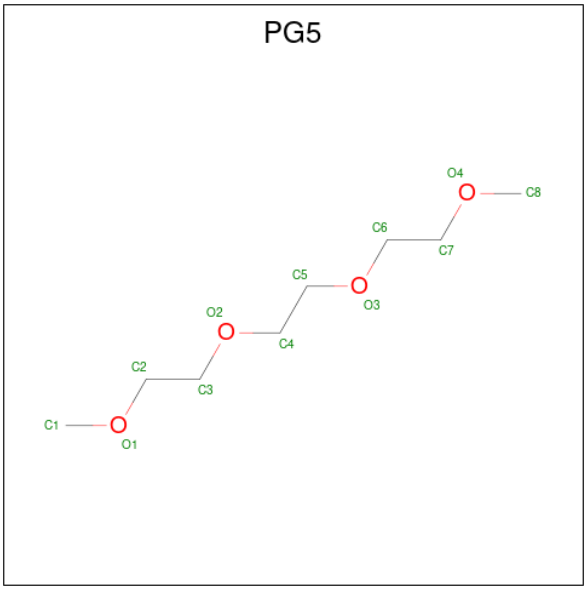
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C H O 4 1 1 2	0	0
8	C	1	Total C H O 4 1 1 2	0	0
8	D	1	Total C H O 4 1 1 2	0	0
8	A	1	Total C H O 4 1 1 2	0	0
8	A	1	Total C H O 4 1 1 2	0	0
8	A	1	Total C H O 4 1 1 2	0	0

- Molecule 9 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



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

- Molecule 10 is water.

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

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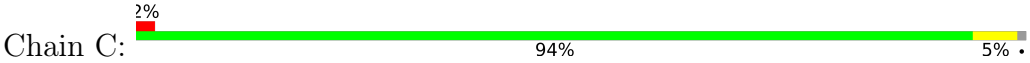
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	276	Total O 276 276	0	0
10	A	733	Total O 733 733	0	0
10	B	262	Total O 262 262	0	0

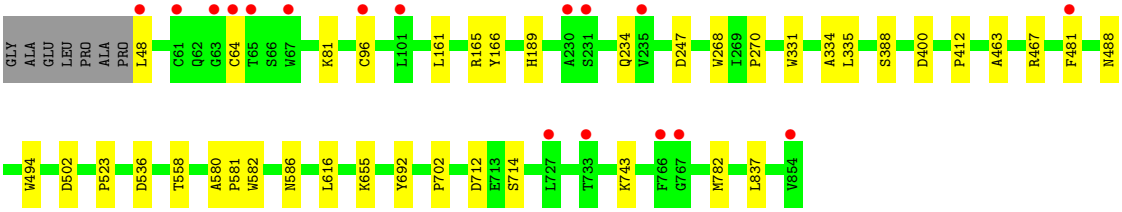
3 Residue-property plots (i)

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: ArrA

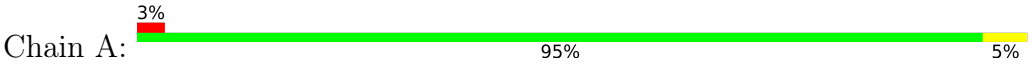
Chain C:

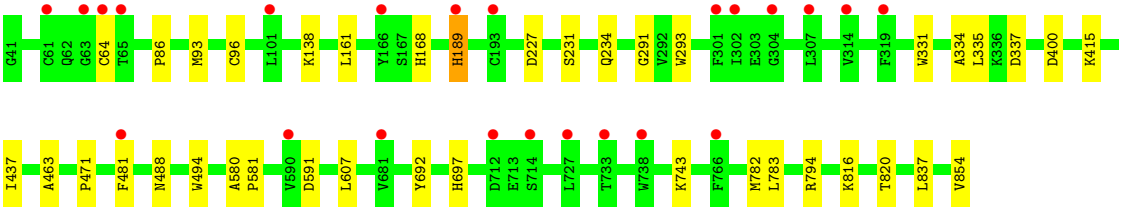




• Molecule 1: ArrA

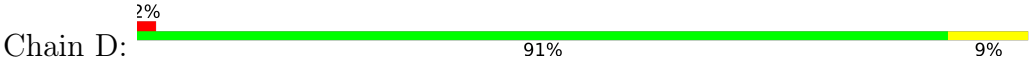
Chain A:

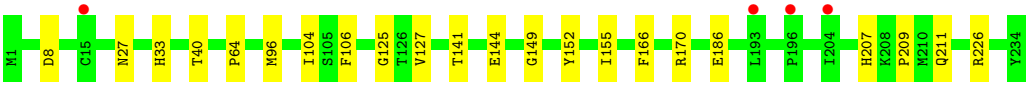




• Molecule 2: 4Fe-4S ferredoxin, iron-sulfur binding domain protein

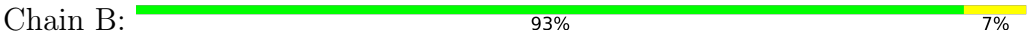
Chain D:

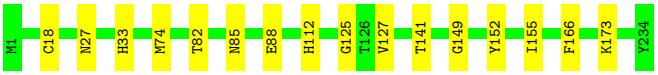




• Molecule 2: 4Fe-4S ferredoxin, iron-sulfur binding domain protein

Chain B:





4 Data and refinement statistics (i)

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 39.52 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.10-1.78) 99.9 (39.52-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 1.78Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.137 , 0.168 0.133 , 0.164	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)	0.37 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*l,-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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MO, O, MGD, PG5, FMT, ART, SF4

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	0.45	0/6621	0.55	1/8979 (0.0%)
1	C	0.48	0/6621	0.59	1/8969 (0.0%)
2	B	0.44	0/1892	0.60	0/2567
2	D	0.46	0/1818	0.61	0/2473
All	All	0.46	0/16952	0.58	2/22988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	536	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	6423	6229	6247	19	0
1	C	6410	6252	6274	21	0
2	B	1826	1783	1796	10	0
2	D	1770	1682	1691	19	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	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	4	1
10	D	276	0	0	6	0
All	All	19011	16074	16137	68	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 (68) 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:A:138:LYS:NZ	10:A:1004:HOH:O	2.28	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:GLU:CD	10:D:405:HOH:O	2.41	0.59
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
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: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: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
2:D:207:HIS:C	10:D:402:HOH:O	2.52	0.48
1:C:463:ALA:HB2	1:C:494:TRP:CE2	2.49	0.48
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
2:B:27[B]:ASN:ND2	2:B:112:HIS:NE2	2.64	0.45
1:C:712:ASP:OD1	1:C:714:SER:OG	2.33	0.44
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:268:TRP:CZ2	1:C:270:PRO:HB3	2.52	0.44
1:A:783:LEU:C	1:A:783:LEU:HD12	2.39	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
2:D:96:MET:SD	2:D:106:PHE:HB2	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:O	2:B:173:LYS:HG3	2.20	0.41
1:A:86:PRO:HG3	1:A:93:MET:HE2	2.02	0.41
1:C:388:SER:HA	1:C:702:PRO:HB3	2.02	0.41
1:C:161:LEU:C	1:C:161:LEU:HD13	2.40	0.41
1:A:692:TYR:CE1	1:A:837:LEU:HG	2.55	0.41
1:A:161:LEU:C	1:A:161:LEU:HD13	2.41	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:189:HIS:C	1:A:189:HIS:CD2	2.94	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 (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	820/814 (101%)	790 (96%)	29 (4%)	1 (0%)	51	35
1	C	818/814 (100%)	788 (96%)	29 (4%)	1 (0%)	51	35
2	B	241/234 (103%)	236 (98%)	3 (1%)	2 (1%)	19	7
2	D	235/234 (100%)	230 (98%)	3 (1%)	2 (1%)	17	5
All	All	2114/2096 (101%)	2044 (97%)	64 (3%)	6 (0%)	41	25

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	669/672 (100%)	660 (99%)	9 (1%)	69	59
1	C	671/672 (100%)	663 (99%)	8 (1%)	71	62
2	B	208/201 (104%)	205 (99%)	3 (1%)	67	56
2	D	195/201 (97%)	192 (98%)	3 (2%)	65	53
All	All	1743/1746 (100%)	1720 (99%)	23 (1%)	69	59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	96	CYS
1	C	189	HIS
1	C	234	GLN
1	C	400	ASP
1	C	481	PHE
1	C	488	ASN
1	C	743	LYS
1	C	782	MET
2	D	33	HIS
2	D	141	THR
2	D	166	PHE
1	A	96	CYS
1	A	189	HIS
1	A	234	GLN
1	A	400	ASP
1	A	481	PHE

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	743	LYS
1	A	782	MET
1	A	854	VAL
2	B	33	HIS
2	B	141	THR
2	B	166	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
9	PG5	C	911	-	11,11,11	0.50	0	10,10,10	0.20	0
3	SF4	D	303	2	0,12,12	-	-	-		
3	SF4	D	302	2	0,12,12	-	-	-		
8	FMT	A	909	-	2,2,2	0.80	0	1,1,1	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ART	A	904[A]	-	0,4,4	-	-	0,6,6	-	-
3	SF4	A	901	1	0,12,12	-	-	-		
8	FMT	A	910	-	2,2,2	0.66	0	1,1,1	0.32	0
8	FMT	A	908	-	2,2,2	0.67	0	1,1,1	0.43	0
4	MGD	A	903	6	41,52,52	5.00	26 (63%)	40,81,81	2.94	14 (35%)
4	MGD	A	902	6	41,52,52	4.82	28 (68%)	40,81,81	2.57	11 (27%)
8	FMT	C	909	-	2,2,2	0.73	0	1,1,1	0.31	0
3	SF4	C	901	1	0,12,12	-	-	-		
9	PG5	A	911	-	11,11,11	0.49	0	10,10,10	0.37	0
3	SF4	B	304	2	0,12,12	-	-	-		
8	FMT	D	305	-	2,2,2	0.65	0	1,1,1	0.62	0
5	ART	C	904[A]	-	0,4,4	-	-	0,6,6	-	-
3	SF4	B	301	10,2	0,12,12	-	-	-		
8	FMT	C	910	-	2,2,2	0.53	0	1,1,1	0.63	0
3	SF4	B	303	2	0,12,12	-	-	-		
5	ART	A	904[B]	-	0,4,4	-	-	0,6,6	-	-
5	ART	C	904[B]	-	0,4,4	-	-	0,6,6	-	-
8	FMT	C	908	-	2,2,2	0.97	0	1,1,1	0.50	0
3	SF4	D	304	2	0,12,12	-	-	-		
4	MGD	C	903	6	41,52,52	4.76	24 (58%)	40,81,81	2.68	11 (27%)
3	SF4	B	302	2	0,12,12	-	-	-		
3	SF4	D	301	2	0,12,12	-	-	-		
4	MGD	C	902	6	41,52,52	4.54	28 (68%)	40,81,81	2.60	11 (27%)

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	D	302	2	-	-	0/6/5/5
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	C	903	6	-	2/18/66/66	0/6/6/6
3	SF4	A	901	1	-	-	0/6/5/5
3	SF4	B	304	2	-	-	0/6/5/5
3	SF4	B	302	2	-	-	0/6/5/5
4	MGD	A	903	6	-	1/18/66/66	0/6/6/6
4	MGD	A	902	6	-	4/18/66/66	0/6/6/6
3	SF4	C	901	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	D	301	2	-	-	0/6/5/5
9	PG5	A	911	-	-	5/9/9/9	-
4	MGD	C	902	6	-	3/18/66/66	0/6/6/6
3	SF4	B	301	10,2	-	-	0/6/5/5
3	SF4	D	303	2	-	-	0/6/5/5

