wwPDB X-ray Structure Validation Summary Report (i)

Jan 26, 2023 – 04:18 am GMT

PDB ID	:	7QWI
Title	:	Vanadate complex of the vanadium-dependent bromoperoxidase from Corallina pilulifera
Authors	:	Isupov, M.N.; Mitchell, D.; Littelchild, J.A.; Garcia-Rodriguez, E.
Deposited on	:	2022-01-25
Resolution	:	2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

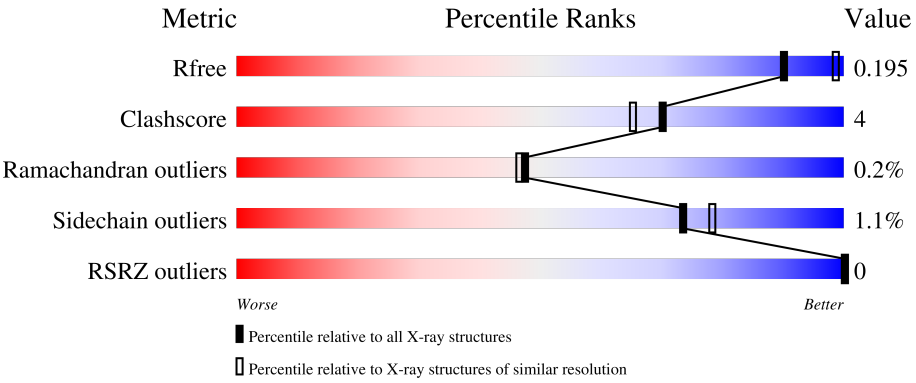
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	AAA	598	93% 6% •
1	BBB	598	93% 6% •
1	CCC	598	93% 7% •
1	DDD	598	93% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PEG	AAA	622	-	-	X	-
8	EDO	CCC	615	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 22153 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

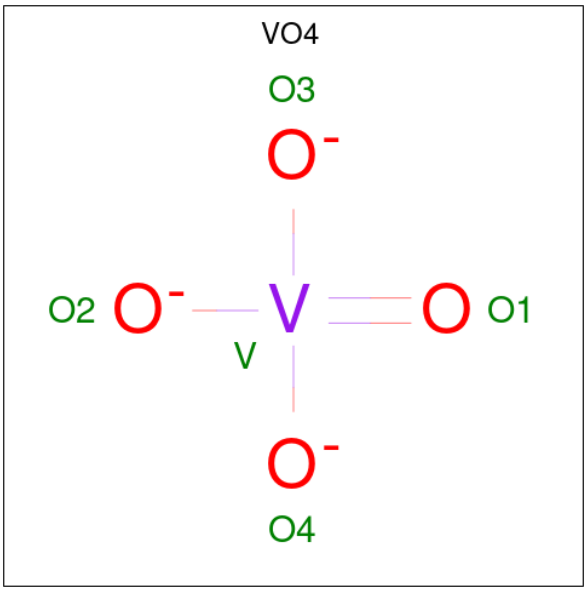
- Molecule 1 is a protein called Vanadium-dependent bromoperoxidase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	AAA	597	Total	Br	C	N	O	S	V	0	20	0
			4724	2	3009	777	928	7	1			
1	BBB	597	Total	Br	C	N	O	S	V	0	14	0
			4693	2	2984	775	924	7	1			
1	CCC	597	Total	Br	C	N	O	S	V	0	14	0
			4695	2	2996	774	915	7	1			
1	DDD	597	Total	Br	C	N	O	S	V	0	18	0
			4724	2	3014	780	920	7	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	423	ALA	PRO	engineered mutation	UNP O81959
BBB	423	ALA	PRO	engineered mutation	UNP O81959
CCC	423	ALA	PRO	engineered mutation	UNP O81959
DDD	423	ALA	PRO	engineered mutation	UNP O81959

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O V 5 4 1	0	0
2	BBB	1	Total O V 5 4 1	0	0
2	CCC	1	Total O V 5 4 1	0	0
2	DDD	1	Total O V 5 4 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0
3	BBB	1	Total Ca 1 1	0	0
3	CCC	1	Total Ca 1 1	0	0
3	DDD	1	Total Ca 1 1	0	0

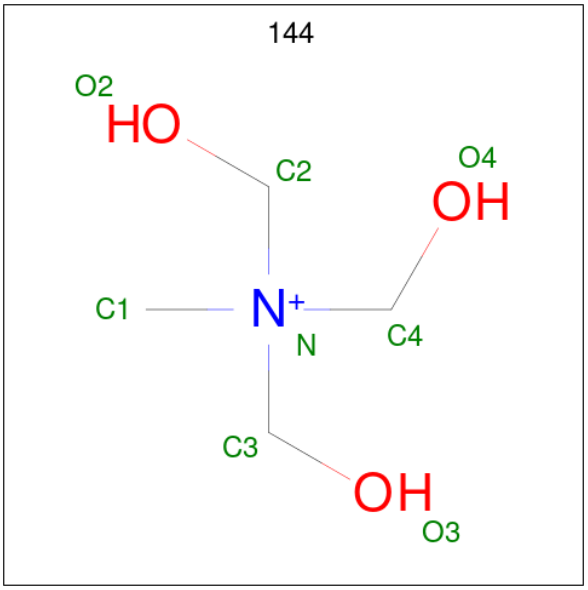
- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	3	Total Br 3 3	0	0
4	BBB	3	Total Br 3 3	0	0
4	CCC	3	Total Br 3 3	0	0
4	DDD	3	Total Br 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	4	Total Na 4 4	0	0
5	BBB	5	Total Na 5 5	0	0
5	CCC	4	Total Na 4 4	0	0
5	DDD	5	Total Na 5 5	0	0

- Molecule 6 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C N O 8 4 1 3	0	0

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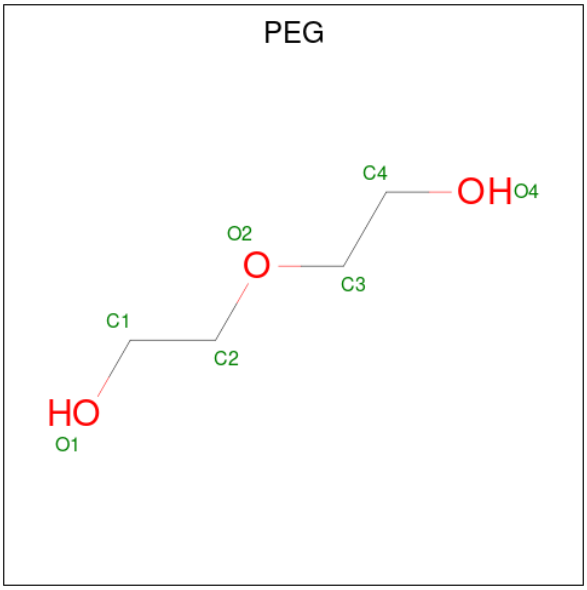
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C N O 8 4 1 3	0	0
6	BBB	1	Total C N O 8 4 1 3	0	0
6	BBB	1	Total C N O 8 4 1 3	0	0
6	BBB	1	Total C N O 8 4 1 3	0	0
6	BBB	1	Total C N O 8 4 1 3	0	0
6	CCC	1	Total C N O 8 4 1 3	0	0
6	CCC	1	Total C N O 8 4 1 3	0	0
6	DDD	1	Total C N O 8 4 1 3	0	0
6	DDD	1	Total C N O 8 4 1 3	0	0
6	DDD	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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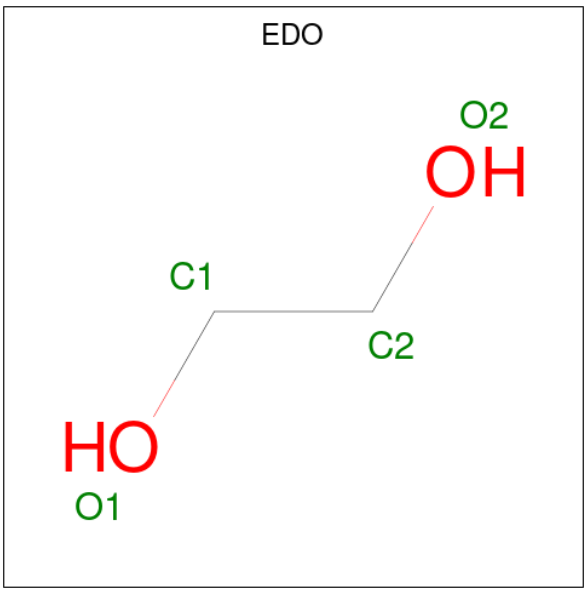
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			7	4	3		
7	AAA	1	Total	C	O	0	0
			7	4	3		
7	AAA	1	Total	C	O	0	0
			7	4	3		
7	AAA	1	Total	C	O	0	0
			7	4	3		
7	AAA	1	Total	C	O	0	0
			7	4	3		
7	BBB	1	Total	C	O	0	0
			7	4	3		
7	BBB	1	Total	C	O	0	0
			7	4	3		
7	BBB	1	Total	C	O	0	0
			7	4	3		
7	CCC	1	Total	C	O	0	0
			7	4	3		
7	CCC	1	Total	C	O	0	0
			7	4	3		
7	CCC	1	Total	C	O	0	0
			7	4	3		
7	DDD	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total C O 4 2 2	0	0
8	AAA	1	Total C O 4 2 2	0	0
8	AAA	1	Total C O 4 2 2	0	0
8	AAA	1	Total C O 4 2 2	0	0
8	AAA	1	Total C O 4 2 2	0	0
8	AAA	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	BBB	1	Total C O 4 2 2	0	0
8	CCC	1	Total C O 4 2 2	0	0
8	CCC	1	Total C O 4 2 2	0	0
8	CCC	1	Total C O 4 2 2	0	0
8	CCC	1	Total C O 4 2 2	0	0
8	CCC	1	Total C O 4 2 2	0	0
8	DDD	1	Total C O 4 2 2	0	0
8	DDD	1	Total C O 4 2 2	0	0
8	DDD	1	Total C O 4 2 2	0	0
8	DDD	1	Total C O 4 2 2	0	0
8	DDD	1	Total C O 4 2 2	0	0

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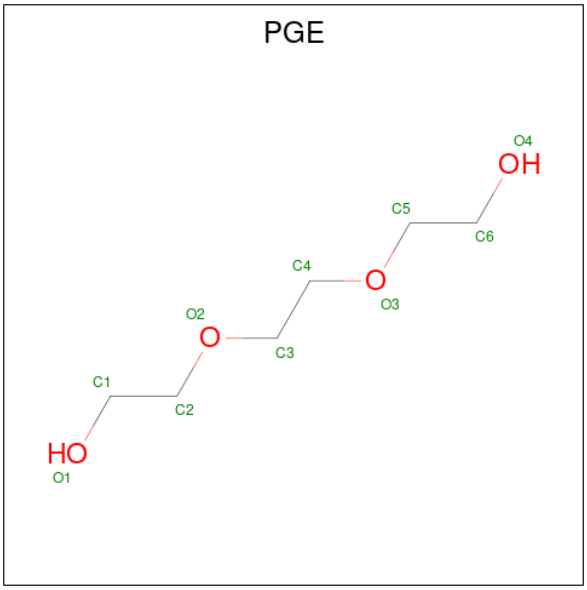
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	DDD	1	Total C O 4 2 2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	1	Total C O 10 6 4	0	0
9	BBB	1	Total C O 10 6 4	0	0
9	CCC	1	Total C O 10 6 4	0	0
9	DDD	1	Total C O 10 6 4	0	0

- Molecule 10 is water.

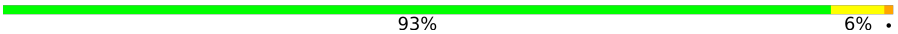
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	712	Total O 712 712	0	0
10	BBB	715	Total O 715 715	0	0
10	CCC	730	Total O 730 730	0	0
10	DDD	795	Total O 795 795	0	0

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.

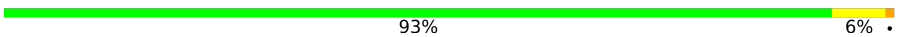
• Molecule 1: Vanadium-dependent bromoperoxidase

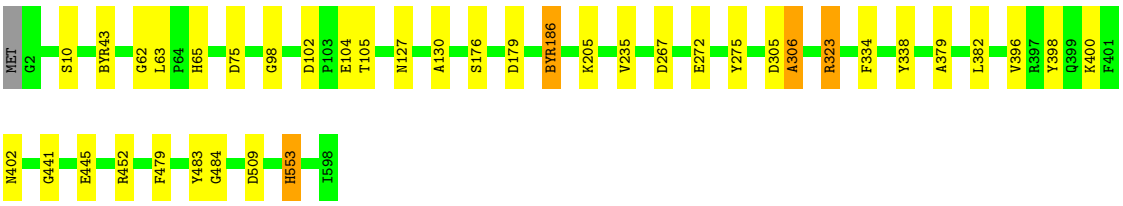
Chain AAA:



• Molecule 1: Vanadium-dependent bromoperoxidase

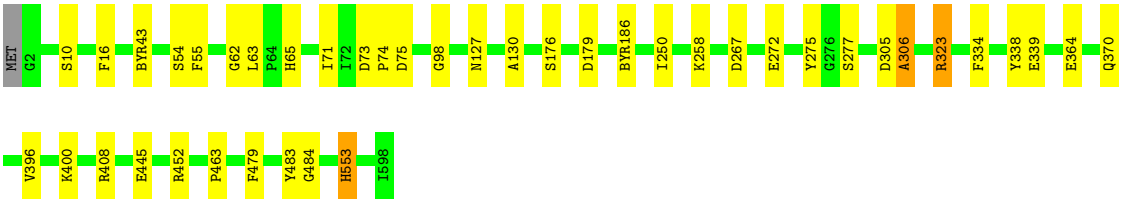
Chain BBB:





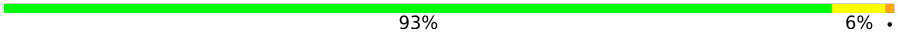
• Molecule 1: Vanadium-dependent bromoperoxidase

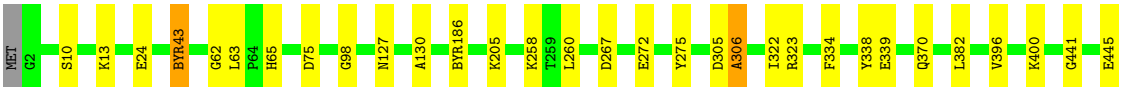
Chain CCC:

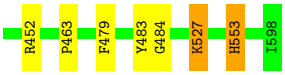


• Molecule 1: Vanadium-dependent bromoperoxidase

Chain DDD:






R452
P463
F479
Y483
G484
K527
H553
I598

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	199.60Å 199.60Å 199.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 2.15 14.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.9 (14.96-2.15) 99.2 (14.96-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.144 , 0.195 0.144 , 0.195	Depositor DCC
R_{free} test set	7104 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22153	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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: VO4, PEG, NA, I4O, PGE, BR, 144, CA, BYR, EDO

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	AAA	0.39	0/4824	0.60	0/6550
1	BBB	0.38	0/4775	0.60	0/6484
1	CCC	0.39	0/4780	0.61	0/6491
1	DDD	0.38	0/4821	0.62	0/6539
All	All	0.39	0/19200	0.61	0/26064

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

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	AAA	4724	0	4629	29	0
1	BBB	4693	0	4574	33	0
1	CCC	4695	0	4613	32	0
1	DDD	4724	0	4656	25	0
2	AAA	5	0	0	1	0
2	BBB	5	0	0	1	0
2	CCC	5	0	0	1	0
2	DDD	5	0	0	0	0
3	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	3	0	0	1	0
4	BBB	3	0	0	1	0
4	CCC	3	0	0	1	0
4	DDD	3	0	0	1	0
5	AAA	4	0	0	0	0
5	BBB	5	0	0	0	0
5	CCC	4	0	0	0	0
5	DDD	5	0	0	0	0
6	AAA	16	0	24	3	0
6	BBB	32	0	48	7	0
6	CCC	16	0	24	6	0
6	DDD	24	0	36	8	0
7	AAA	42	0	60	14	0
7	BBB	21	0	30	2	0
7	CCC	21	0	30	2	0
7	DDD	7	0	10	0	0
8	AAA	24	0	36	2	0
8	BBB	24	0	36	5	0
8	CCC	20	0	30	4	0
8	DDD	24	0	36	2	0
9	AAA	10	0	14	0	0
9	BBB	10	0	14	2	0
9	CCC	10	0	14	1	0
9	DDD	10	0	14	1	0
10	AAA	712	0	0	5	0
10	BBB	715	0	0	10	0
10	CCC	730	0	0	12	0
10	DDD	795	0	0	11	0
All	All	22153	0	18928	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:24[A]:GLU:OE1	10:DDD:701:HOH:O	1.52	1.27
1:AAA:553[A]:I4O:O1	2:AAA:601:VO4:O1	1.58	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:553[A]:I4O:O1	2:BBB:602:VO4:O3	1.58	1.19
1:CCC:553[A]:I4O:O1	2:CCC:601:VO4:O3	1.59	1.18
1:DDD:43:BYR:BR	10:DDD:1416:HOH:O	2.22	1.12

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	611/598 (102%)	604 (99%)	6 (1%)	1 (0%)	47	46
1	BBB	605/598 (101%)	598 (99%)	6 (1%)	1 (0%)	47	46
1	CCC	606/598 (101%)	598 (99%)	7 (1%)	1 (0%)	47	46
1	DDD	610/598 (102%)	601 (98%)	8 (1%)	1 (0%)	47	46
All	All	2432/2392 (102%)	2401 (99%)	27 (1%)	4 (0%)	47	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	306	ALA
1	DDD	306	ALA
1	AAA	306	ALA
1	CCC	306	ALA

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	AAA	506/488 (104%)	501 (99%)	5 (1%)	76	81
1	BBB	500/488 (102%)	493 (99%)	7 (1%)	67	72
1	CCC	501/488 (103%)	496 (99%)	5 (1%)	76	81
1	DDD	505/488 (104%)	497 (98%)	8 (2%)	62	67
All	All	2012/1952 (103%)	1987 (99%)	25 (1%)	73	76

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	370	GLN
1	DDD	323	ARG
1	DDD	527[C]	LYS
1	CCC	479	PHE
1	DDD	338	TYR

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)

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	BYR	AAA	186	1	12,13,14	0.61	0	14,17,19	1.75	1 (7%)
1	BYR	DDD	43	1	12,13,14	0.92	0	14,17,19	0.90	1 (7%)
1	BYR	CCC	43	1	12,13,14	0.81	0	14,17,19	0.93	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	BYR	AAA	43	1	12,13,14	0.89	0	14,17,19	0.92	1 (7%)
1	BYR	DDD	186	1	12,13,14	0.64	0	14,17,19	1.97	3 (21%)
1	I4O	BBB	553[A]	1,2	8,15,16	8.61	3 (37%)	3,24,26	3.73	1 (33%)
1	I4O	CCC	553[A]	1,2	8,15,16	8.71	3 (37%)	3,24,26	3.65	1 (33%)
1	I4O	BBB	553[B]	1	5,10,16	0.59	0	3,12,26	4.16	2 (66%)
1	BYR	CCC	186	1	12,13,14	0.53	0	14,17,19	1.90	2 (14%)
1	I4O	CCC	553[B]	1	5,10,16	0.62	0	3,12,26	4.02	2 (66%)
1	I4O	AAA	553[A]	1,2	8,15,16	8.52	3 (37%)	3,24,26	3.64	1 (33%)
1	I4O	DDD	553[A]	1,2	8,15,16	8.49	3 (37%)	3,24,26	3.81	1 (33%)
1	BYR	BBB	43	1	12,13,14	0.89	0	14,17,19	0.89	0
1	BYR	BBB	186	1	12,13,14	0.61	0	14,17,19	1.91	1 (7%)
1	I4O	AAA	553[B]	1	5,10,16	0.67	0	3,12,26	4.18	2 (66%)
1	I4O	DDD	553[B]	1	5,10,16	0.66	0	3,12,26	4.34	3 (100%)

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
1	BYR	AAA	186	1	-	0/5/6/8	0/1/1/1
1	BYR	DDD	43	1	-	0/5/6/8	0/1/1/1
1	BYR	CCC	43	1	-	0/5/6/8	0/1/1/1
1	BYR	AAA	43	1	-	0/5/6/8	0/1/1/1
1	BYR	DDD	186	1	-	0/5/6/8	0/1/1/1
1	I4O	BBB	553[A]	1,2	-	1/5/14/16	0/1/1/1
1	I4O	CCC	553[A]	1,2	-	1/5/14/16	0/1/1/1
1	I4O	BBB	553[B]	1	-	1/5/6/16	0/1/1/1
1	BYR	CCC	186	1	-	0/5/6/8	0/1/1/1
1	I4O	CCC	553[B]	1	-	2/5/6/16	0/1/1/1
1	I4O	AAA	553[A]	1,2	-	1/5/14/16	0/1/1/1
1	I4O	DDD	553[A]	1,2	-	1/5/14/16	0/1/1/1
1	BYR	BBB	43	1	-	0/5/6/8	0/1/1/1
1	BYR	BBB	186	1	-	0/5/6/8	0/1/1/1
1	I4O	AAA	553[B]	1	-	2/5/6/16	0/1/1/1
1	I4O	DDD	553[B]	1	-	2/5/6/16	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	553[A]	I4O	O5-V9	22.99	1.90	1.58
1	BBB	553[A]	I4O	O5-V9	22.81	1.90	1.58
1	AAA	553[A]	I4O	O5-V9	22.54	1.90	1.58
1	DDD	553[A]	I4O	O5-V9	22.43	1.90	1.58
1	CCC	553[A]	I4O	CE1-ND1	7.50	1.47	1.35

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	553[B]	I4O	CD2-NE2-CE1	6.74	116.29	105.78
1	DDD	553[B]	I4O	CD2-NE2-CE1	6.69	116.21	105.78
1	BBB	553[B]	I4O	CD2-NE2-CE1	6.65	116.15	105.78
1	CCC	553[B]	I4O	CD2-NE2-CE1	6.57	116.03	105.78
1	DDD	553[A]	I4O	CE1-NE2-CD2	6.43	116.77	105.31

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	553[B]	I4O	N-CA-CB-CG
1	AAA	553[A]	I4O	C-CA-CB-CG
1	AAA	553[B]	I4O	C-CA-CB-CG
1	BBB	553[A]	I4O	C-CA-CB-CG
1	BBB	553[B]	I4O	C-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	DDD	43	BYR	1	0
1	BBB	553[A]	I4O	2	0
1	CCC	553[A]	I4O	3	0
1	AAA	553[A]	I4O	3	0
1	DDD	553[A]	I4O	1	0
1	BBB	43	BYR	1	0
1	BBB	186	BYR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 34 are monoatomic - leaving 55 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	$\#\|Z\| > 2$
6	144	AAA	611	-	1,7,7	0.21	0	3,9,9	0.22	0
7	PEG	CCC	609	-	6,6,6	0.18	0	5,5,5	0.10	0
6	144	DDD	609	-	1,7,7	0.10	0	3,9,9	0.33	0
7	PEG	CCC	617	-	6,6,6	0.12	0	5,5,5	0.11	0
6	144	BBB	623	-	1,7,7	0.28	0	3,9,9	0.22	0
6	144	CCC	606	-	1,7,7	0.44	0	3,9,9	0.70	0
7	PEG	AAA	622	-	6,6,6	0.38	0	5,5,5	0.40	0
8	EDO	BBB	620	-	3,3,3	0.07	0	2,2,2	0.14	0
8	EDO	BBB	619	-	3,3,3	0.33	0	2,2,2	0.23	0
8	EDO	CCC	615	-	3,3,3	0.27	0	2,2,2	0.11	0
7	PEG	AAA	621	-	6,6,6	0.13	0	5,5,5	0.08	0
8	EDO	DDD	618	-	3,3,3	0.07	0	2,2,2	0.21	0
7	PEG	AAA	623	-	6,6,6	0.23	0	5,5,5	0.17	0
8	EDO	AAA	614	-	3,3,3	0.17	0	2,2,2	0.39	0
8	EDO	CCC	614	-	3,3,3	0.42	0	2,2,2	0.51	0
8	EDO	BBB	617	-	3,3,3	0.08	0	2,2,2	0.35	0
7	PEG	AAA	612	-	6,6,6	0.16	0	5,5,5	0.07	0
8	EDO	CCC	613	-	3,3,3	0.33	0	2,2,2	1.00	0
8	EDO	AAA	620	-	3,3,3	0.13	0	2,2,2	0.41	0
9	PGE	CCC	618	-	9,9,9	0.29	0	8,8,8	0.36	0
8	EDO	DDD	616	-	3,3,3	0.13	0	2,2,2	0.56	0
8	EDO	BBB	615	-	3,3,3	0.08	0	2,2,2	0.10	0
8	EDO	CCC	616	-	3,3,3	0.08	0	2,2,2	0.06	0
2	VO4	AAA	601	1	1,4,4	4.78	1 (100%)	-		
7	PEG	BBB	612	-	6,6,6	0.10	0	5,5,5	0.15	0
6	144	BBB	601	-	1,7,7	0.30	0	3,9,9	0.22	0
8	EDO	DDD	619	-	3,3,3	0.10	0	2,2,2	0.39	0
7	PEG	BBB	622	-	6,6,6	0.38	0	5,5,5	0.35	0
6	144	BBB	607	-	1,7,7	0.57	0	3,9,9	0.60	0
6	144	DDD	602	-	1,7,7	0.38	0	3,9,9	0.49	0
6	144	DDD	610	-	1,7,7	0.31	0	3,9,9	0.10	0
9	PGE	AAA	617	-	9,9,9	0.20	0	8,8,8	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PEG	AAA	609	-	6,6,6	0.20	0	5,5,5	0.07	0
8	EDO	BBB	616	-	3,3,3	0.23	0	2,2,2	0.53	0
8	EDO	DDD	620	-	3,3,3	0.15	0	2,2,2	0.19	0
6	144	CCC	619	-	1,7,7	0.34	0	3,9,9	0.03	0
8	EDO	AAA	618	-	3,3,3	0.06	0	2,2,2	0.18	0
8	EDO	AAA	619	-	3,3,3	0.09	0	2,2,2	0.21	0
2	VO4	BBB	602	1	1,4,4	4.46	1 (100%)	-		
2	VO4	CCC	601	1	1,4,4	4.19	1 (100%)	-		
7	PEG	AAA	607	-	6,6,6	0.16	0	5,5,5	0.07	0
7	PEG	CCC	607	-	6,6,6	0.19	0	5,5,5	0.16	0
2	VO4	DDD	604	1	1,4,4	4.52	1 (100%)	-		
6	144	AAA	606	-	1,7,7	0.34	0	3,9,9	0.45	0
9	PGE	DDD	611	-	9,9,9	0.24	0	8,8,8	0.19	0
6	144	BBB	608	-	1,7,7	0.07	0	3,9,9	0.43	0
8	EDO	DDD	603	-	3,3,3	0.09	0	2,2,2	0.26	0
8	EDO	BBB	618	-	3,3,3	0.04	0	2,2,2	0.20	0
8	EDO	DDD	617	-	3,3,3	0.32	0	2,2,2	0.39	0
8	EDO	CCC	612	-	3,3,3	0.11	0	2,2,2	0.17	0
9	PGE	BBB	621	-	9,9,9	0.19	0	8,8,8	0.29	0
7	PEG	BBB	609	-	6,6,6	0.13	0	5,5,5	0.09	0
7	PEG	DDD	612	-	6,6,6	0.28	0	5,5,5	0.16	0
8	EDO	AAA	616	-	3,3,3	0.13	0	2,2,2	0.27	0
8	EDO	AAA	615	-	3,3,3	0.11	0	2,2,2	0.61	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
6	144	AAA	611	-	-	0/0/9/9	-
7	PEG	CCC	609	-	-	1/4/4/4	-
6	144	DDD	609	-	-	0/0/9/9	-
7	PEG	CCC	617	-	-	3/4/4/4	-
6	144	BBB	623	-	-	0/0/9/9	-
7	PEG	AAA	622	-	-	3/4/4/4	-
6	144	CCC	606	-	-	0/0/9/9	-
8	EDO	BBB	620	-	-	0/1/1/1	-
8	EDO	BBB	619	-	-	1/1/1/1	-
8	EDO	CCC	615	-	-	1/1/1/1	-
7	PEG	AAA	621	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	DDD	618	-	-	1/1/1/1	-
7	PEG	AAA	623	-	-	2/4/4/4	-
8	EDO	AAA	614	-	-	1/1/1/1	-
8	EDO	CCC	614	-	-	1/1/1/1	-
8	EDO	BBB	617	-	-	1/1/1/1	-
7	PEG	AAA	612	-	-	3/4/4/4	-
8	EDO	CCC	613	-	-	1/1/1/1	-
8	EDO	AAA	620	-	-	1/1/1/1	-
9	PGE	CCC	618	-	-	5/7/7/7	-
8	EDO	DDD	616	-	-	0/1/1/1	-
8	EDO	BBB	615	-	-	1/1/1/1	-
8	EDO	CCC	616	-	-	1/1/1/1	-
7	PEG	BBB	612	-	-	1/4/4/4	-
6	144	BBB	601	-	-	0/0/9/9	-
8	EDO	DDD	619	-	-	1/1/1/1	-
7	PEG	BBB	622	-	-	3/4/4/4	-
6	144	BBB	607	-	-	0/0/9/9	-
6	144	DDD	602	-	-	0/0/9/9	-
6	144	DDD	610	-	-	0/0/9/9	-
9	PGE	AAA	617	-	-	2/7/7/7	-
7	PEG	AAA	609	-	-	3/4/4/4	-
8	EDO	BBB	616	-	-	1/1/1/1	-
8	EDO	DDD	620	-	-	1/1/1/1	-
6	144	CCC	619	-	-	0/0/9/9	-
8	EDO	AAA	618	-	-	1/1/1/1	-
8	EDO	AAA	619	-	-	1/1/1/1	-
7	PEG	AAA	607	-	-	3/4/4/4	-
7	PEG	CCC	607	-	-	2/4/4/4	-
6	144	AAA	606	-	-	0/0/9/9	-
9	PGE	DDD	611	-	-	4/7/7/7	-
6	144	BBB	608	-	-	0/0/9/9	-
8	EDO	DDD	603	-	-	0/1/1/1	-
8	EDO	BBB	618	-	-	0/1/1/1	-
8	EDO	DDD	617	-	-	0/1/1/1	-
8	EDO	CCC	612	-	-	1/1/1/1	-
9	PGE	BBB	621	-	-	4/7/7/7	-
7	PEG	BBB	609	-	-	3/4/4/4	-
7	PEG	DDD	612	-	-	3/4/4/4	-
8	EDO	AAA	616	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	AAA	615	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	601	VO4	O1-V	4.78	1.91	1.63
2	DDD	604	VO4	O1-V	4.52	1.89	1.63
2	BBB	602	VO4	O1-V	4.46	1.89	1.63
2	CCC	601	VO4	O1-V	4.19	1.87	1.63