All (106) 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	902	MGD	O11-C11	12.13	1.60	1.43
4	C	902	MGD	O11-C11	12.10	1.59	1.43
4	A	903	MGD	C16-C21	11.99	1.59	1.38
4	C	903	MGD	O11-C11	11.98	1.59	1.43
4	A	903	MGD	O11-C11	11.86	1.59	1.43
4	C	903	MGD	C16-C21	11.71	1.58	1.38
4	C	902	MGD	C16-C21	11.45	1.58	1.38
4	A	903	MGD	C14-N15	11.16	1.59	1.46
4	C	902	MGD	C23-C14	-11.15	1.44	1.53
4	A	903	MGD	O11-C23	-11.14	1.27	1.43
4	C	903	MGD	O11-C23	-10.86	1.28	1.43
4	C	903	MGD	C14-N15	10.53	1.58	1.46
4	A	902	MGD	C23-C14	-9.19	1.46	1.53
4	A	903	MGD	C3'-C4'	-8.46	1.31	1.53
4	A	903	MGD	C23-N22	8.22	1.59	1.45
4	C	902	MGD	C3'-C4'	-8.12	1.32	1.53
4	C	903	MGD	C3'-C4'	-8.12	1.32	1.53
4	A	902	MGD	C3'-C4'	-8.09	1.32	1.53
4	A	902	MGD	C14-N15	7.73	1.55	1.46
4	A	903	MGD	O4'-C4'	7.72	1.62	1.45
4	A	902	MGD	O4'-C4'	7.56	1.61	1.45
4	C	903	MGD	O4'-C4'	7.14	1.61	1.45
4	C	902	MGD	O4'-C4'	6.91	1.60	1.45
4	C	903	MGD	C23-N22	6.70	1.56	1.45
4	A	902	MGD	C23-N22	6.17	1.55	1.45
4	A	902	MGD	C19-N20	6.00	1.47	1.33
4	A	902	MGD	C19-N18	6.00	1.52	1.37
4	A	903	MGD	C19-N20	5.99	1.47	1.33
4	C	903	MGD	C19-N20	5.76	1.47	1.33
4	C	902	MGD	C21-N20	5.56	1.44	1.36
4	C	902	MGD	C14-N15	5.51	1.52	1.46
4	A	903	MGD	C19-N18	5.50	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	902	MGD	C23-N22	5.43	1.54	1.45
4	C	902	MGD	C19-N20	5.35	1.46	1.33
4	C	903	MGD	C19-N18	5.15	1.50	1.37
4	A	903	MGD	C6-N1	4.91	1.45	1.37
4	A	903	MGD	C2-N2	4.82	1.45	1.34
4	A	902	MGD	C21-N20	4.74	1.43	1.36
4	A	902	MGD	C6-N1	4.71	1.44	1.37
4	C	903	MGD	C2-N2	4.67	1.45	1.34
4	C	902	MGD	C19-N18	4.59	1.49	1.37
4	A	903	MGD	C19-N19	4.58	1.45	1.34
4	C	903	MGD	C21-N20	4.56	1.42	1.36
4	A	903	MGD	C21-N20	4.45	1.42	1.36
4	A	903	MGD	C21-N22	4.44	1.40	1.35
4	A	902	MGD	C2-N2	4.44	1.44	1.34
4	C	903	MGD	C6-N1	4.39	1.44	1.37
4	A	903	MGD	C2-N3	4.32	1.43	1.33
4	A	902	MGD	C21-N22	4.29	1.40	1.35
4	A	902	MGD	C4-N3	4.28	1.47	1.37
4	A	902	MGD	C19-N19	4.16	1.44	1.34
4	A	902	MGD	C2-N3	4.09	1.43	1.33
4	C	902	MGD	C2-N3	4.03	1.43	1.33
4	C	902	MGD	C2-N2	3.97	1.43	1.34
4	C	902	MGD	C4-N3	3.96	1.47	1.37
4	C	902	MGD	C19-N19	3.92	1.43	1.34
4	C	903	MGD	C17-N18	3.89	1.46	1.38
4	A	902	MGD	O3'-C3'	3.82	1.52	1.43
4	C	902	MGD	C17-N18	3.79	1.45	1.38
4	A	902	MGD	C17-N18	3.76	1.45	1.38
4	A	902	MGD	O17-C17	-3.63	1.16	1.23
4	C	903	MGD	C4-N3	3.63	1.46	1.37
4	C	903	MGD	C19-N19	3.61	1.42	1.34
4	C	903	MGD	C5-C6	3.54	1.54	1.47
4	C	902	MGD	C6-N1	3.52	1.43	1.37
4	A	902	MGD	O4'-C1'	-3.50	1.36	1.41
4	C	903	MGD	C2-N3	3.49	1.41	1.33
4	C	903	MGD	C21-N22	3.40	1.39	1.35
4	A	902	MGD	C5-C6	3.39	1.54	1.47
4	A	903	MGD	O4'-C1'	-3.36	1.36	1.41
4	A	903	MGD	C5-C6	3.36	1.54	1.47
4	A	903	MGD	C17-N18	3.33	1.45	1.38
4	C	902	MGD	O3'-C3'	3.32	1.50	1.43
4	A	903	MGD	O17-C17	-3.26	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	MGD	O2'-C2'	-3.21	1.35	1.43
4	A	903	MGD	C4-N3	3.18	1.45	1.37
4	C	903	MGD	C16-C17	3.07	1.50	1.42
4	C	902	MGD	C21-N22	3.02	1.38	1.35
4	C	902	MGD	C5-C4	-2.99	1.35	1.43
4	C	902	MGD	C5-C6	2.97	1.53	1.47
4	C	903	MGD	O17-C17	-2.83	1.18	1.23
4	A	902	MGD	O6-C6	-2.80	1.17	1.23
4	C	902	MGD	C8-N7	2.71	1.39	1.35
4	A	902	MGD	C5-C4	-2.65	1.36	1.43
4	A	903	MGD	C16-C17	2.64	1.49	1.42
4	A	902	MGD	C16-C17	2.59	1.49	1.42
4	A	902	MGD	C12-C13	2.51	1.51	1.35
4	C	902	MGD	O17-C17	-2.49	1.18	1.23
4	A	903	MGD	C5-C4	-2.45	1.36	1.43
4	C	902	MGD	C12-C13	2.39	1.51	1.35
4	C	903	MGD	C5-C4	-2.39	1.37	1.43
4	A	903	MGD	C12-C13	2.36	1.50	1.35
4	A	903	MGD	O3'-C3'	2.35	1.48	1.43
4	C	902	MGD	C16-C17	2.33	1.48	1.42
4	C	903	MGD	C8-N7	2.31	1.39	1.35
4	C	902	MGD	O6-C6	-2.20	1.18	1.23
4	A	903	MGD	C2'-C1'	-2.19	1.50	1.53
4	C	902	MGD	C2-N1	2.18	1.43	1.37
4	A	902	MGD	C8-N7	2.17	1.38	1.35
4	C	902	MGD	O2'-C2'	-2.15	1.37	1.43
4	C	902	MGD	O11-C23	-2.12	1.40	1.43
4	C	903	MGD	C2-N1	2.06	1.42	1.37
4	C	903	MGD	C12-C13	2.02	1.48	1.35
4	A	903	MGD	C8-N7	2.01	1.38	1.35
4	A	902	MGD	C2'-C1'	-2.01	1.50	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	903	MGD	O11-C23-C14	13.18	117.75	108.96
4	C	902	MGD	O11-C23-N22	-11.32	96.94	108.57
4	C	903	MGD	O11-C23-C14	11.22	116.45	108.96
4	A	902	MGD	O11-C23-N22	-11.08	97.18	108.57
4	C	903	MGD	O11-C23-N22	8.17	116.96	108.57
4	A	903	MGD	O11-C23-N22	7.72	116.50	108.57
4	C	902	MGD	C2'-C3'-C4'	5.39	113.12	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	902	MGD	O11-C23-C14	4.81	112.17	108.96
4	C	902	MGD	N2-C2-N1	4.52	126.33	116.71
4	A	903	MGD	C19-N20-C21	4.30	121.19	113.43
4	A	903	MGD	N2-C2-N1	4.19	125.64	116.71
4	A	902	MGD	C19-N20-C21	3.99	120.63	113.43
4	A	902	MGD	C2'-C3'-C4'	3.98	110.38	102.64
4	A	902	MGD	N2-C2-N1	3.90	125.02	116.71
4	C	903	MGD	C19-N20-C21	3.77	120.23	113.43
4	C	903	MGD	N2-C2-N1	3.74	124.67	116.71
4	C	902	MGD	C19-N20-C21	3.48	119.70	113.43
4	C	902	MGD	O11-C23-C14	3.42	111.24	108.96
4	C	902	MGD	N2-C2-N3	-3.12	113.67	119.74
4	A	902	MGD	C5-C6-N1	2.85	118.99	113.95
4	A	903	MGD	C17-C16-N15	2.70	124.00	116.76
4	C	902	MGD	C5-C6-N1	2.69	118.70	113.95
4	C	903	MGD	C17-C16-N15	2.68	123.97	116.76
4	C	902	MGD	N18-C19-N20	-2.61	118.46	123.32
4	A	903	MGD	N19-C19-N18	2.60	122.24	116.71
4	A	903	MGD	N1-C2-N3	-2.57	118.51	123.32
4	A	903	MGD	C5-C6-N1	2.52	118.40	113.95
4	C	902	MGD	C8-N7-C5	2.44	107.64	102.99
4	A	903	MGD	C8-N7-C5	2.43	107.63	102.99
4	A	903	MGD	O2'-C2'-C1'	-2.43	101.88	110.85
4	C	903	MGD	C5-C6-N1	2.38	118.15	113.95
4	A	902	MGD	O17-C17-C16	-2.36	121.83	127.24
4	C	902	MGD	N19-C19-N18	2.35	121.72	116.71
4	A	902	MGD	N1-C2-N3	-2.32	118.99	123.32
4	A	902	MGD	C16-C17-N18	2.31	119.20	112.31
4	C	903	MGD	O3'-C3'-C2'	-2.29	104.41	111.82
4	A	902	MGD	C8-N7-C5	2.27	107.31	102.99
4	A	902	MGD	N19-C19-N18	2.25	121.51	116.71
4	A	903	MGD	C3'-C2'-C1'	2.22	104.32	100.98
4	C	903	MGD	N19-C19-N18	2.17	121.33	116.71
4	C	903	MGD	O2'-C2'-C1'	-2.16	102.86	110.85
4	C	903	MGD	N1-C2-N3	-2.14	119.32	123.32
4	C	902	MGD	C3'-C2'-C1'	-2.12	97.78	100.98
4	A	903	MGD	N18-C19-N20	-2.11	119.39	123.32
4	A	903	MGD	C16-C17-N18	2.09	118.55	112.31
4	A	903	MGD	N2-C2-N3	-2.04	115.78	119.74
4	C	903	MGD	C8-N7-C5	2.03	106.86	102.99

There are no chirality outliers.

All (21) 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
9	A	911	PG5	O3-C6-C7-O4
4	C	903	MGD	C3'-C4'-C5'-O5'
9	C	911	PG5	O3-C6-C7-O4
9	C	911	PG5	C4-C5-O3-C6
9	C	911	PG5	C6-C7-O4-C8
9	A	911	PG5	O2-C4-C5-O3
4	C	903	MGD	O4'-C4'-C5'-O5'
9	C	911	PG5	C2-C3-O2-C4
4	A	902	MGD	O4'-C4'-C5'-O5'
9	C	911	PG5	O2-C4-C5-O3
9	A	911	PG5	C3-C2-O1-C1
4	A	902	MGD	C3'-C4'-C5'-O5'
4	C	902	MGD	PB-O3B-PA-O1A
4	A	902	MGD	PB-O3B-PA-O1A
9	A	911	PG5	C2-C3-O2-C4
9	A	911	PG5	O1-C2-C3-O2
4	C	902	MGD	O4'-C4'-C5'-O5'
4	A	903	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

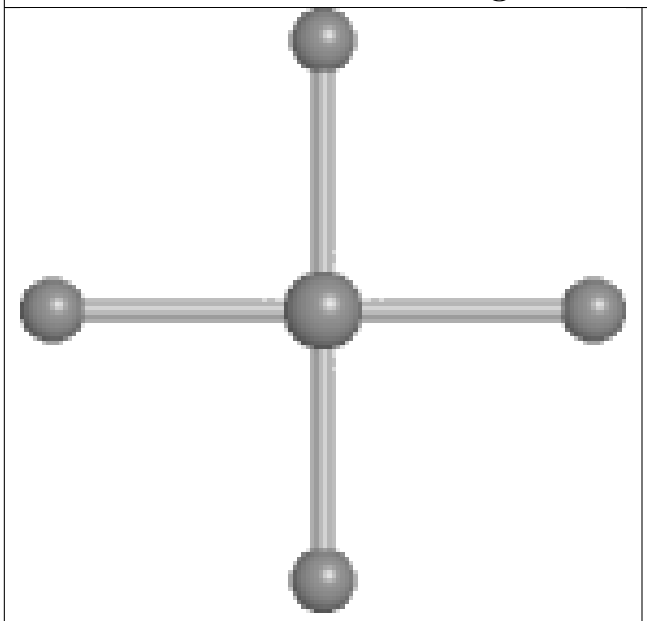
8 monomers are involved in 9 short contacts:

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

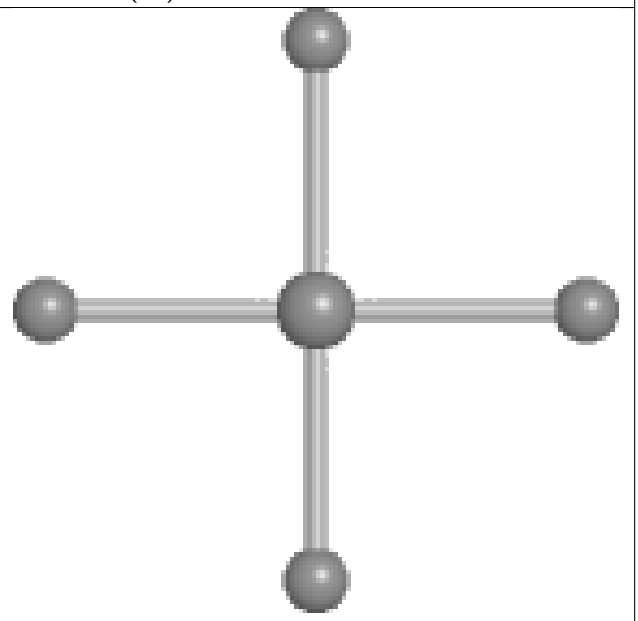
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

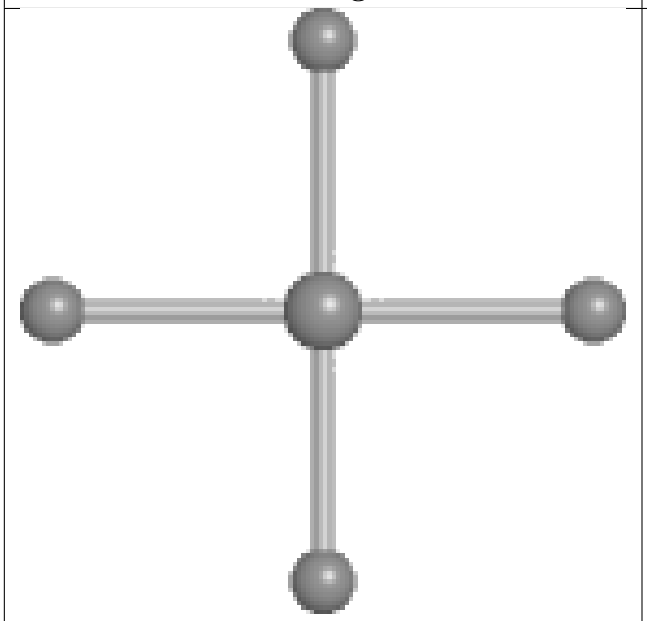
Ligand ART A 904 (A)