There are no bond angle outliers.

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	BBB	621	PGE	C1-C2-O2-C3
7	AAA	622	PEG	C1-C2-O2-C3
9	DDD	611	PGE	O2-C3-C4-O3
9	CCC	618	PGE	O2-C3-C4-O3
7	AAA	609	PEG	C4-C3-O2-C2

There are no ring outliers.

31 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	611	144	1	0
6	DDD	609	144	2	0
7	CCC	617	PEG	1	0
6	BBB	623	144	2	0
6	CCC	606	144	2	0
7	AAA	622	PEG	13	0
8	BBB	619	EDO	3	0
8	CCC	615	EDO	4	0
7	AAA	612	PEG	1	0
8	AAA	620	EDO	1	0
9	CCC	618	PGE	1	0
8	BBB	615	EDO	1	0
2	AAA	601	VO4	1	0
6	BBB	601	144	1	0
8	DDD	619	EDO	1	0
7	BBB	622	PEG	1	0

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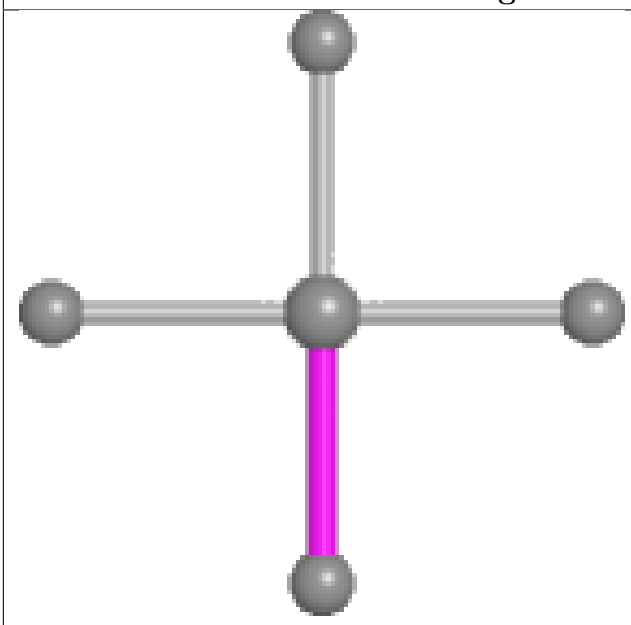
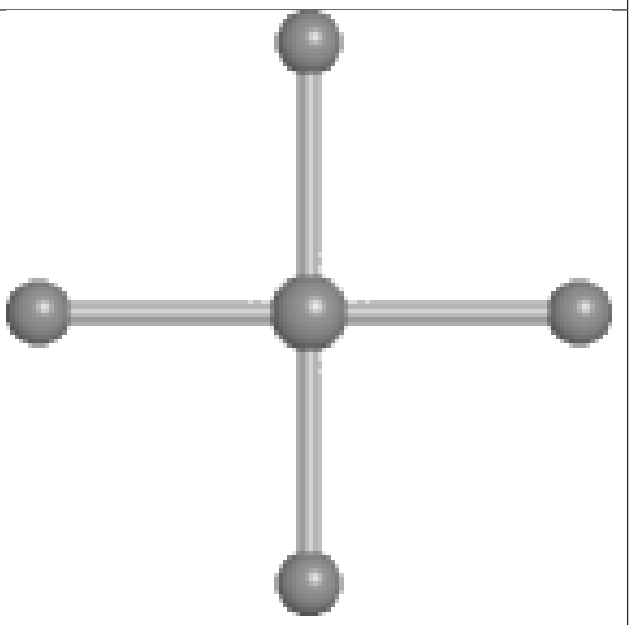
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	607	144	2	0
6	DDD	602	144	3	0
6	DDD	610	144	3	0
6	CCC	619	144	4	0
8	AAA	619	EDO	1	0
2	BBB	602	VO4	1	0
2	CCC	601	VO4	1	0
7	CCC	607	PEG	1	0
6	AAA	606	144	2	0
9	DDD	611	PGE	1	0
6	BBB	608	144	2	0
8	BBB	618	EDO	1	0
8	DDD	617	EDO	1	0
9	BBB	621	PGE	2	0
7	BBB	609	PEG	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.