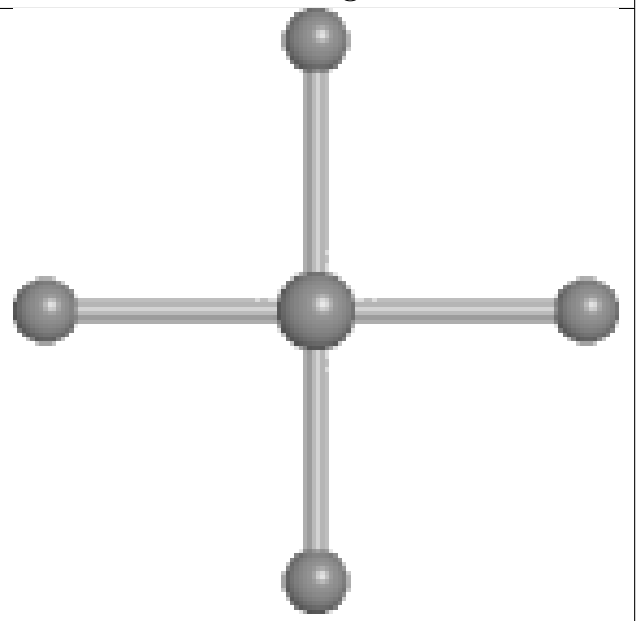
Bond lengths



Bond angles

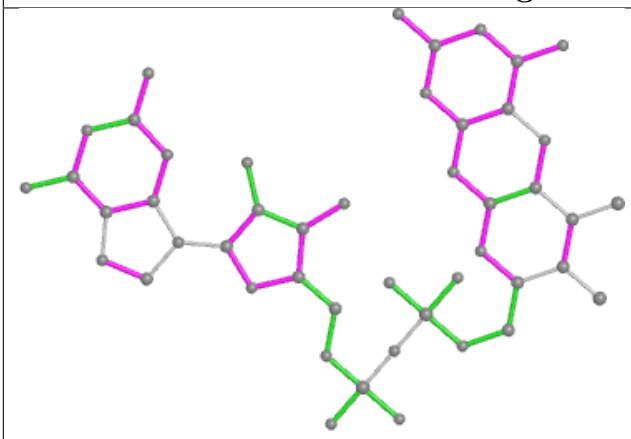


Torsions

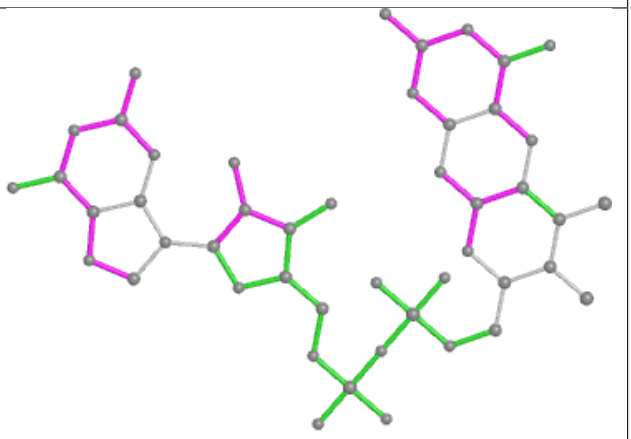


Rings

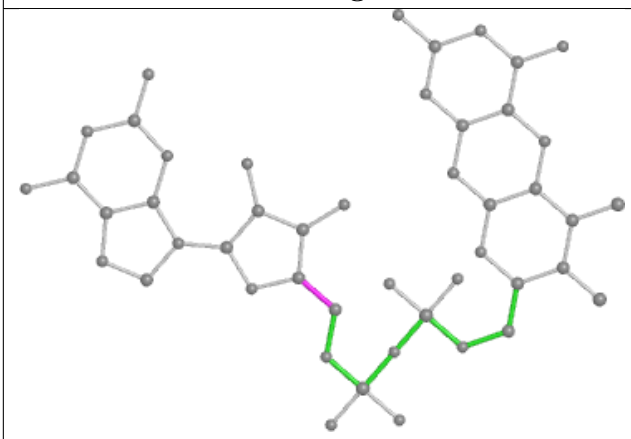
Ligand MGD A 903



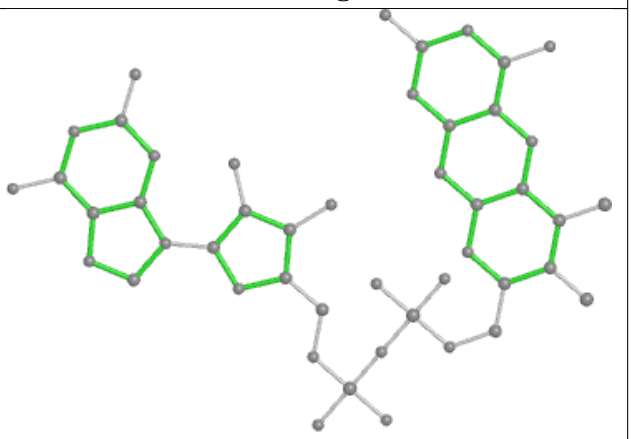
Bond lengths



Bond angles

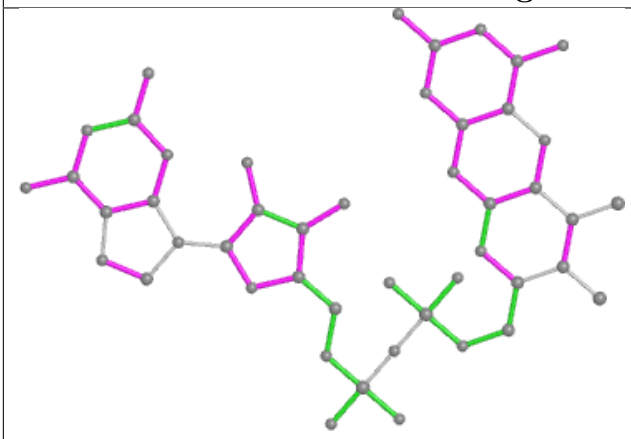


Torsions

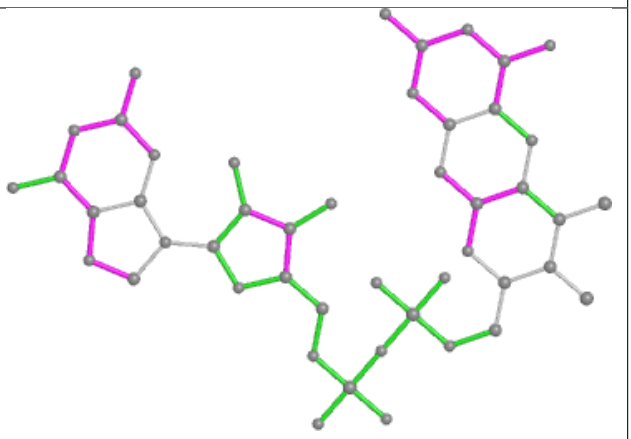


Rings

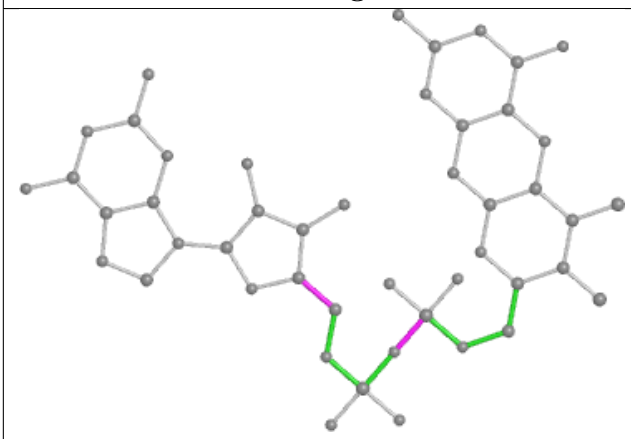
Ligand MGD A 902



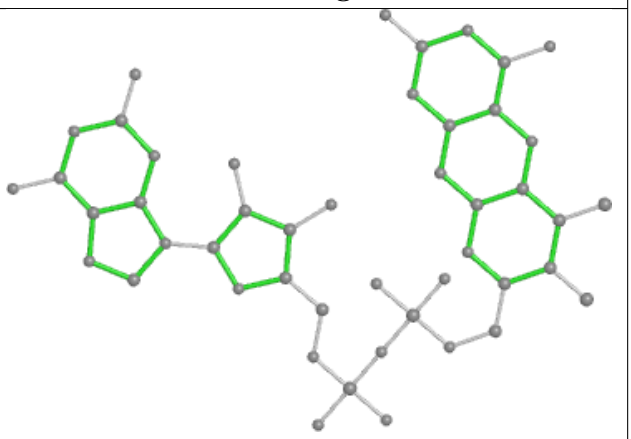
Bond lengths



Bond angles

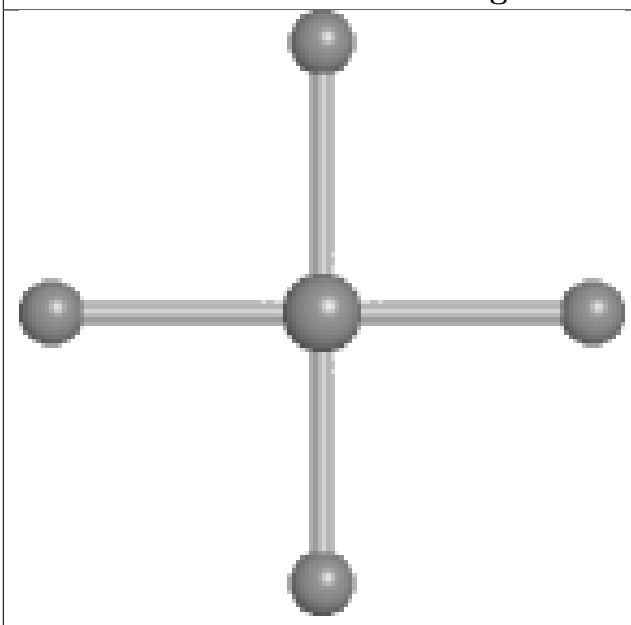


Torsions

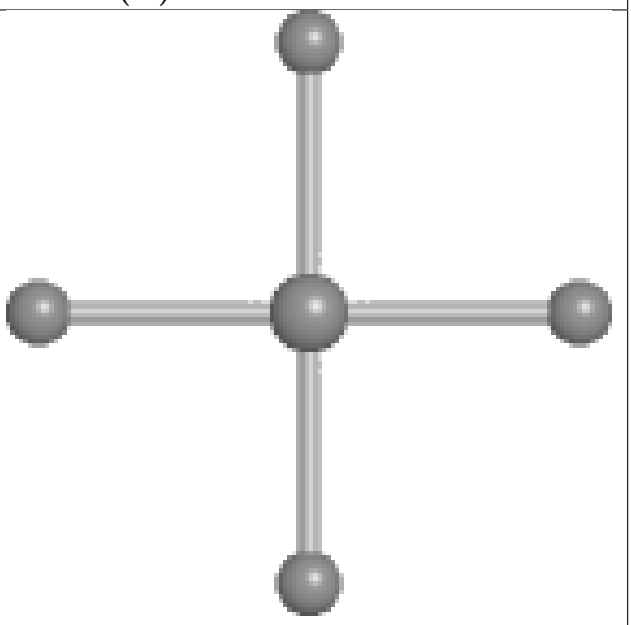


Rings

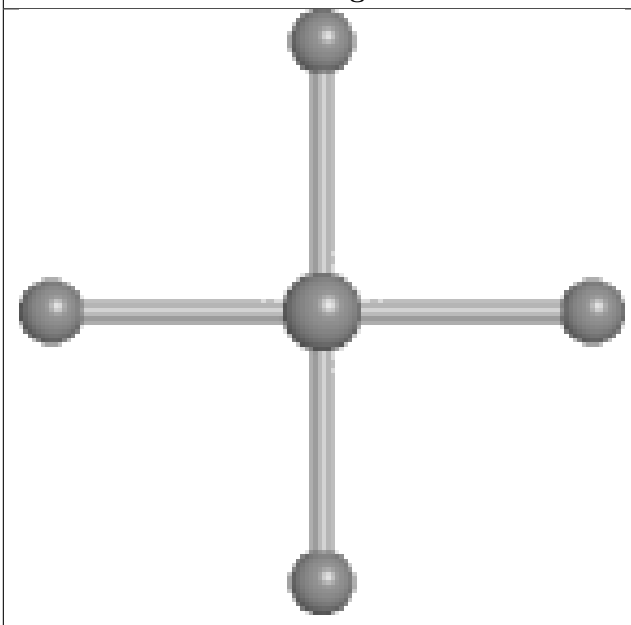
Ligand ART C 904 (A)



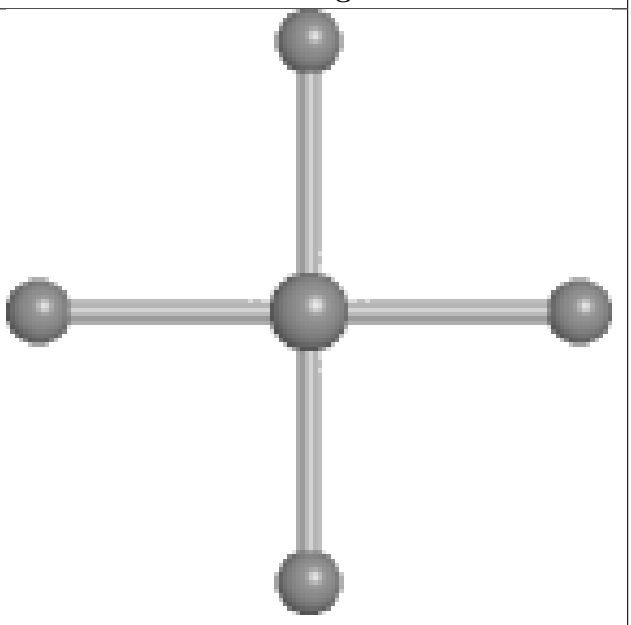
Bond lengths



Bond angles

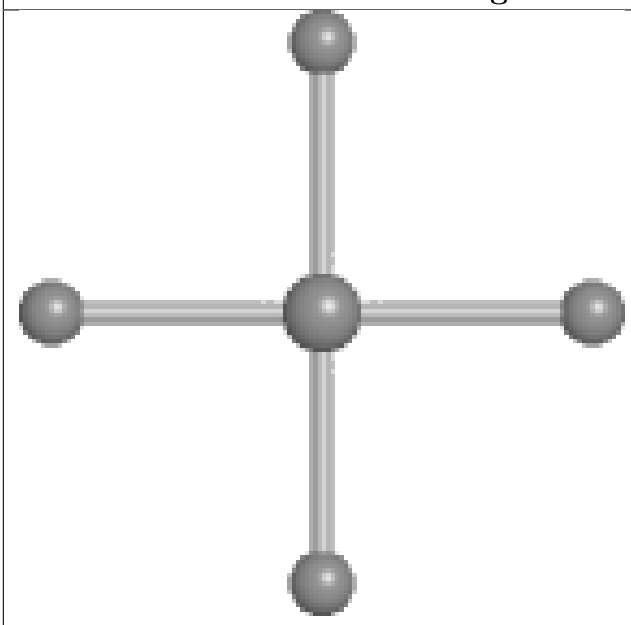


Torsions

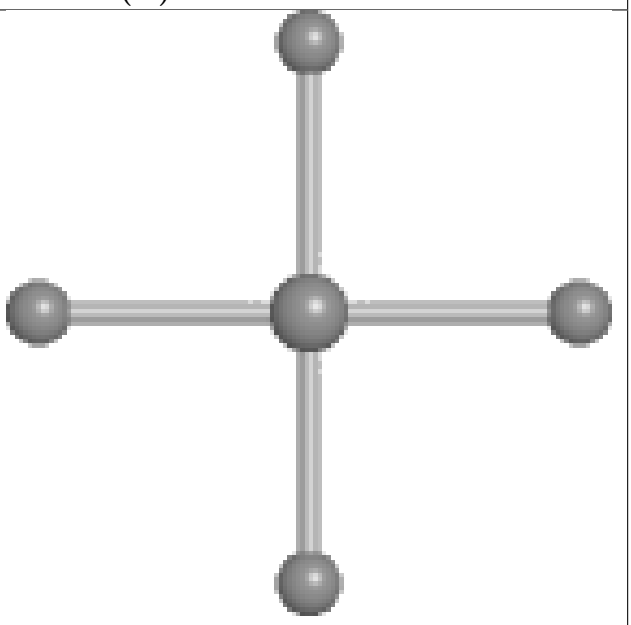


Rings

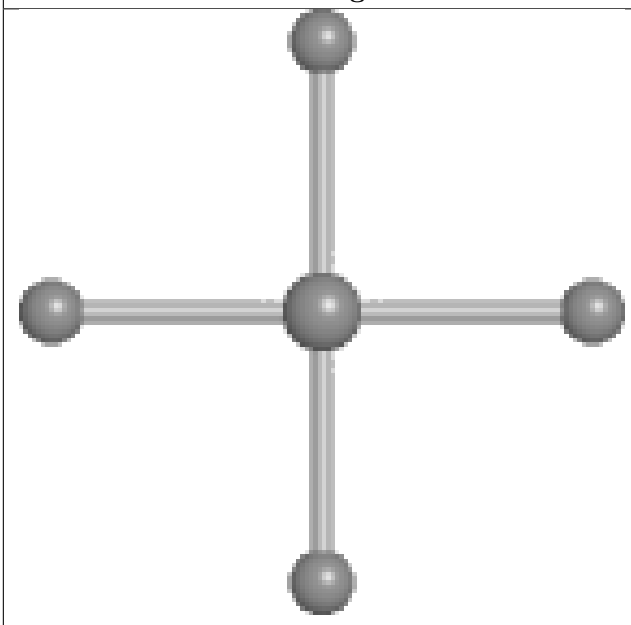
Ligand ART A 904 (B)



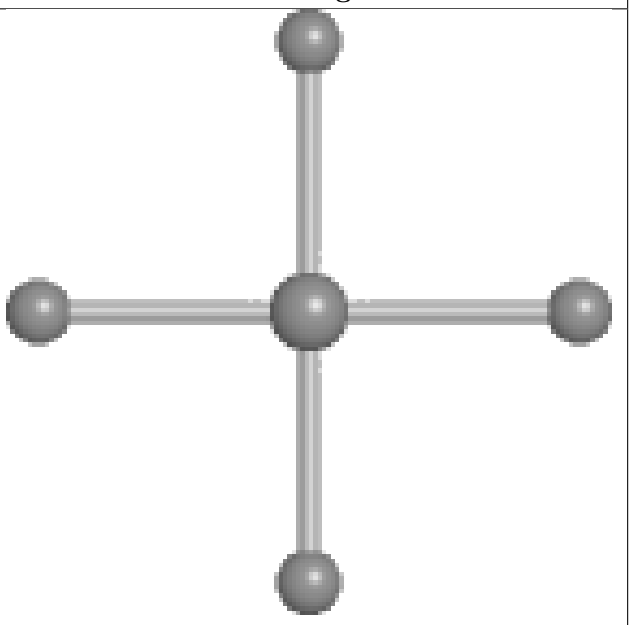
Bond lengths



Bond angles

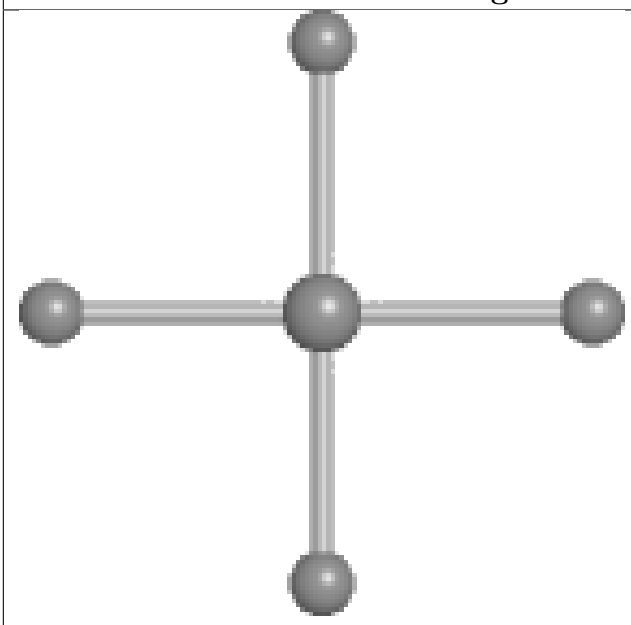


Torsions

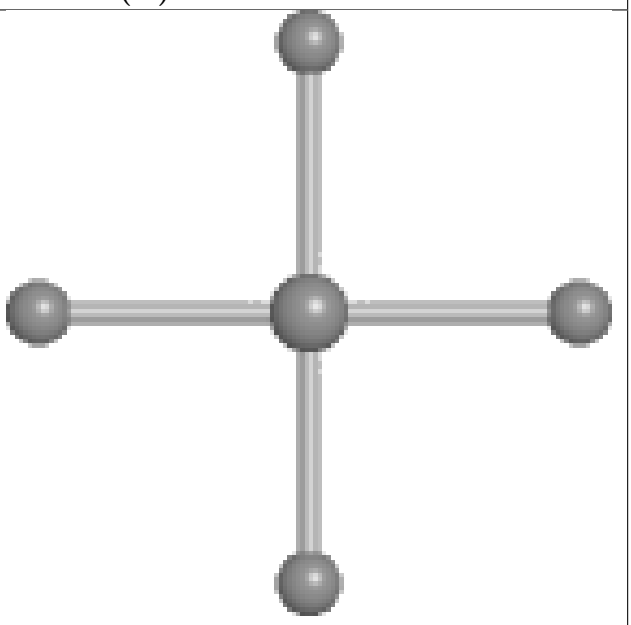


Rings

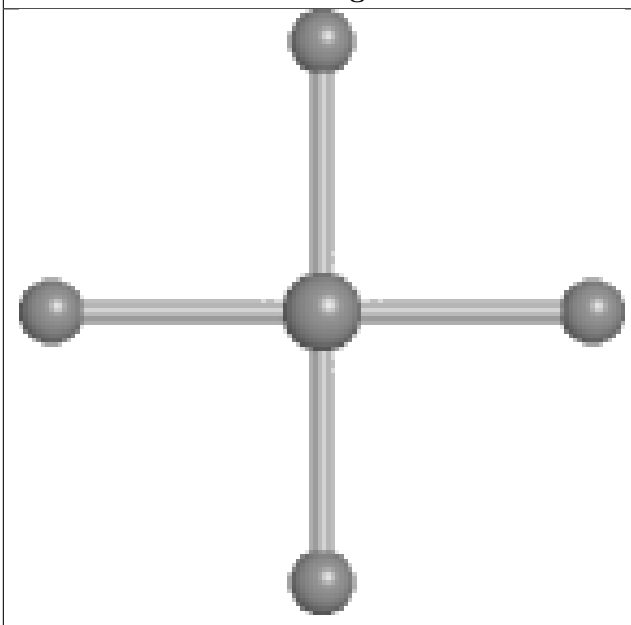
Ligand ART C 904 (B)