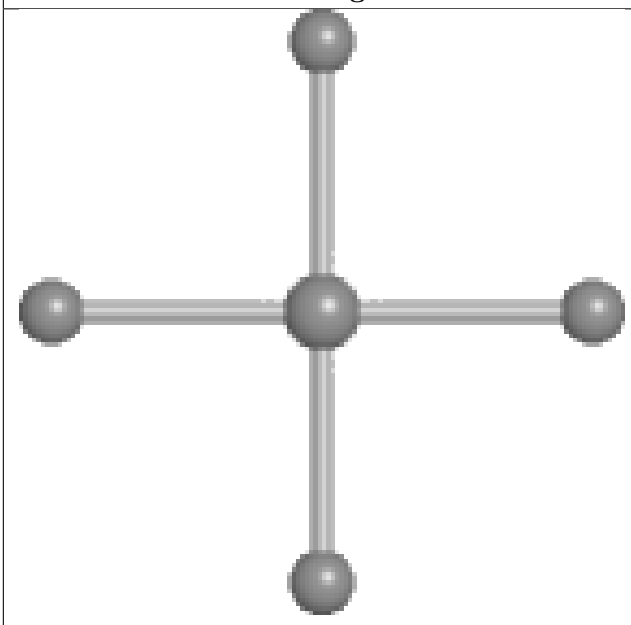
Ligand VO4 AAA 601



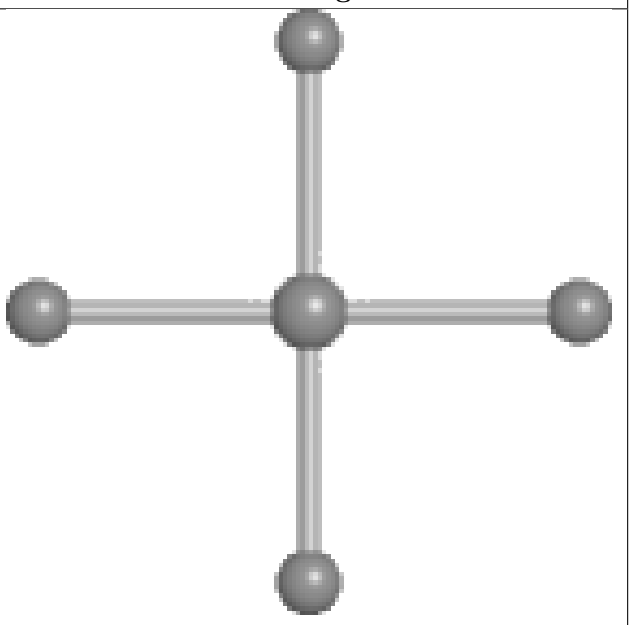
Bond lengths



Bond angles

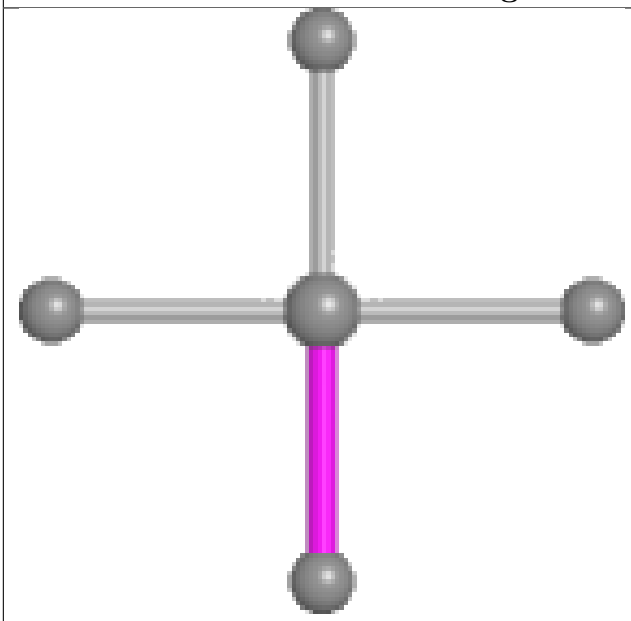


Torsions

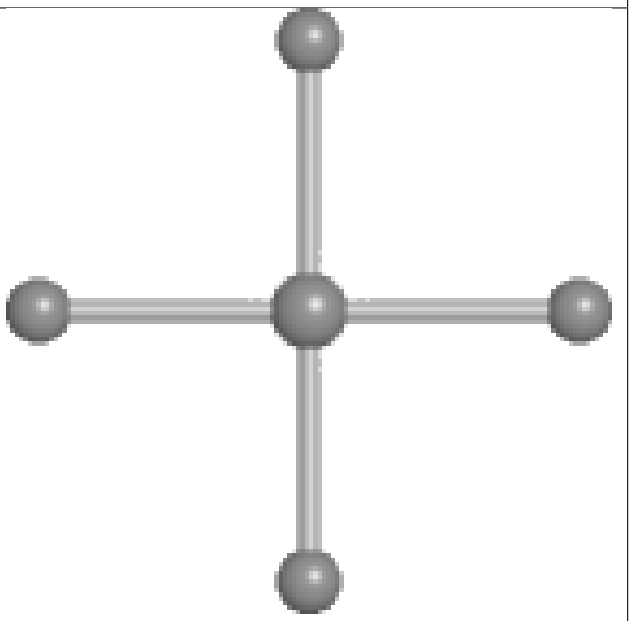


Rings

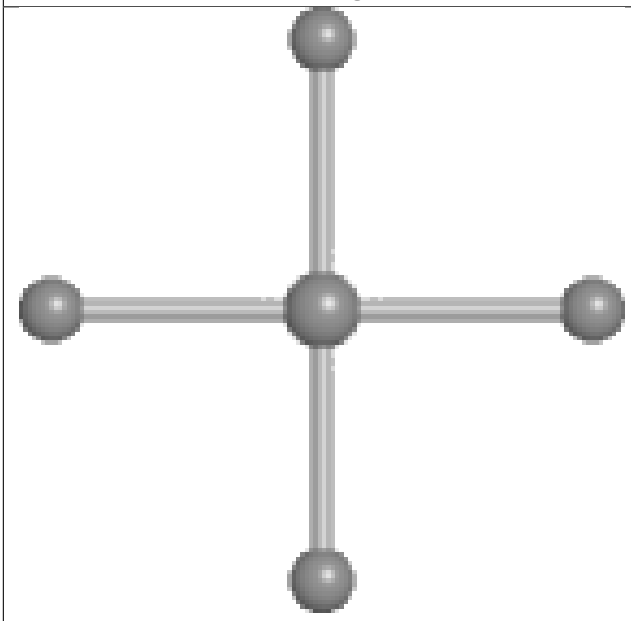
Ligand VO4 BBB 602



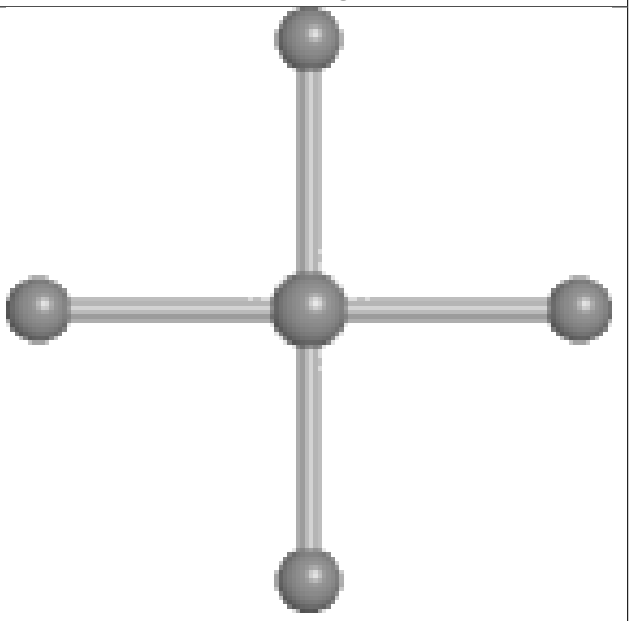
Bond lengths



Bond angles

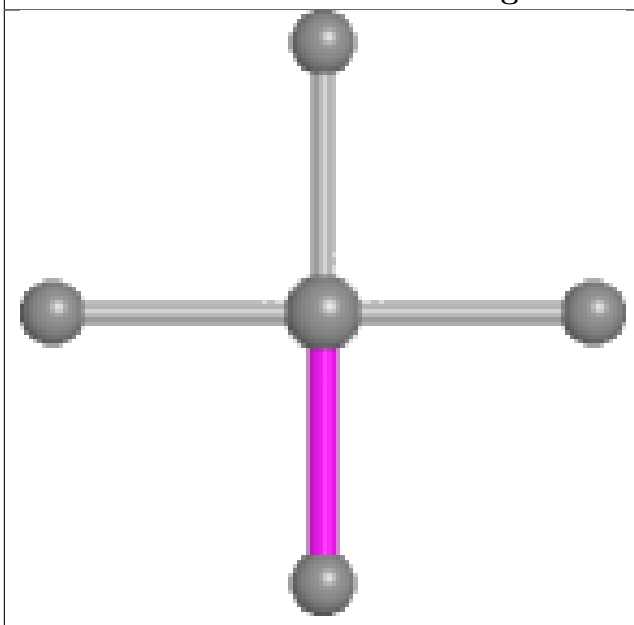


Torsions

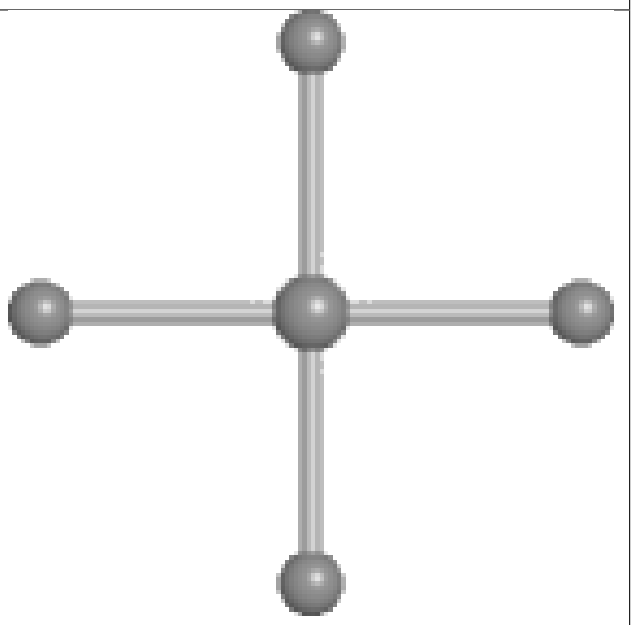


Rings

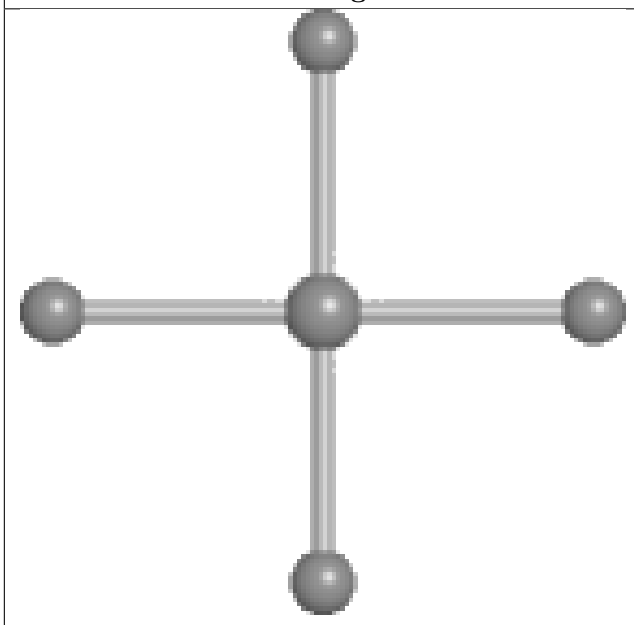
Ligand VO4 CCC 601



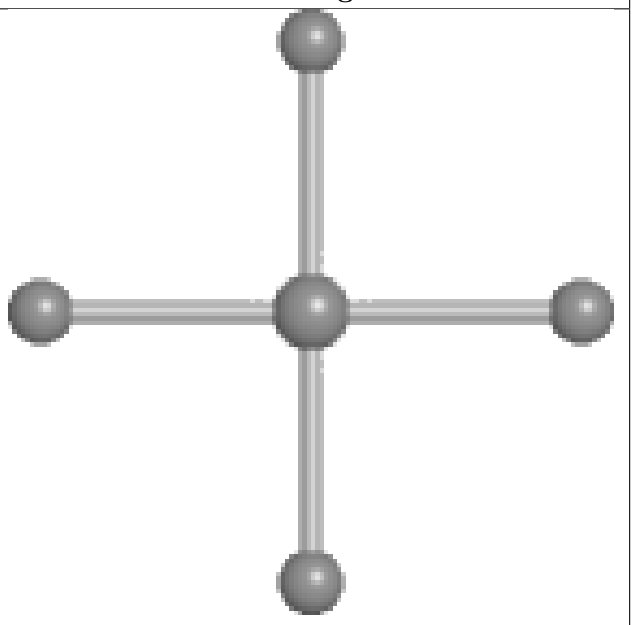
Bond lengths



Bond angles

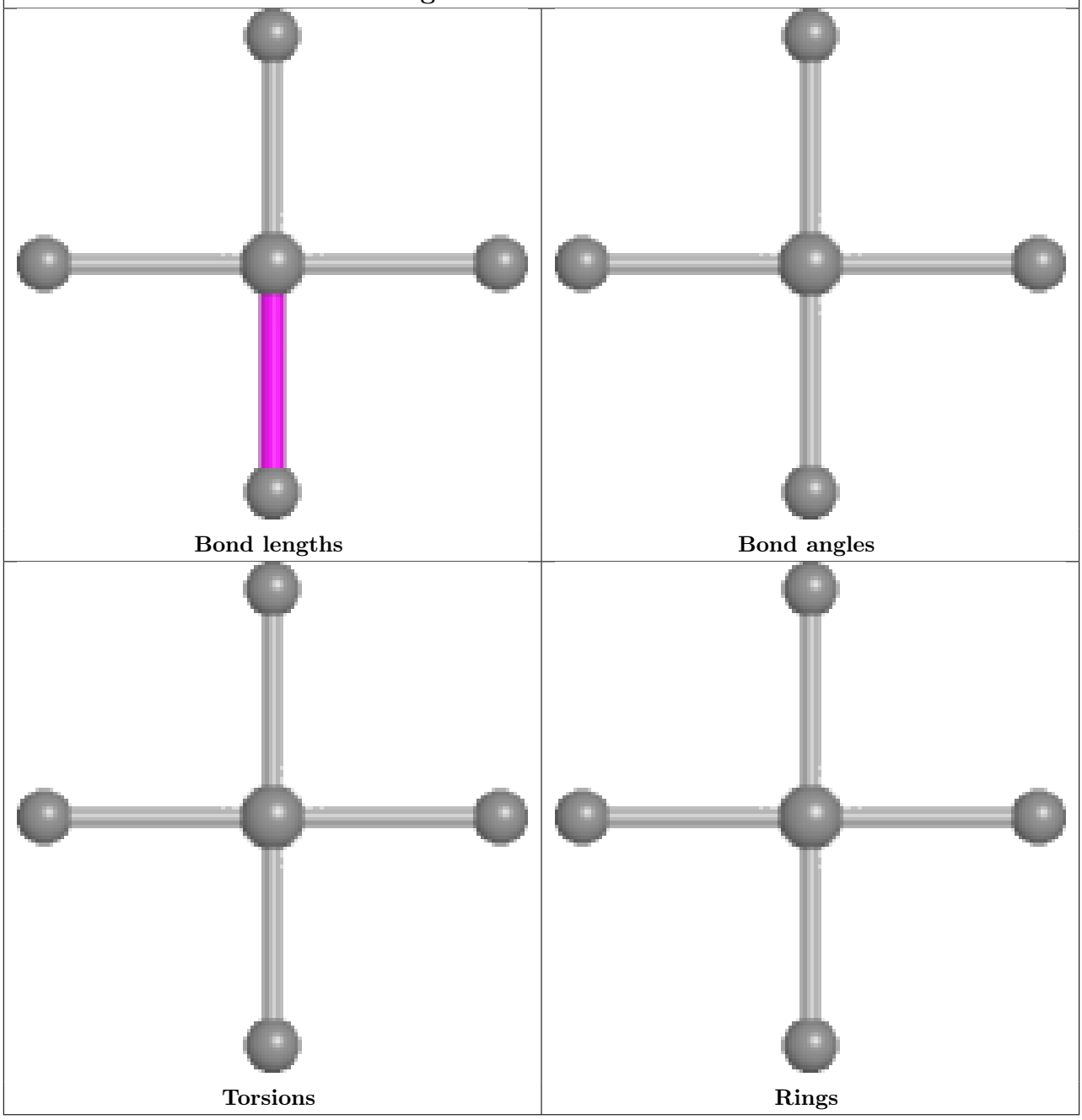


Torsions



Rings

Ligand VO4 DDD 604



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	AAA	594/598 (99%)	-0.94	0	100	100	10, 16, 29, 75	0
1	BBB	594/598 (99%)	-0.94	0	100	100	10, 16, 30, 62	0
1	CCC	594/598 (99%)	-0.97	0	100	100	10, 15, 31, 76	0
1	DDD	594/598 (99%)	-0.98	0	100	100	10, 15, 28, 53	0
All	All	2376/2392 (99%)	-0.96	0	100	100	10, 16, 29, 76	0

There are no RSRZ outliers to report.

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

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	BYR	DDD	186	13/14	0.94	0.09	17,21,32,35	1
1	BYR	BBB	186	13/14	0.95	0.10	18,27,41,42	1
1	BYR	AAA	186	13/14	0.95	0.09	14,22,32,35	1
1	BYR	AAA	43	13/14	0.96	0.07	11,15,20,28	1
1	BYR	DDD	43	13/14	0.96	0.07	13,14,19,31	1
1	BYR	BBB	43	13/14	0.96	0.08	12,15,23,25	1
1	I4O	CCC	553[A]	15/16	0.97	0.09	13,17,31,40	15
1	I4O	CCC	553[B]	10/16	0.97	0.09	9,10,11,13	10
1	BYR	CCC	43	13/14	0.97	0.06	12,15,21,22	1
1	BYR	CCC	186	13/14	0.97	0.09	17,29,40,41	1
1	I4O	BBB	553[A]	15/16	0.98	0.07	12,18,31,38	15
1	I4O	BBB	553[B]	10/16	0.98	0.07	10,12,14,14	10
1	I4O	AAA	553[A]	15/16	0.98	0.08	13,18,26,35	15
1	I4O	AAA	553[B]	10/16	0.98	0.08	11,13,15,16	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	I4O	DDD	553[A]	15/16	0.98	0.07	13,16,27,34	15
1	I4O	DDD	553[B]	10/16	0.98	0.07	8,8,13,15	10

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, 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
8	EDO	AAA	616	4/4	0.66	0.18	49,56,57,57	0
8	EDO	DDD	620	4/4	0.68	0.26	53,61,78,86	0
8	EDO	CCC	614	4/4	0.77	0.26	29,39,43,55	0
8	EDO	DDD	616	4/4	0.78	0.17	41,50,59,71	0
8	EDO	CCC	616	4/4	0.80	0.21	36,46,53,53	0
8	EDO	CCC	612	4/4	0.80	0.15	44,58,60,62	0
7	PEG	BBB	612	7/7	0.80	0.15	36,47,55,75	0
7	PEG	BBB	622	7/7	0.82	0.20	41,45,66,71	0
8	EDO	AAA	614	4/4	0.82	0.13	40,42,47,67	0
8	EDO	BBB	615	4/4	0.83	0.17	44,45,51,56	0
8	EDO	DDD	603	4/4	0.83	0.22	47,54,63,68	0
8	EDO	BBB	617	4/4	0.84	0.17	41,48,52,55	0
8	EDO	BBB	620	4/4	0.84	0.24	41,46,49,68	0
7	PEG	AAA	609	7/7	0.84	0.19	38,46,78,84	0
8	EDO	BBB	616	4/4	0.84	0.15	39,41,46,49	0
7	PEG	CCC	607	7/7	0.85	0.16	46,51,53,66	0
5	NA	DDD	621	1/1	0.85	0.15	49,49,49,49	0
8	EDO	CCC	613	4/4	0.85	0.17	34,39,42,47	0
5	NA	AAA	624	1/1	0.85	0.19	39,39,39,39	0
7	PEG	DDD	612	7/7	0.86	0.16	46,49,52,66	0
8	EDO	DDD	619	4/4	0.86	0.15	45,46,47,63	0
6	144	CCC	619	8/8	0.86	0.17	33,54,63,70	0
7	PEG	AAA	623	7/7	0.87	0.20	35,44,55,66	0
8	EDO	AAA	619	4/4	0.87	0.13	35,43,49,52	0
9	PGE	AAA	617	10/10	0.87	0.16	35,49,57,69	0
9	PGE	DDD	611	10/10	0.87	0.13	36,44,52,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	AAA	612	7/7	0.88	0.18	40,48,56,67	0
7	PEG	BBB	609	7/7	0.89	0.17	38,55,59,75	0
7	PEG	AAA	607	7/7	0.89	0.18	36,51,61,73	0
9	PGE	BBB	621	10/10	0.89	0.16	32,44,59,82	0
7	PEG	CCC	609	7/7	0.89	0.14	34,44,51,59	0
8	EDO	DDD	618	4/4	0.90	0.26	34,39,59,62	0
8	EDO	BBB	618	4/4	0.90	0.15	42,43,58,71	0
7	PEG	CCC	617	7/7	0.91	0.12	38,40,45,55	0
6	144	AAA	611	8/8	0.91	0.20	34,56,74,75	0
9	PGE	CCC	618	10/10	0.92	0.13	22,45,61,65	0
6	144	BBB	608	8/8	0.92	0.11	24,37,43,45	0
8	EDO	AAA	620	4/4	0.93	0.23	46,53,62,62	0
7	PEG	AAA	622	7/7	0.93	0.14	15,24,48,56	0
5	NA	BBB	624	1/1	0.93	0.18	43,43,43,43	0
6	144	DDD	602	8/8	0.93	0.09	24,33,46,48	0
6	144	BBB	607	8/8	0.93	0.12	27,37,45,47	0
8	EDO	BBB	619	4/4	0.93	0.19	31,35,45,59	0
8	EDO	AAA	615	4/4	0.93	0.16	36,40,49,50	0
6	144	AAA	606	8/8	0.93	0.10	23,29,37,40	0
8	EDO	AAA	618	4/4	0.93	0.17	36,41,61,96	0
6	144	BBB	623	8/8	0.93	0.14	22,35,45,48	0
6	144	CCC	606	8/8	0.94	0.11	20,28,37,39	0
7	PEG	AAA	621	7/7	0.94	0.14	31,41,52,71	0
5	NA	CCC	620	1/1	0.95	0.05	36,36,36,36	0
8	EDO	CCC	615	4/4	0.95	0.20	40,42,43,46	0
5	NA	AAA	608	1/1	0.95	0.04	14,14,14,14	0
6	144	DDD	609	8/8	0.95	0.10	23,26,35,40	0
6	144	BBB	601	8/8	0.96	0.09	21,35,36,36	0
5	NA	DDD	613	1/1	0.96	0.08	16,16,16,16	0
5	NA	CCC	608	1/1	0.96	0.07	15,15,15,15	0
6	144	DDD	610	8/8	0.96	0.08	23,29,41,45	0
2	VO4	CCC	601	5/5	0.96	0.10	12,18,19,38	5
5	NA	DDD	601	1/1	0.96	0.06	26,26,26,26	1
8	EDO	DDD	617	4/4	0.96	0.15	20,24,27,35	0
2	VO4	AAA	601	5/5	0.97	0.07	12,14,19,33	5
2	VO4	DDD	604	5/5	0.97	0.08	11,13,21,32	5
5	NA	BBB	611	1/1	0.97	0.05	16,16,16,16	0
2	VO4	BBB	602	5/5	0.98	0.08	14,15,20,29	5
5	NA	AAA	610	1/1	0.98	0.03	9,9,9,9	0
5	NA	CCC	610	1/1	0.98	0.05	9,9,9,9	0
5	NA	DDD	614	1/1	0.98	0.03	8,8,8,8	0
4	BR	DDD	608	1/1	0.99	0.02	26,26,26,26	1