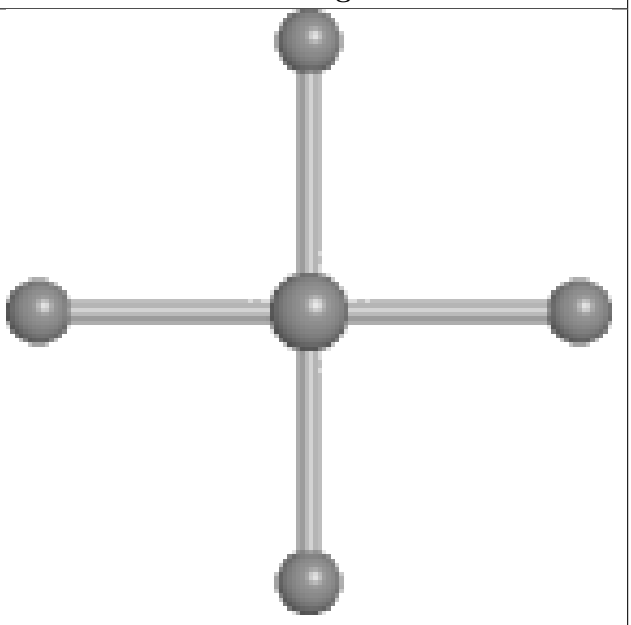
Bond lengths



Bond angles

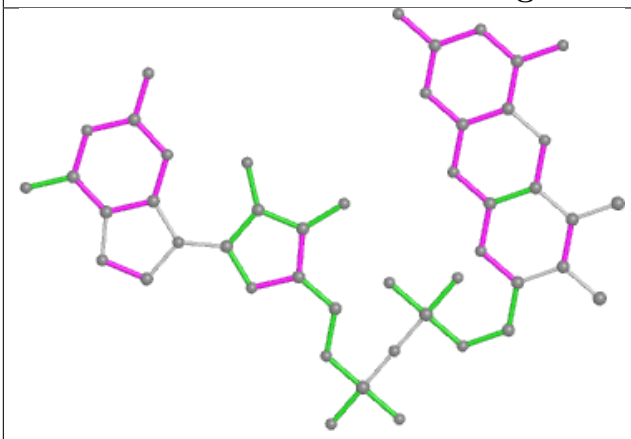


Torsions

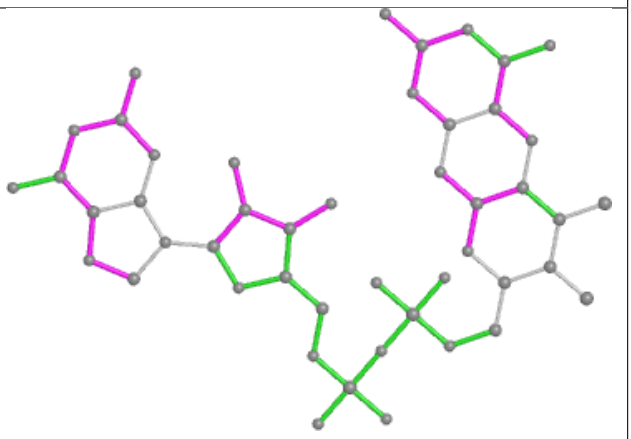


Rings

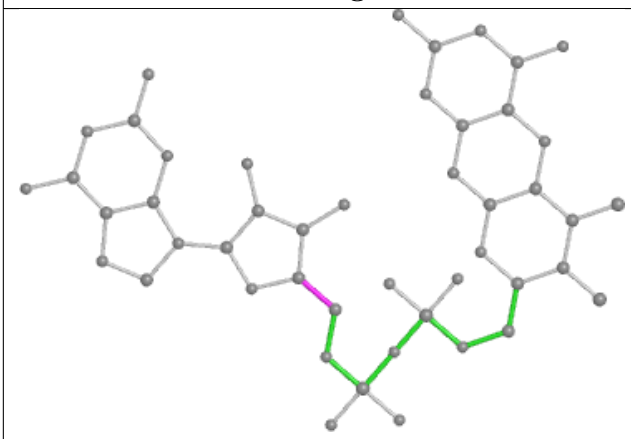
Ligand MGD C 903



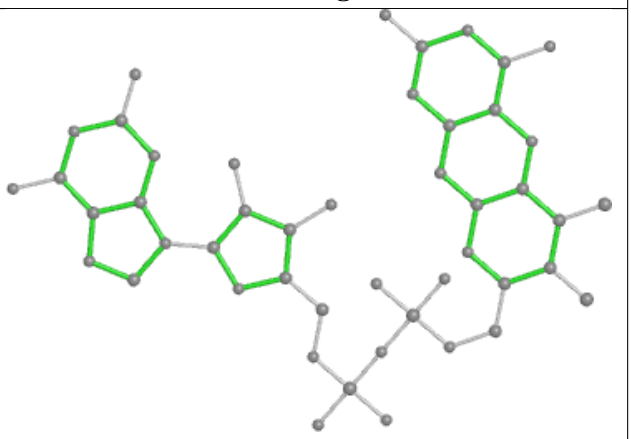
Bond lengths



Bond angles

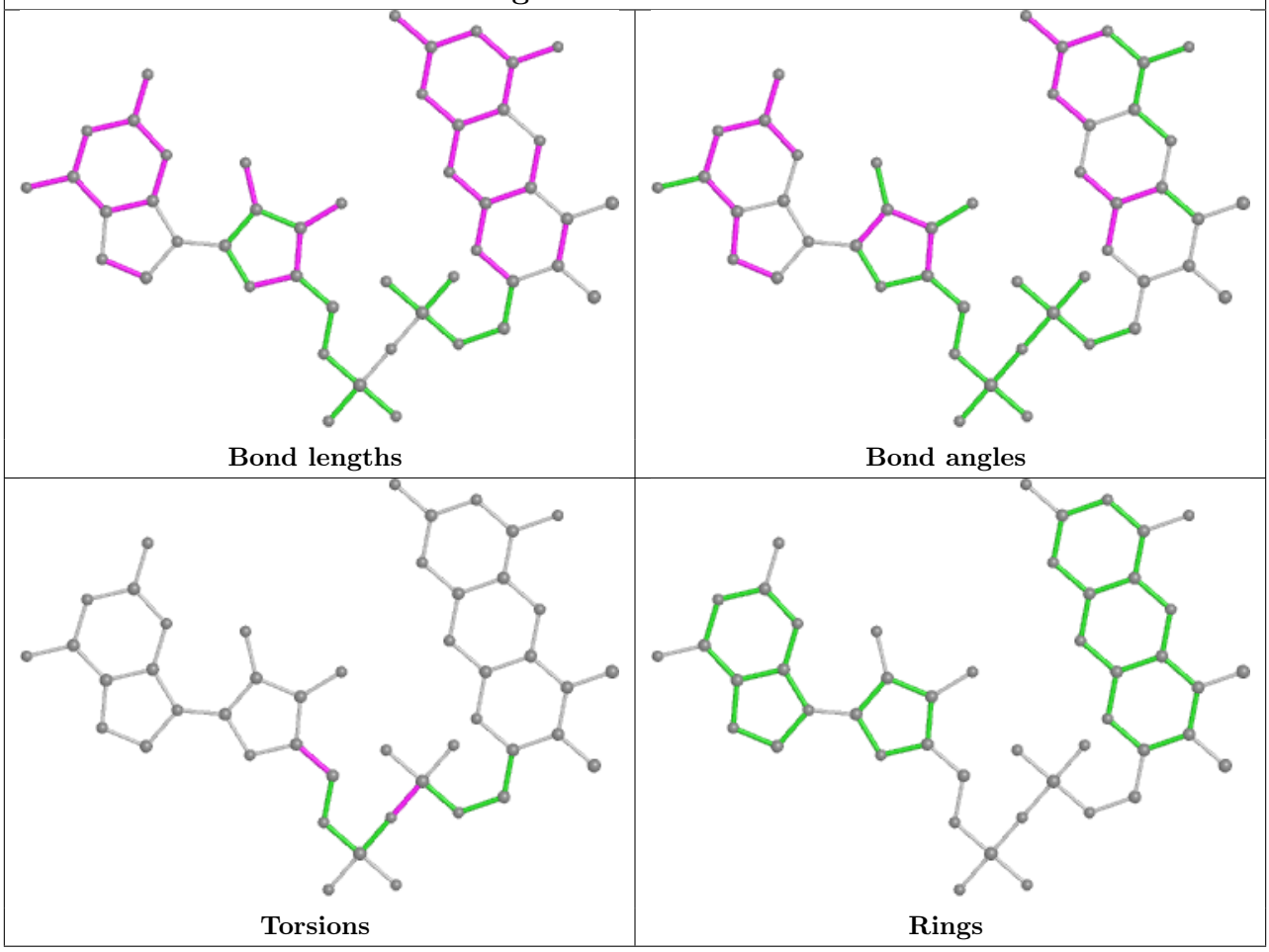


Torsions



Rings

Ligand MGD C 902



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, 95^{th} 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%)	0.00	23 (2%) 53 51	18, 32, 59, 98	0
1	C	807/814 (99%)	-0.25	17 (2%) 63 63	16, 24, 41, 75	0
2	B	234/234 (100%)	-0.30	0 100 100	20, 27, 49, 70	0
2	D	234/234 (100%)	-0.22	4 (1%) 70 70	20, 26, 45, 73	0
All	All	2089/2096 (99%)	-0.16	44 (2%) 63 63	16, 27, 50, 98	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	5.1
1	A	301	PHE	5.1
1	A	302	ILE	4.5
1	A	304	GLY	3.8
1	C	64	CYS	3.6
1	A	314	VAL	3.5
1	A	481	PHE	3.4
1	C	63	GLY	3.2
2	D	204	ILE	3.1
1	C	48	LEU	3.1
1	C	235	VAL	3.0
1	C	96	CYS	3.0
2	D	193	LEU	2.8
1	C	854	VAL	2.7
1	C	67	TRP	2.7
1	C	481	PHE	2.7
1	A	714	SER	2.6
1	C	766	PHE	2.5
1	C	65	THR	2.5
1	A	101	LEU	2.5
1	A	61	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	727	LEU	2.5
1	C	101	LEU	2.4
1	C	733	THR	2.4
1	C	767	GLY	2.4
1	A	64	CYS	2.3
1	A	319	PHE	2.3
1	C	231	SER	2.3
1	C	230	ALA	2.3
1	C	61	CYS	2.3
1	A	590	VAL	2.2
1	A	193	CYS	2.2
1	A	733	THR	2.2
1	A	63	GLY	2.2
1	A	766	PHE	2.2
1	A	681	VAL	2.1
1	A	166	TYR	2.1
1	A	65	THR	2.1
1	A	727	LEU	2.1
2	D	15	CYS	2.1
2	D	196	PRO	2.1
1	A	712	ASP	2.1
1	A	189	HIS	2.0
1	A	738	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

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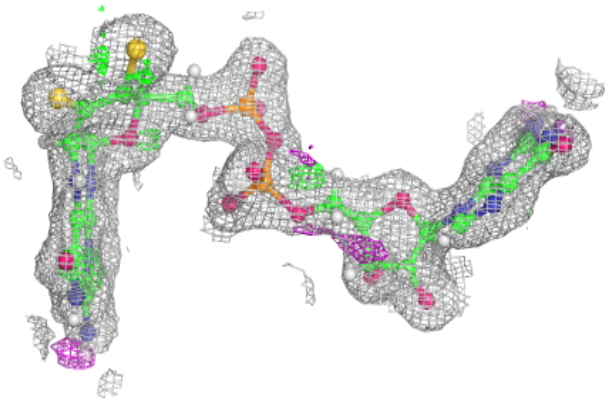
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

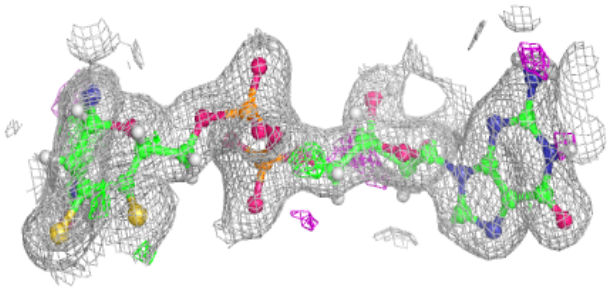
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PG5	C	911	12/12	0.71	0.17	58,81,108,128	0
9	PG5	A	911	12/12	0.75	0.26	53,76,93,93	0
8	FMT	A	910	3/3	0.83	0.19	35,45,66,80	0
7	O	A	912[A]	1/1	0.86	0.63	30,30,30,30	1
8	FMT	C	910	3/3	0.94	0.19	33,35,38,39	0
8	FMT	A	909	3/3	0.95	0.11	39,39,41,50	0
4	MGD	A	902	47/47	0.96	0.15	20,25,33,33	0
8	FMT	D	305	3/3	0.97	0.07	22,23,26,32	0
7	O	C	912[A]	1/1	0.97	0.14	36,36,36,36	1
4	MGD	C	902	47/47	0.97	0.16	16,20,25,28	0
8	FMT	C	909	3/3	0.97	0.11	29,30,35,36	0
4	MGD	A	903	47/47	0.97	0.16	22,25,31,33	0
5	ART	C	904[B]	5/5	0.98	0.13	24,28,42,82	5
4	MGD	C	903	47/47	0.98	0.16	17,19,23,27	0
3	SF4	B	304	8/8	0.98	0.05	29,30,31,32	0
3	SF4	B	301	8/8	0.98	0.05	24,24,25,26	0
5	ART	C	904[A]	5/5	0.98	0.13	14,18,21,24	5
3	SF4	D	303	8/8	0.99	0.04	22,23,23,23	0
7	O	A	906[B]	1/1	0.99	0.18	32,32,32,32	1
7	O	A	907[B]	1/1	0.99	0.15	28,28,28,28	1
3	SF4	D	304	8/8	0.99	0.05	22,22,23,23	0
8	FMT	C	908	3/3	0.99	0.18	18,20,21,21	0
3	SF4	D	301	8/8	0.99	0.07	21,21,23,23	0
3	SF4	B	302	8/8	0.99	0.06	19,20,20,20	0
3	SF4	B	303	8/8	0.99	0.04	22,23,24,24	0
8	FMT	A	908	3/3	0.99	0.19	20,21,24,24	0
3	SF4	D	302	8/8	0.99	0.06	19,20,20,21	0
5	ART	A	904[A]	5/5	0.99	0.18	23,26,29,33	5
5	ART	A	904[B]	5/5	0.99	0.18	29,31,56,84	5
7	O	C	906[B]	1/1	0.99	0.18	33,33,33,33	1
3	SF4	C	901	8/8	1.00	0.11	17,17,17,17	0
7	O	C	907[B]	1/1	1.00	0.14	17,17,17,17	1
3	SF4	A	901	8/8	1.00	0.09	20,20,20,21	0
6	MO	C	905	1/1	1.00	0.10	21,21,21,21	0
6	MO	A	905	1/1	1.00	0.08	26,26,26,26	0

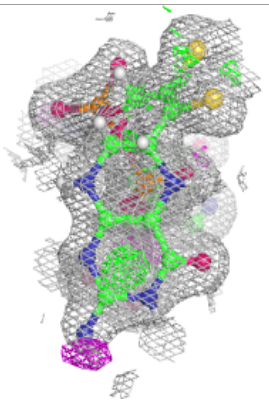
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

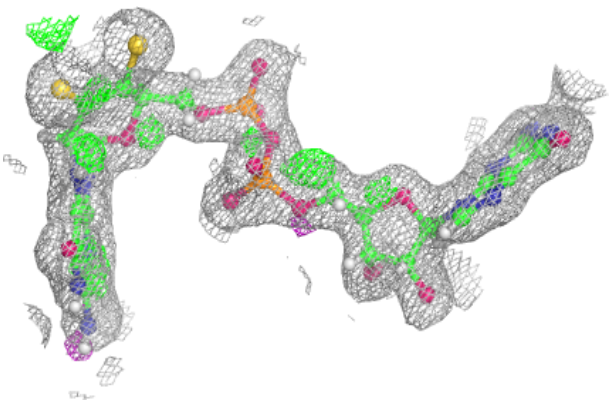


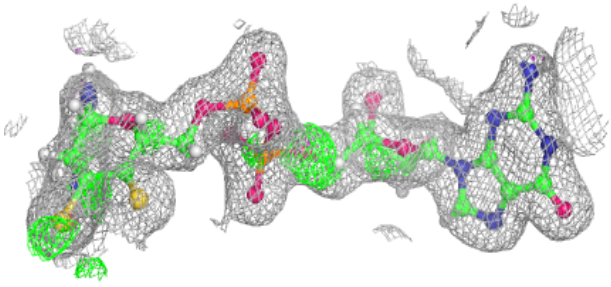


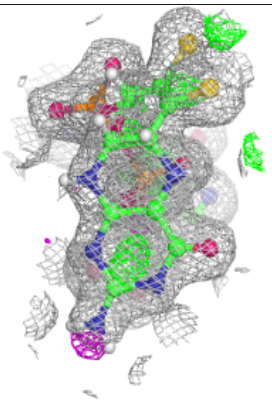


Electron density around MGD C 902:

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

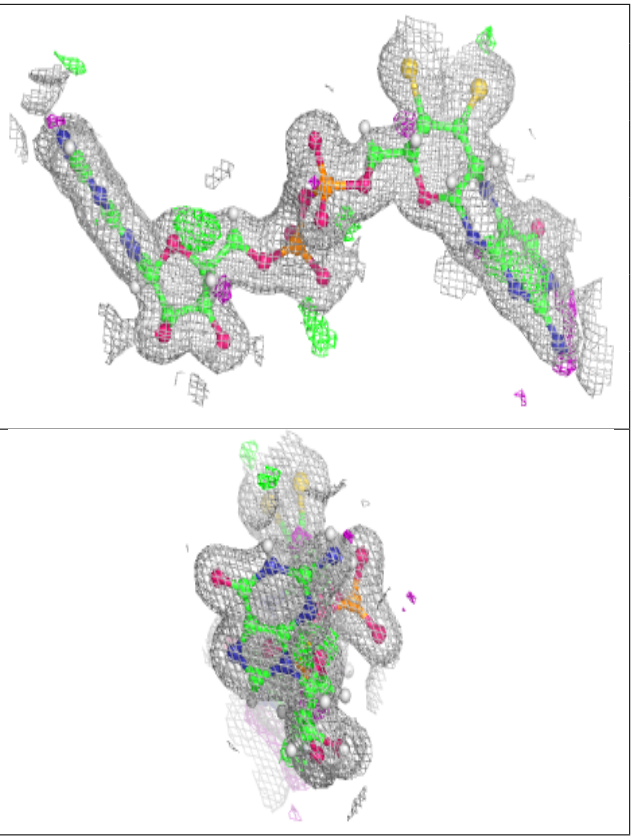


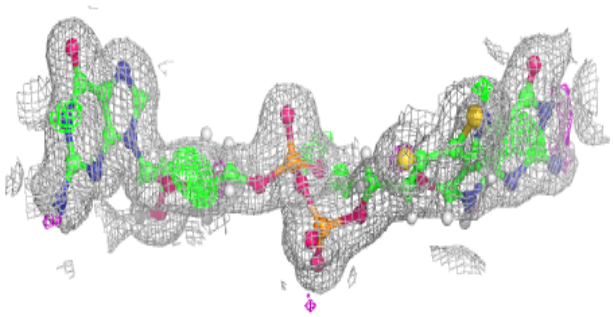




Electron density around MGD A 903:

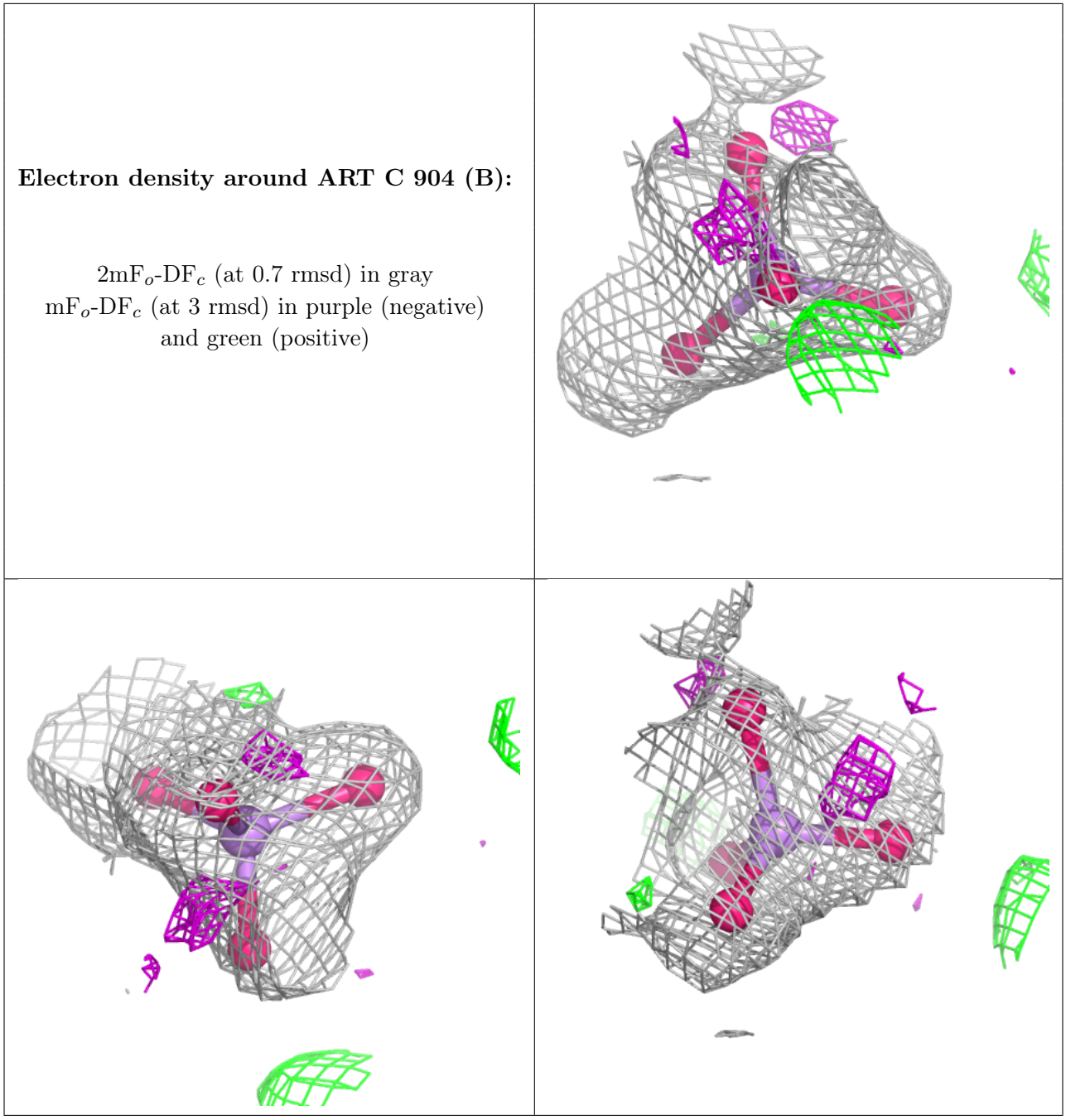
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





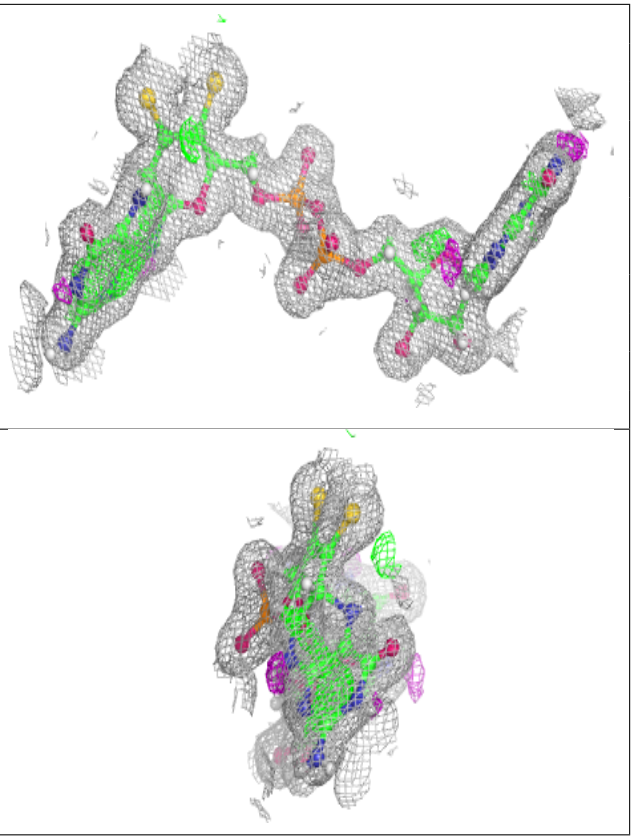
Electron density around ART C 904 (B):

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



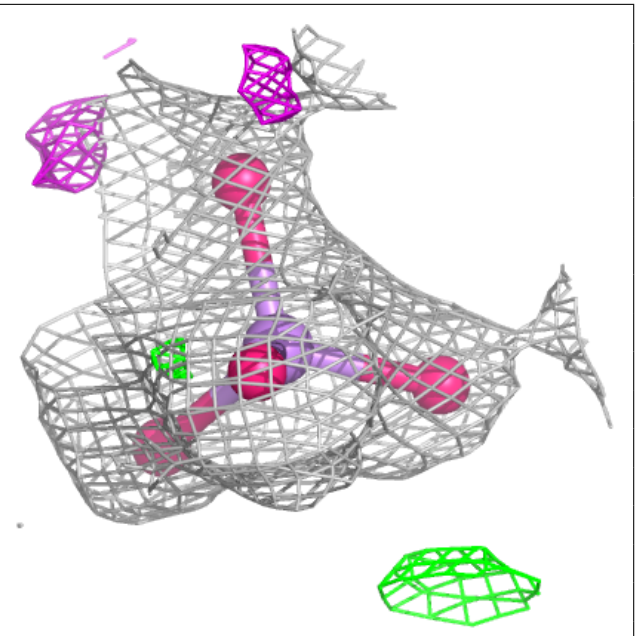
Electron density around MGD C 903:

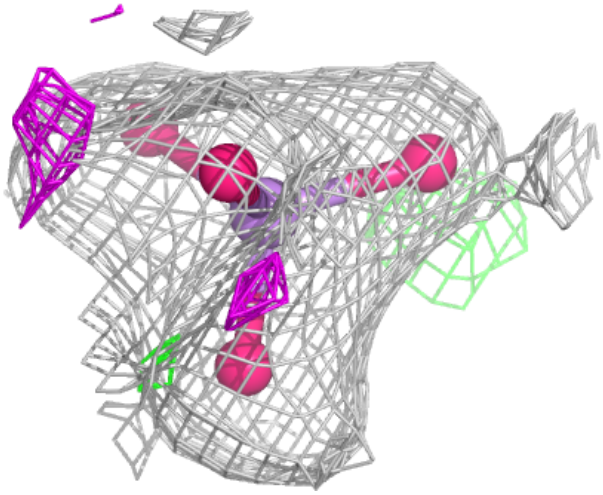
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

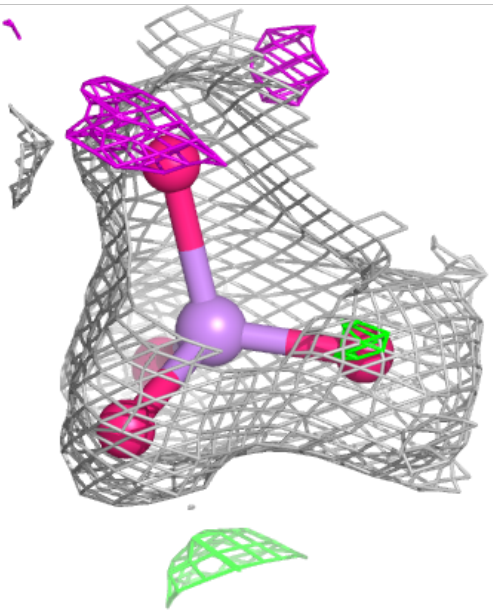


Electron density around ART C 904 (A):

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

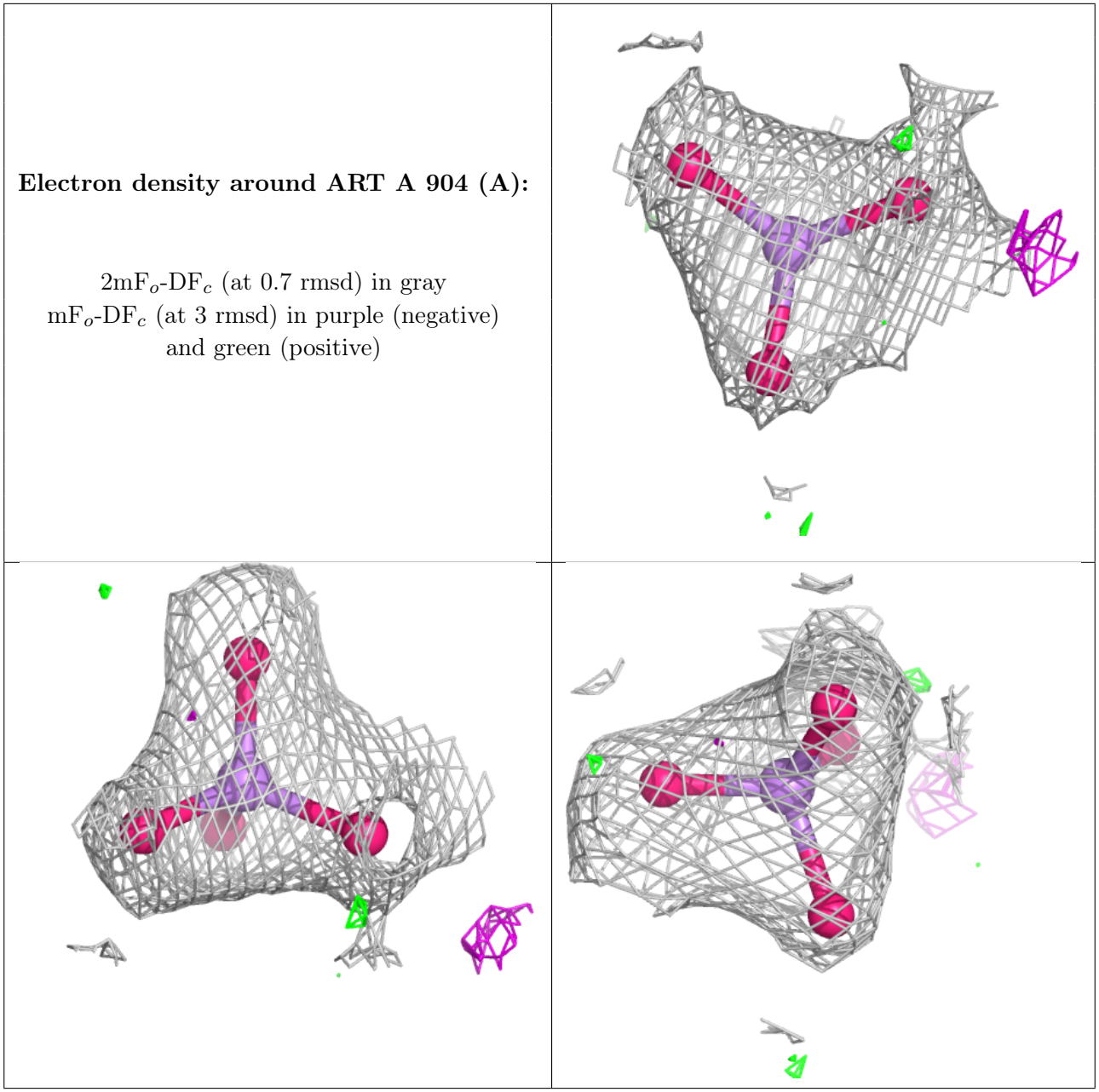






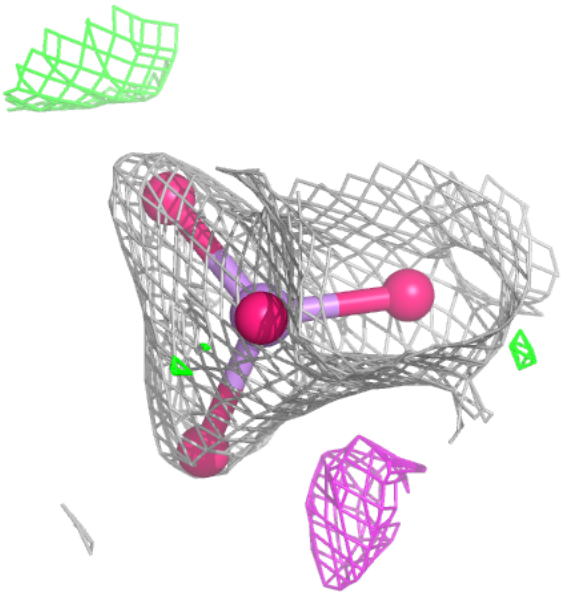
Electron density around ART A 904 (A):

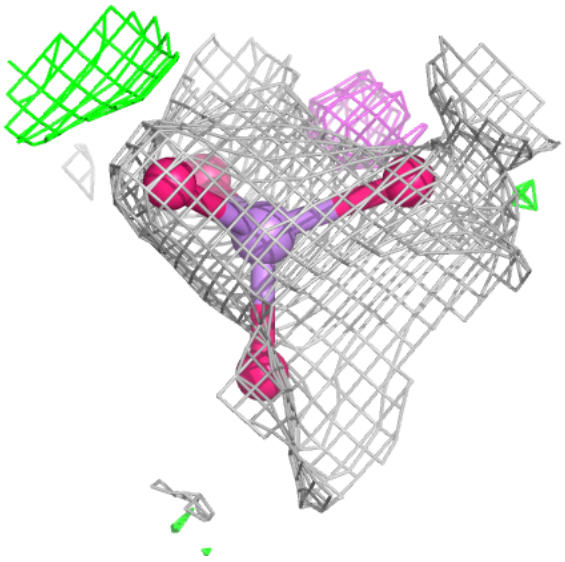
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

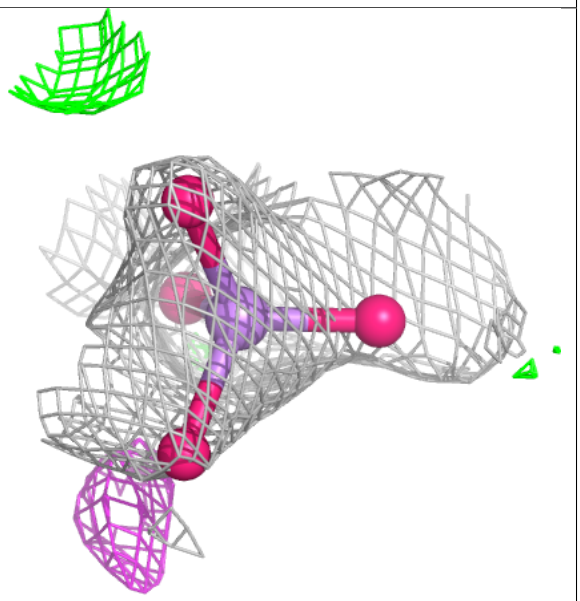


Electron density around ART A 904 (B):

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

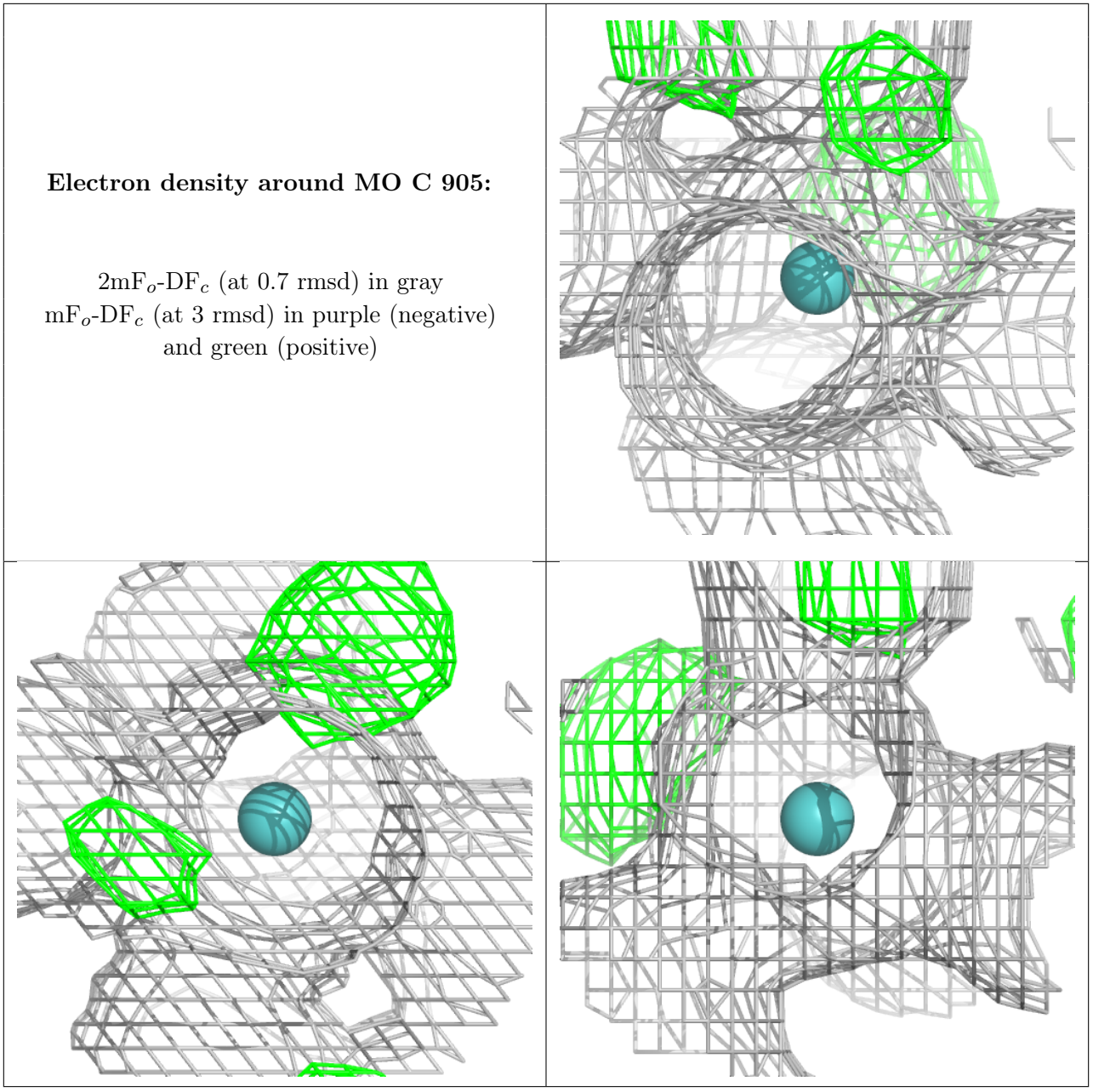






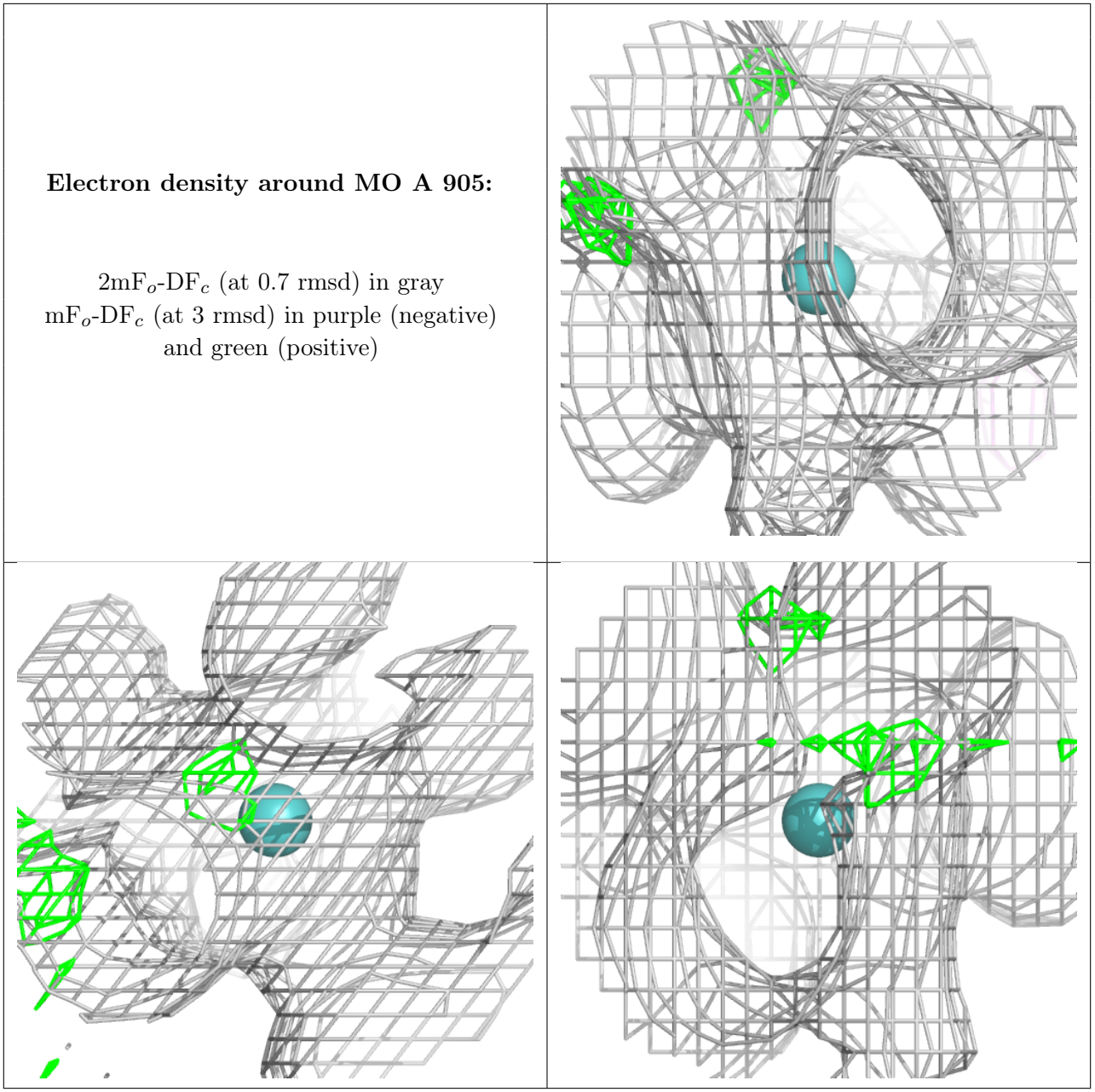
Electron density around MO C 905:

$2mF_o$-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 (i)

There are no such residues in this entry.