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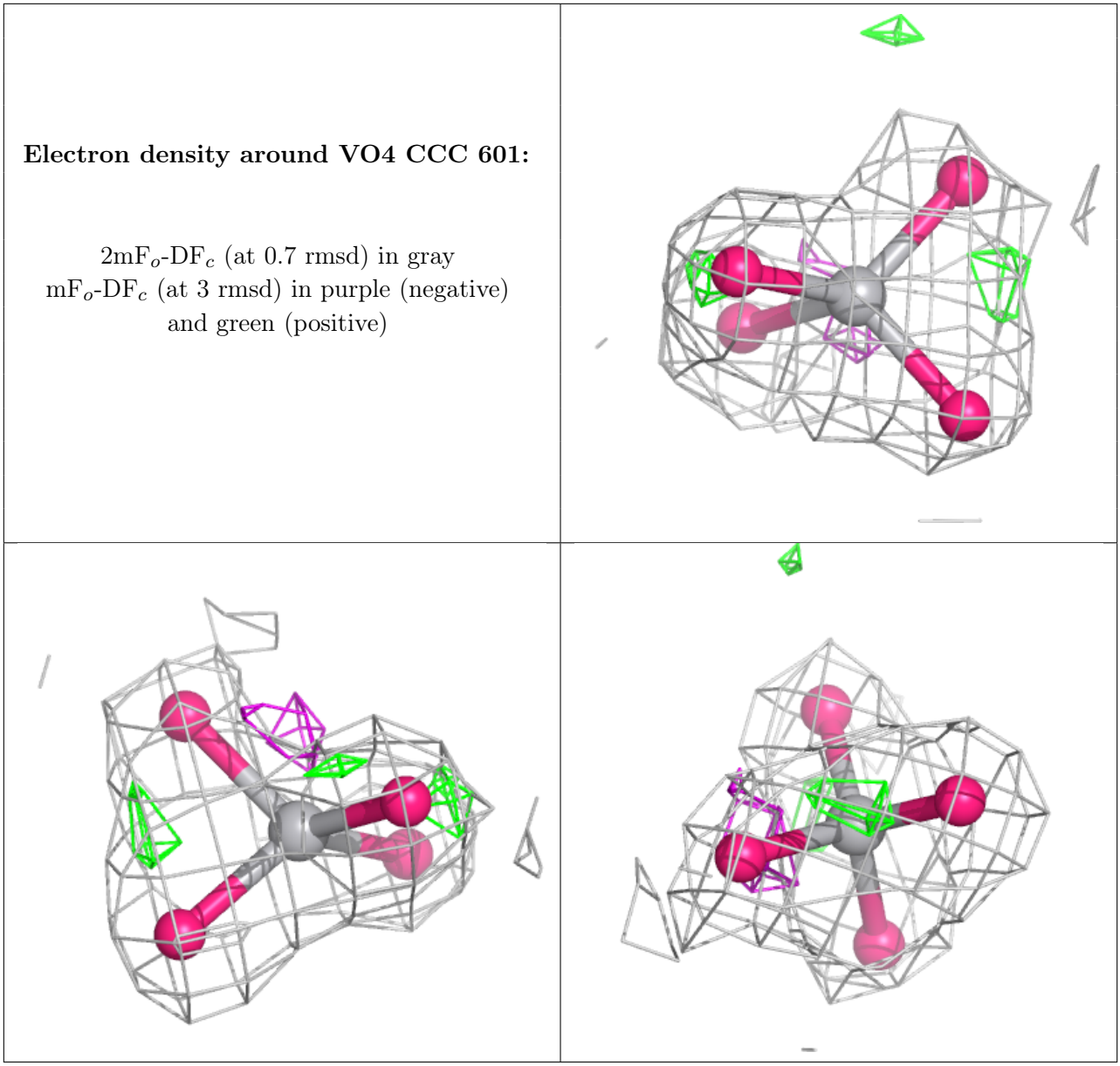
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BR	DDD	615	1/1	0.99	0.03	31,31,31,31	1
5	NA	AAA	604	1/1	0.99	0.07	11,11,11,11	0
3	CA	BBB	603	1/1	0.99	0.02	14,14,14,14	0
4	BR	AAA	613	1/1	0.99	0.09	29,29,29,29	1
5	NA	DDD	607	1/1	0.99	0.04	8,8,8,8	0
4	BR	BBB	614	1/1	0.99	0.04	33,33,33,33	1
5	NA	BBB	605	1/1	0.99	0.10	5,5,5,5	0
4	BR	DDD	606	1/1	0.99	0.03	13,13,13,13	1
5	NA	BBB	613	1/1	0.99	0.05	10,10,10,10	0
5	NA	CCC	604	1/1	1.00	0.10	6,6,6,6	0
4	BR	AAA	603	1/1	1.00	0.03	32,32,32,32	0
4	BR	AAA	605	1/1	1.00	0.03	37,37,37,37	1
3	CA	AAA	602	1/1	1.00	0.03	15,15,15,15	0
4	BR	BBB	604	1/1	1.00	0.04	31,31,31,31	0
4	BR	BBB	606	1/1	1.00	0.06	41,41,41,41	1
3	CA	CCC	602	1/1	1.00	0.02	12,12,12,12	0
4	BR	CCC	603	1/1	1.00	0.05	28,28,28,28	0
5	NA	BBB	610	1/1	1.00	0.03	15,15,15,15	0
4	BR	CCC	605	1/1	1.00	0.02	26,26,26,26	1
4	BR	CCC	611	1/1	1.00	0.05	29,29,29,29	1
3	CA	DDD	605	1/1	1.00	0.01	14,14,14,14	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.

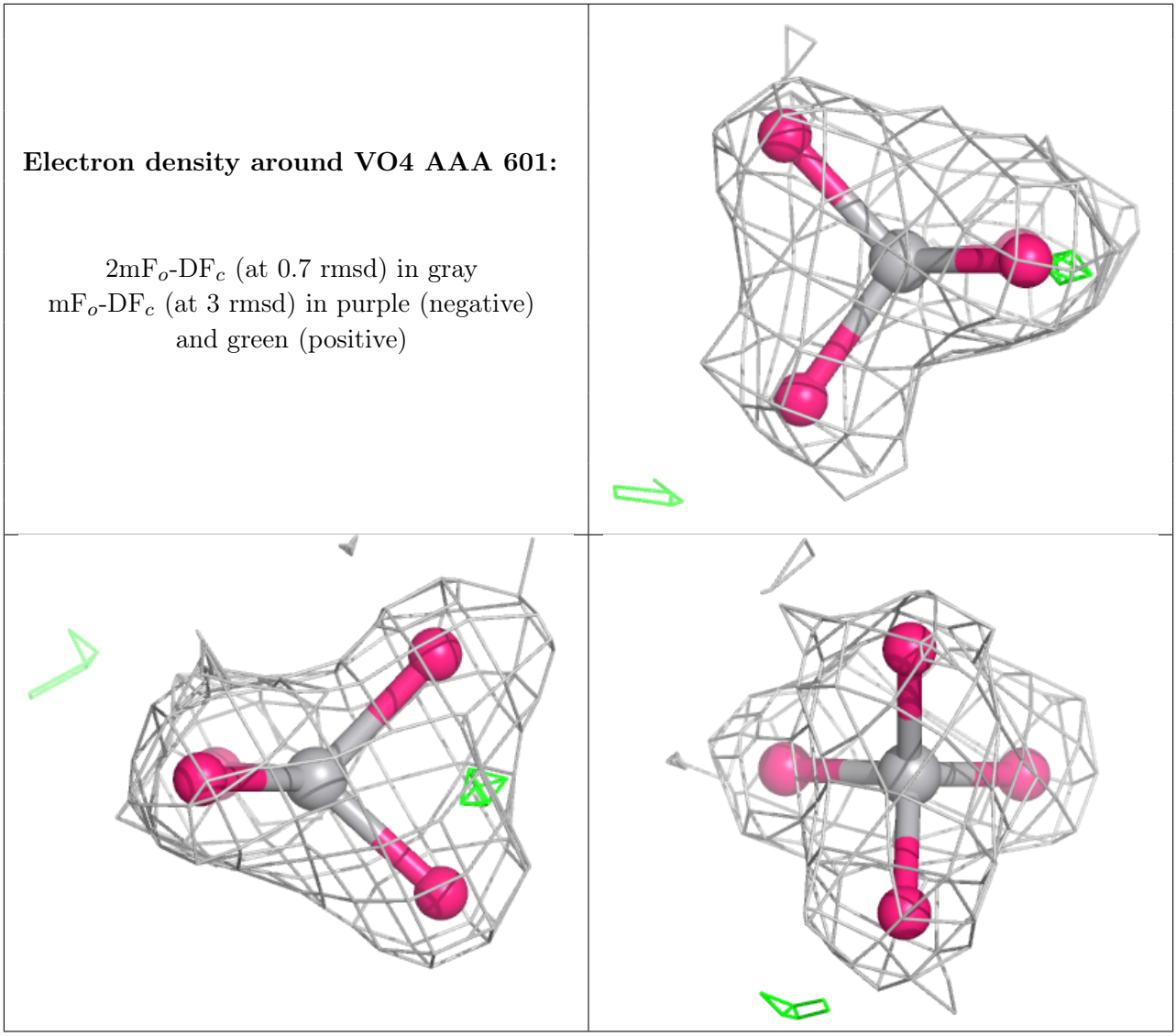
Electron density around VO4 CCC 601:

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



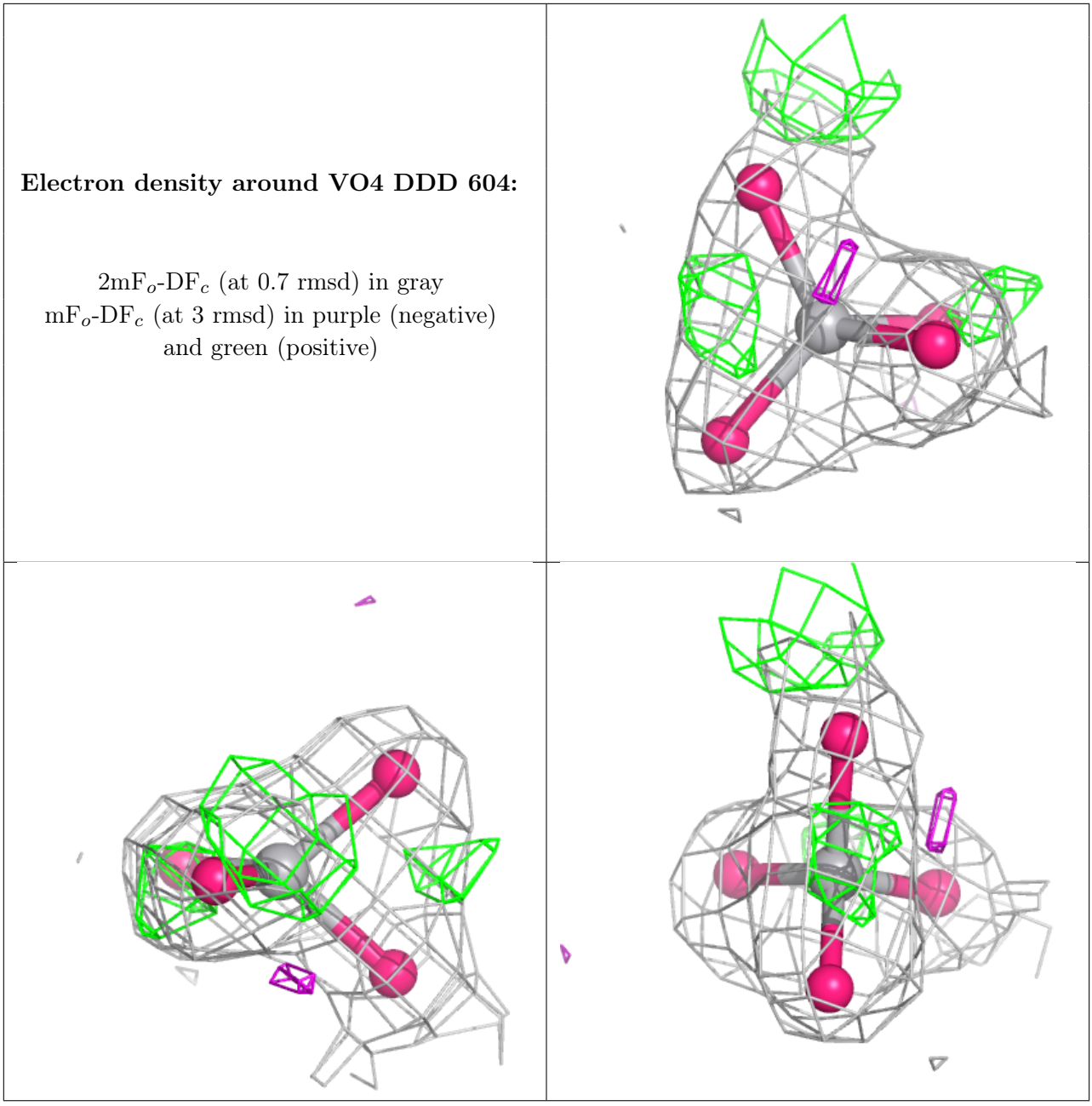
Electron density around VO4 AAA 601:

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



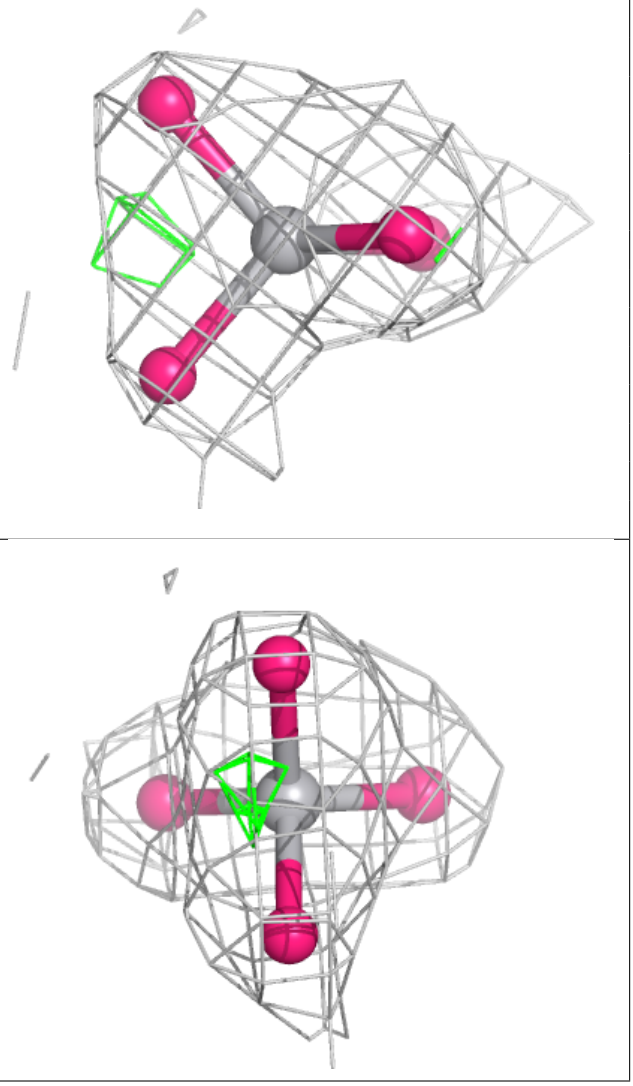
Electron density around VO4 DDD 604:

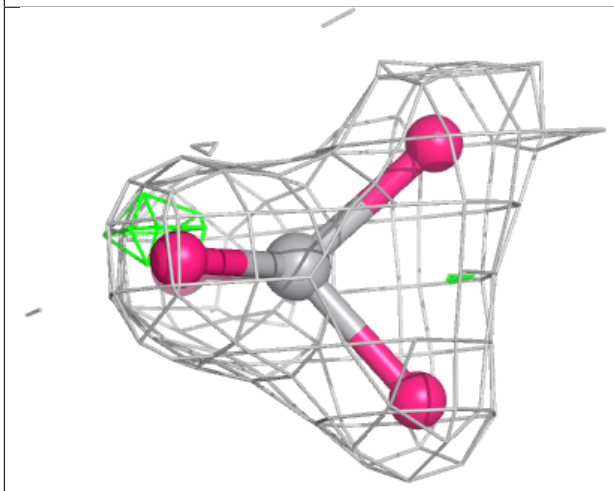
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around VO4 BBB 602:

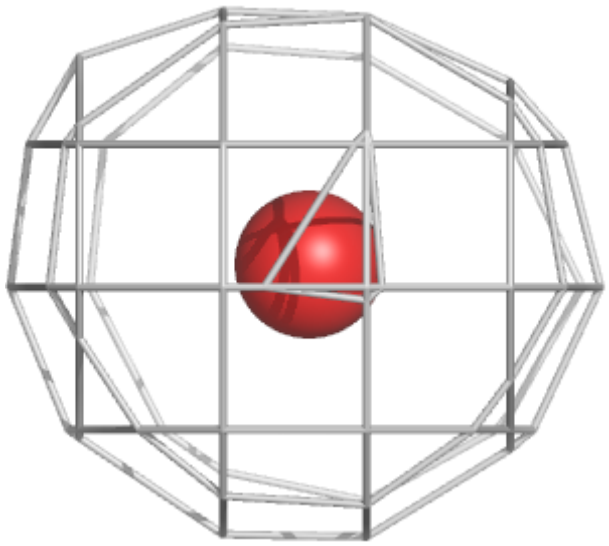
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

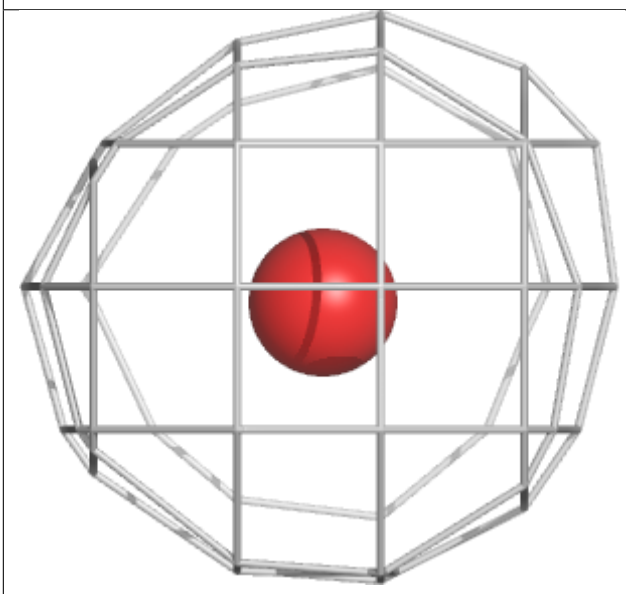


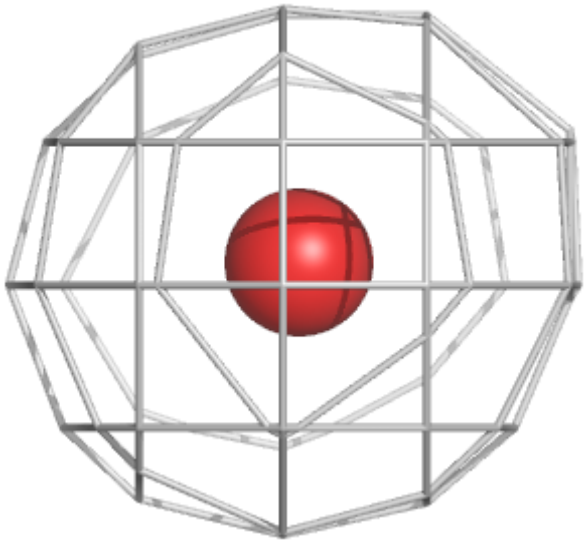


Electron density around BR DDD 608:

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

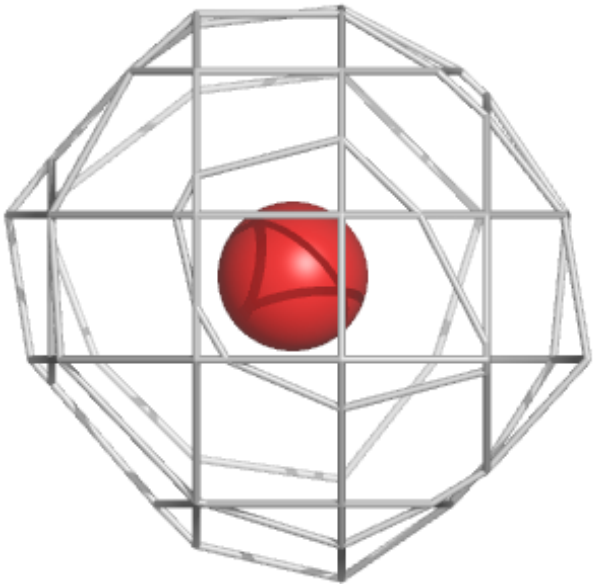


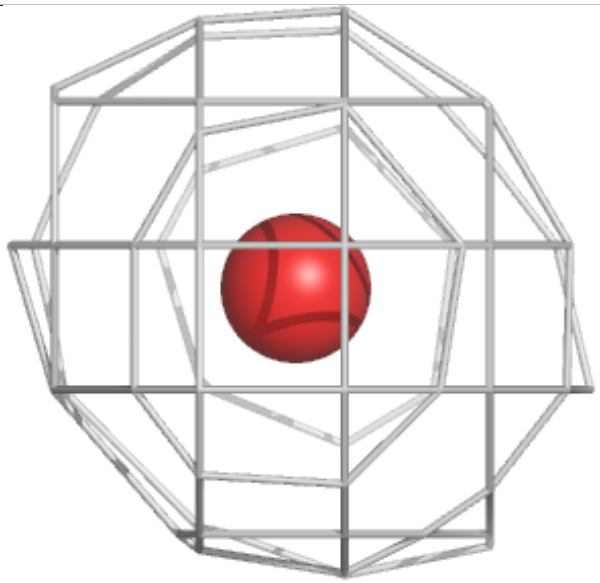


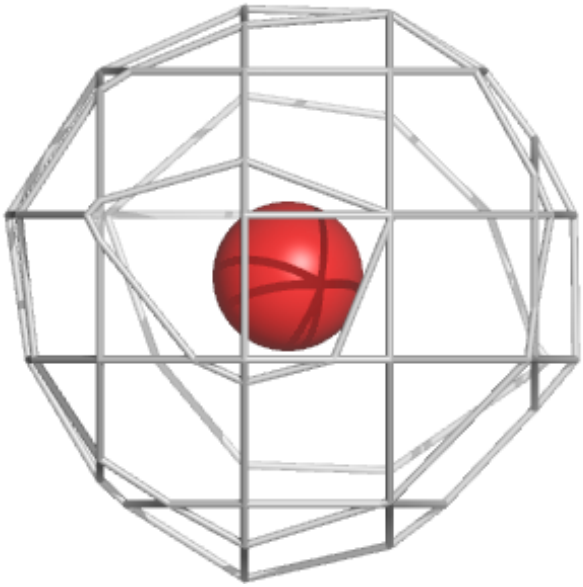


Electron density around BR DDD 615:

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

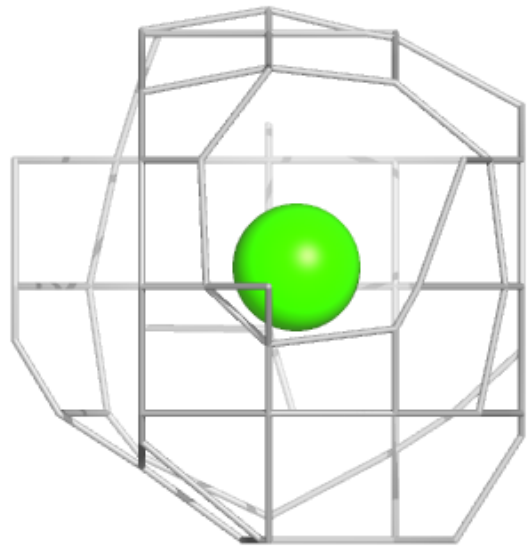


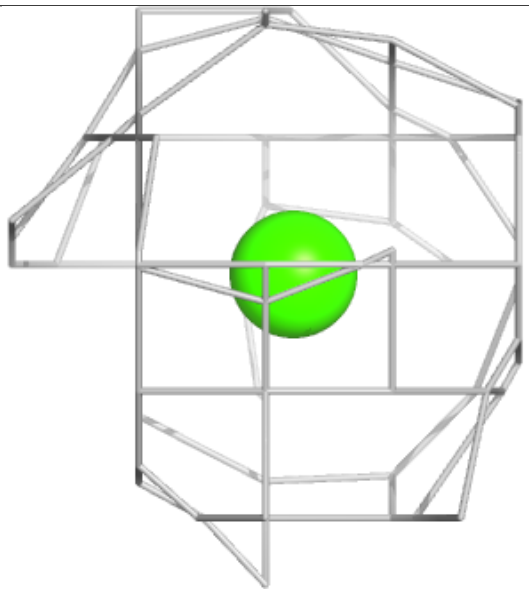


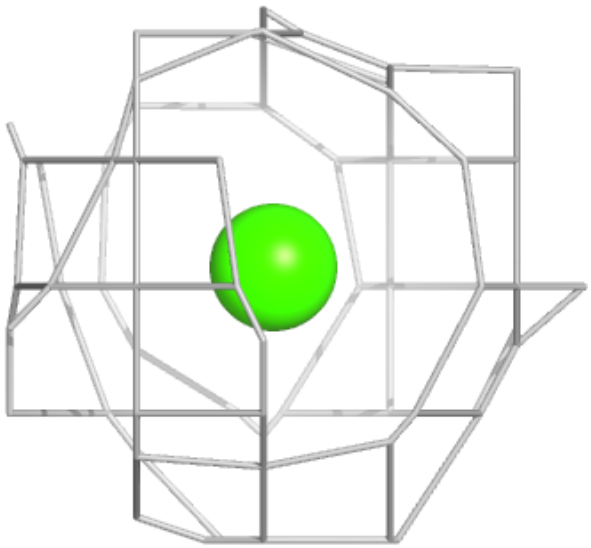


Electron density around CA BBB 603:

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

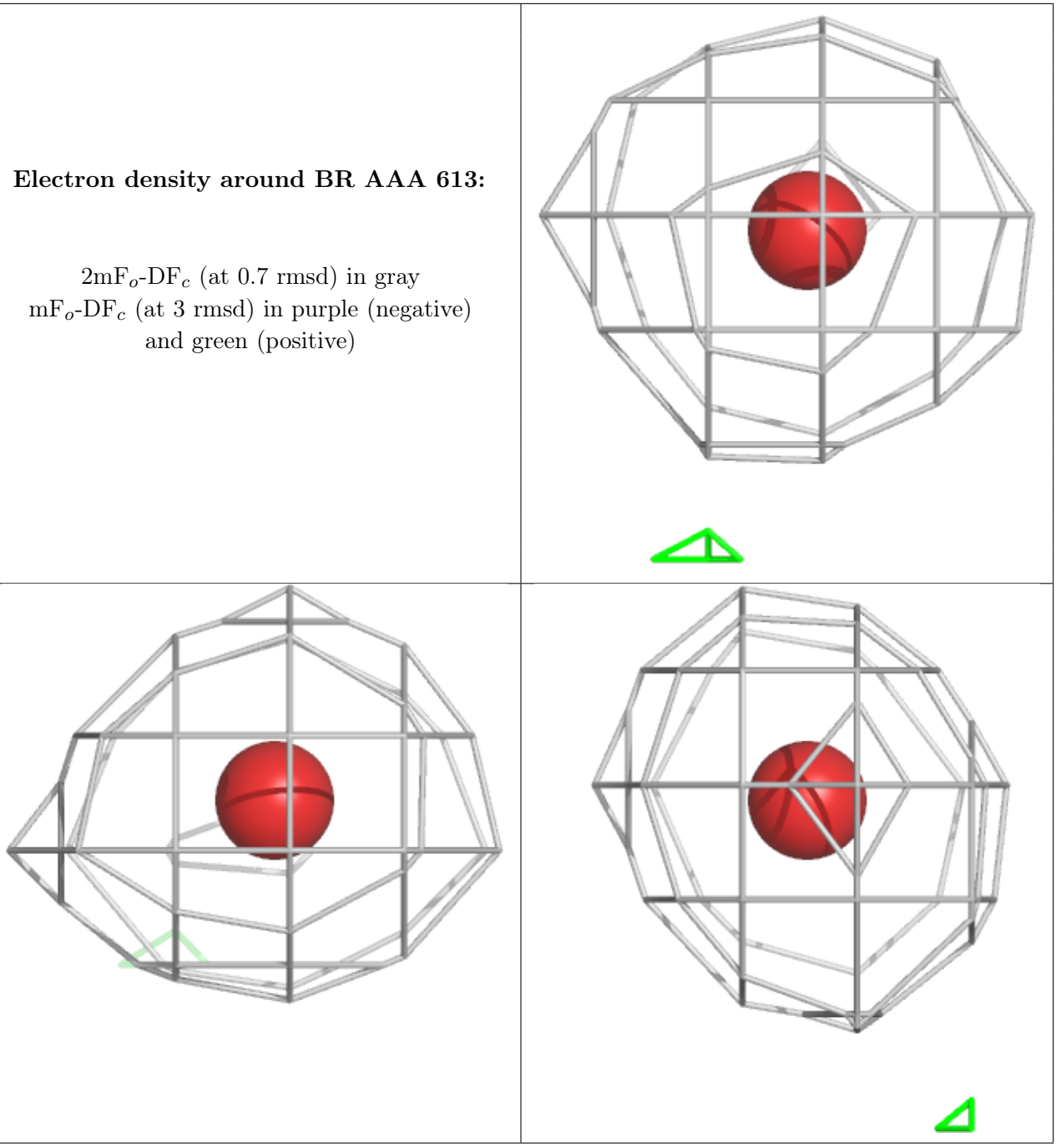






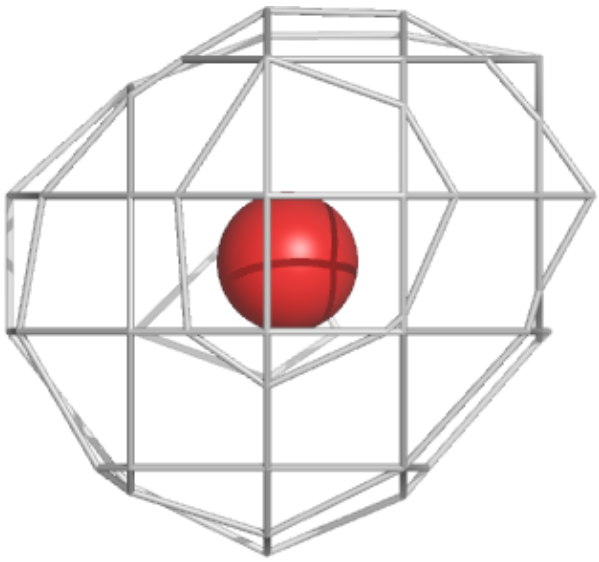
Electron density around BR AAA 613:

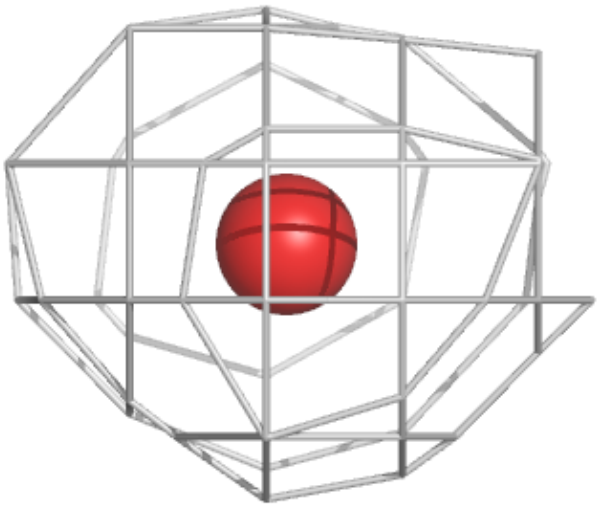
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

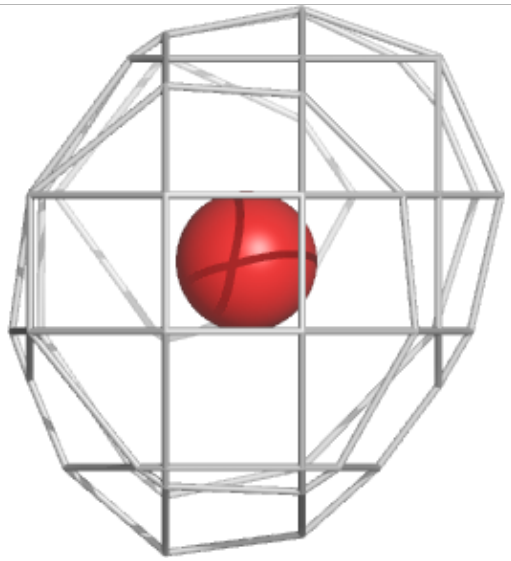


Electron density around BR BBB 614:

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

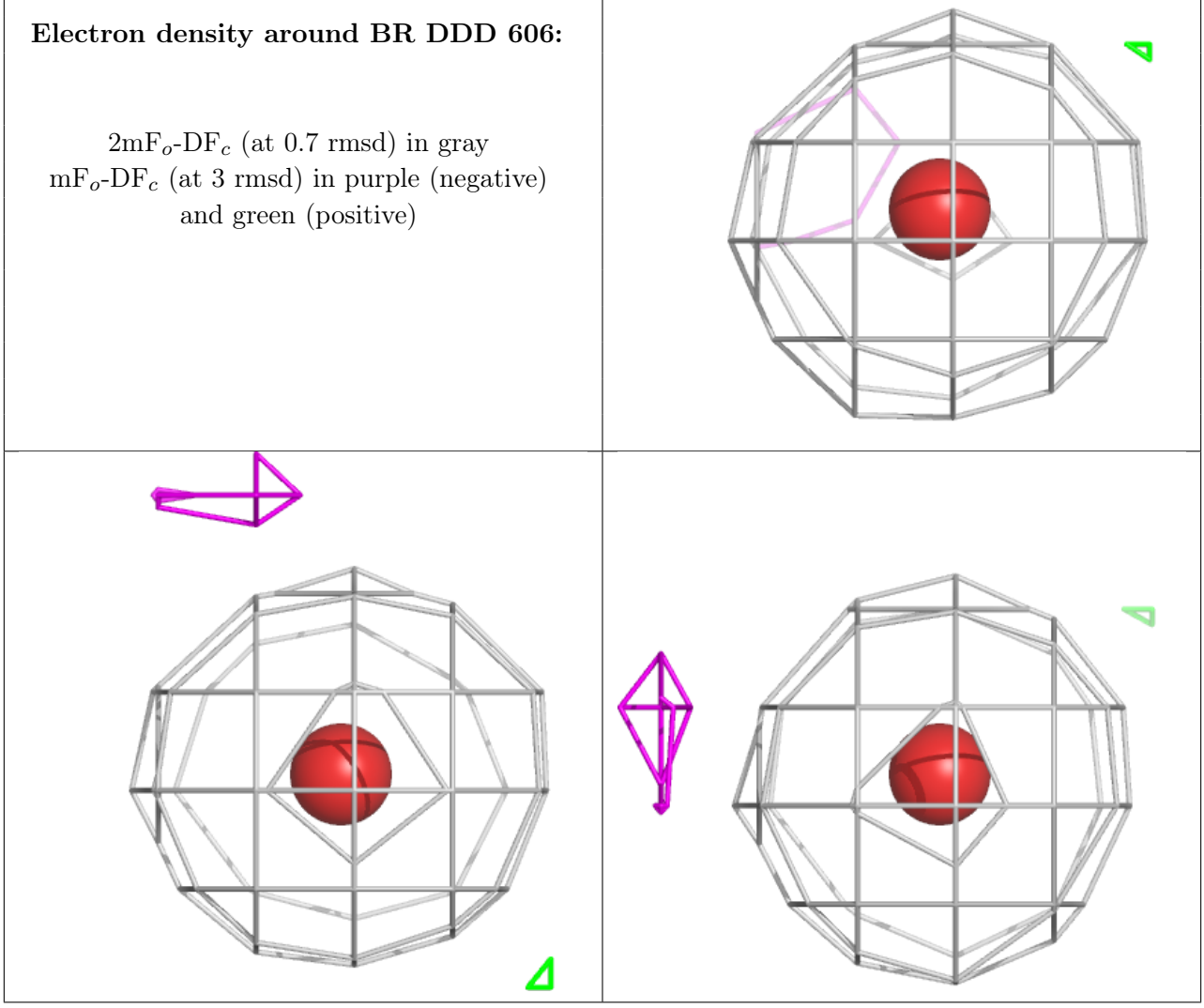






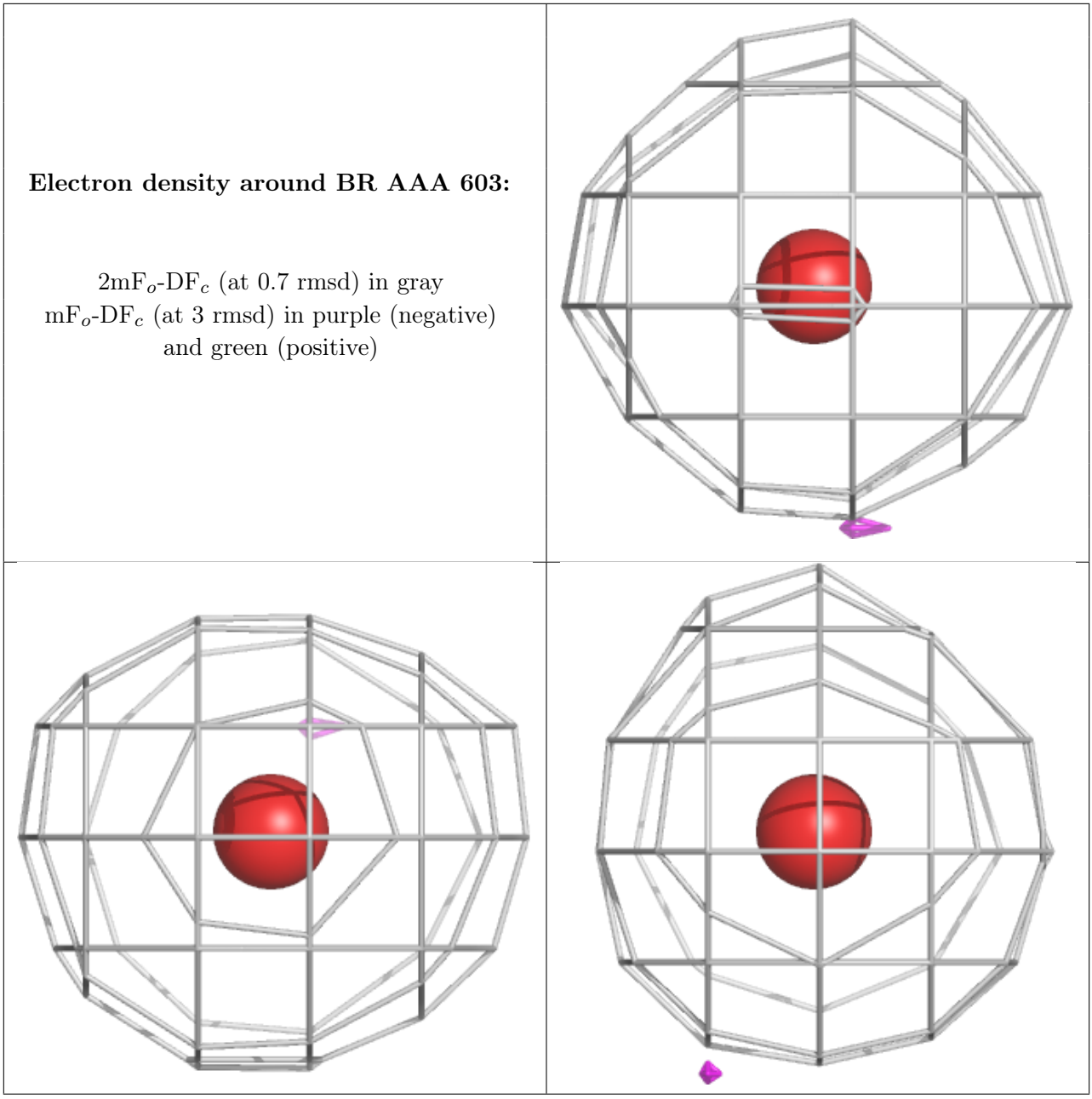
Electron density around BR DDD 606:

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



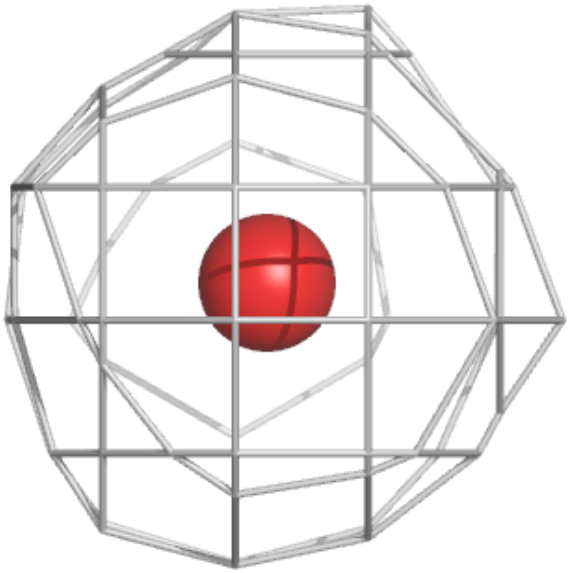
Electron density around BR AAA 603:

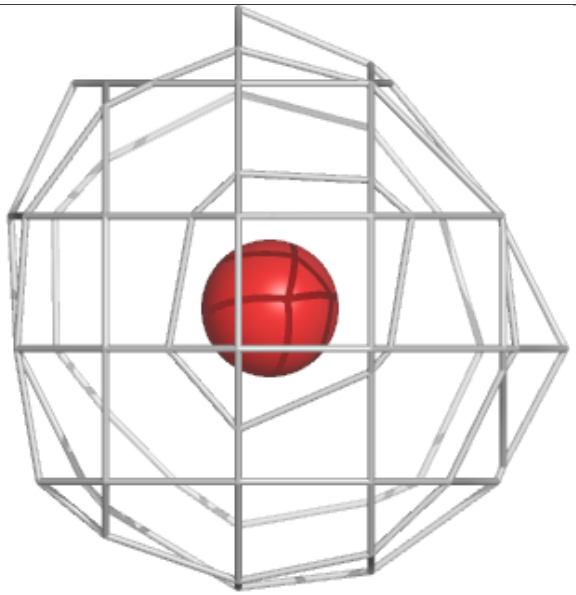
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

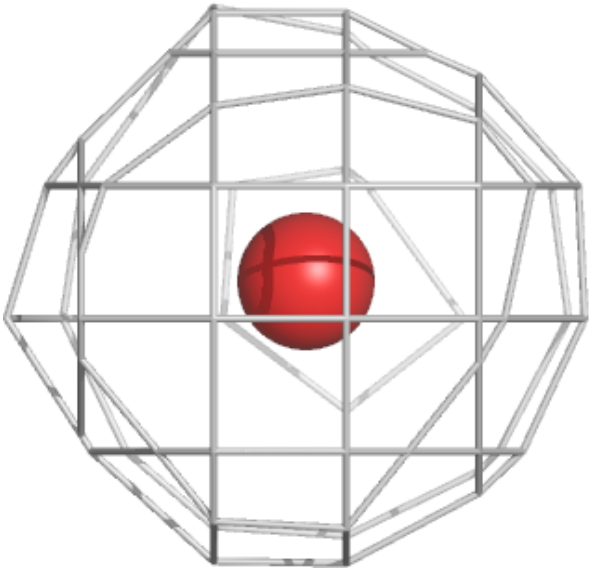


Electron density around BR AAA 605:

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

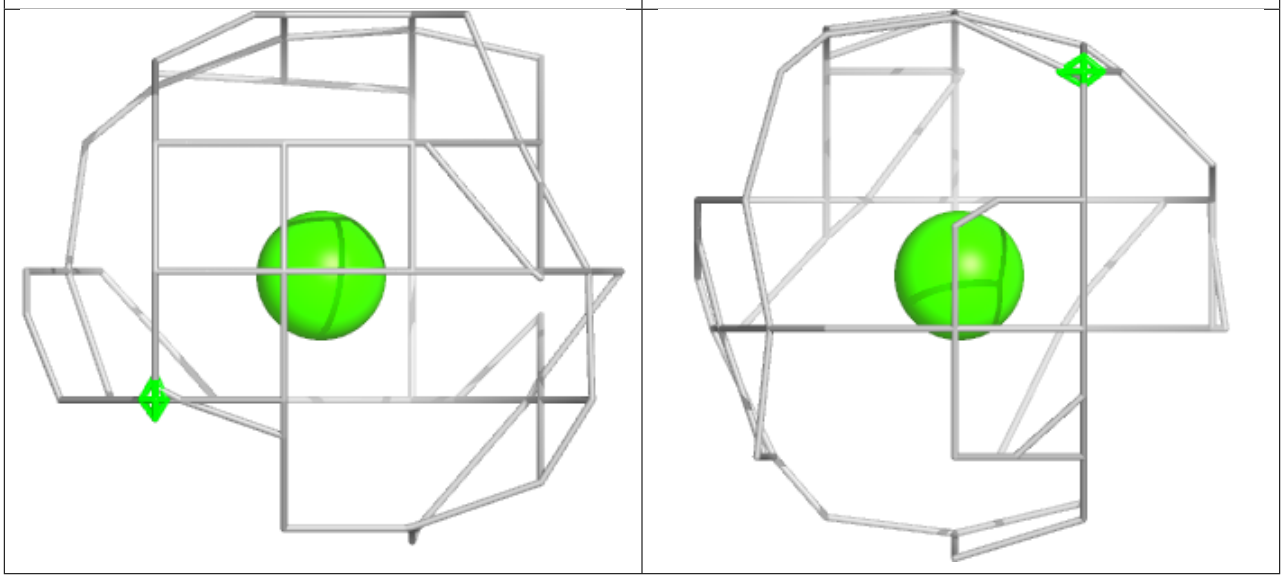






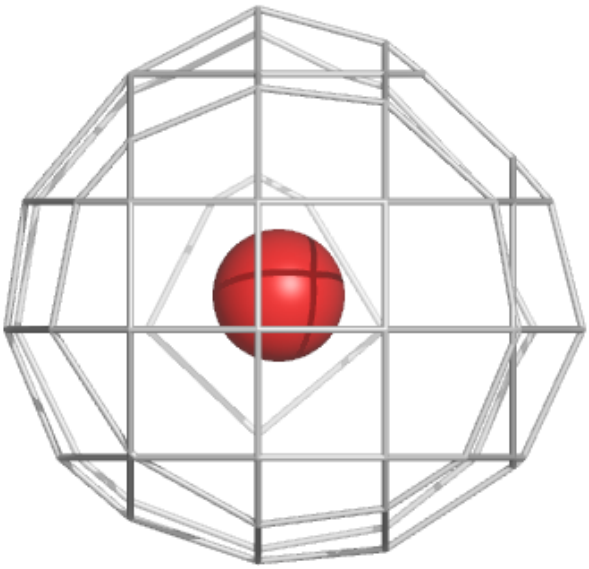
Electron density around CA AAA 602:

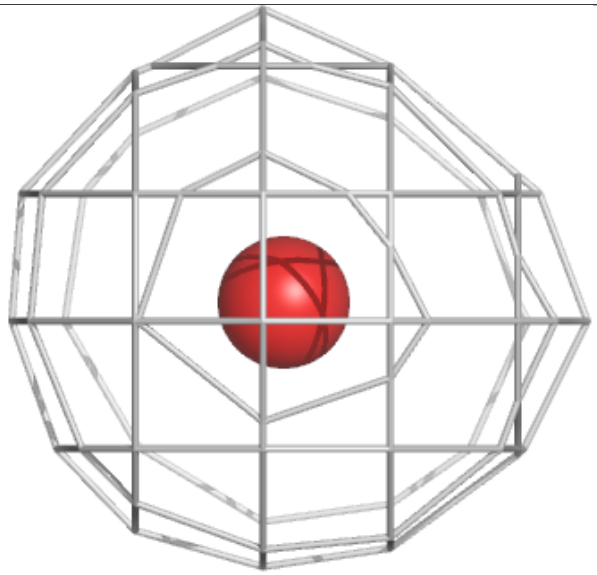
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

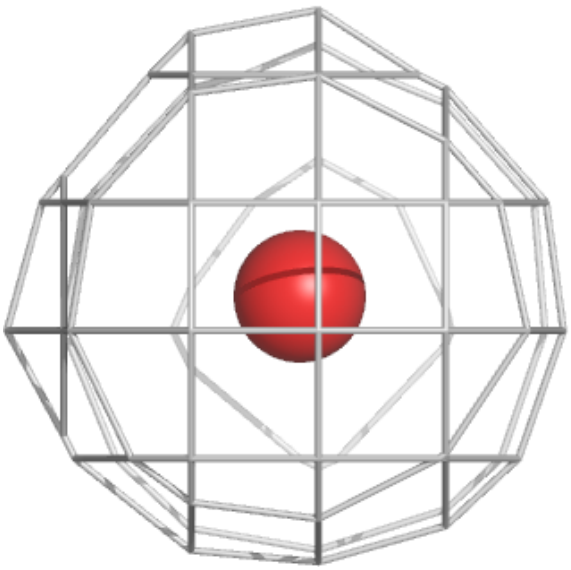


Electron density around BR BBB 604:

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

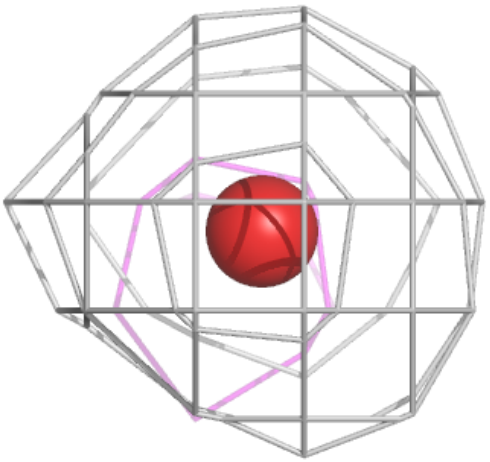


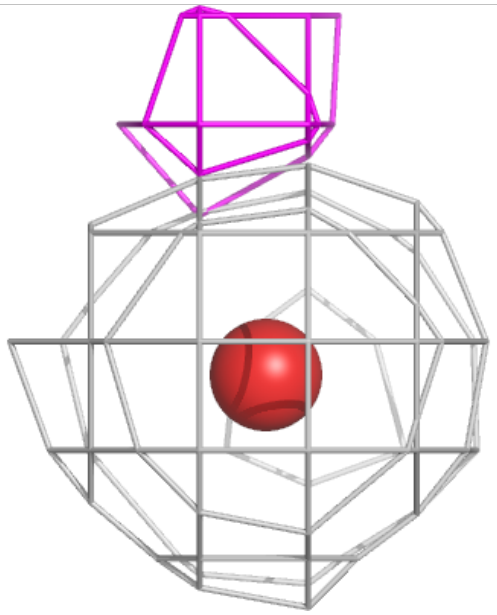


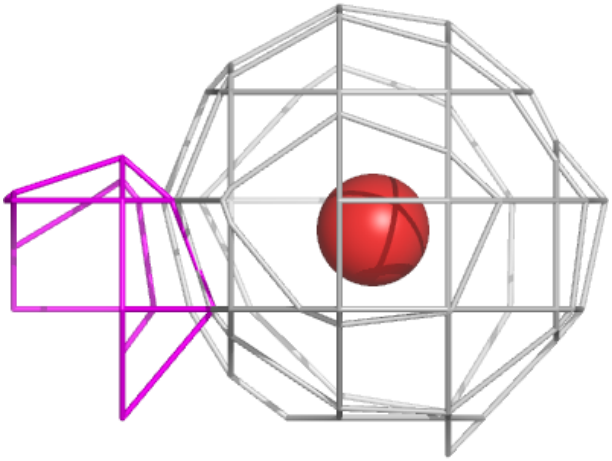


Electron density around BR BBB 606:

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

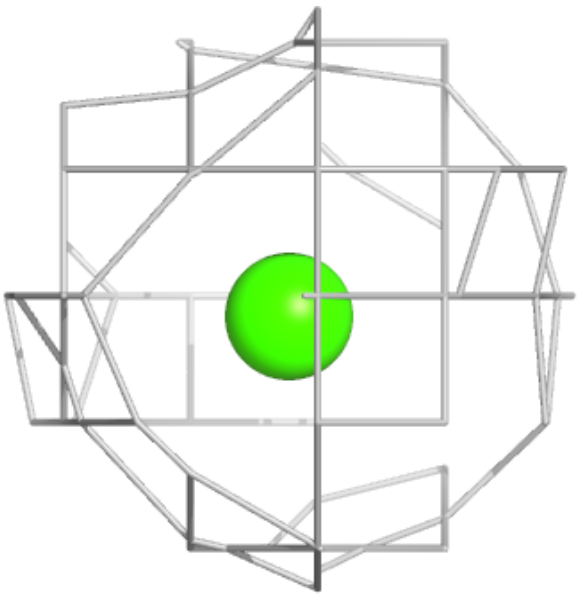


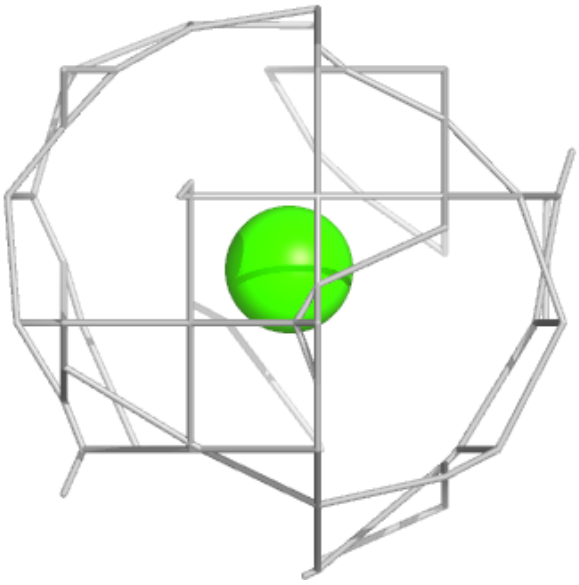


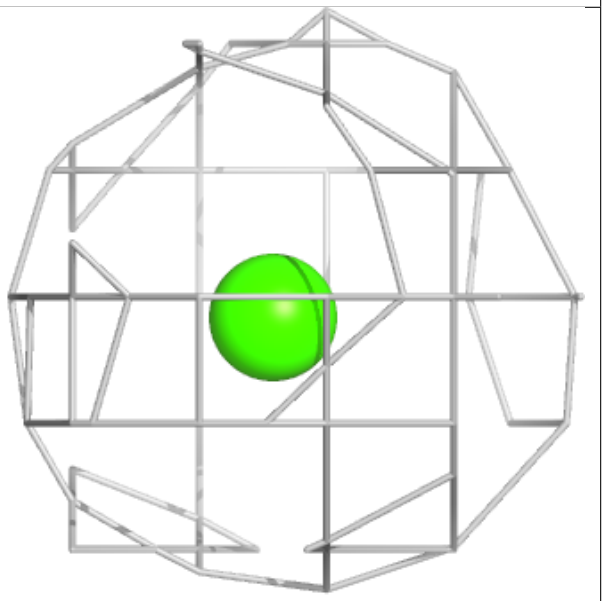


Electron density around CA CCC 602:

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

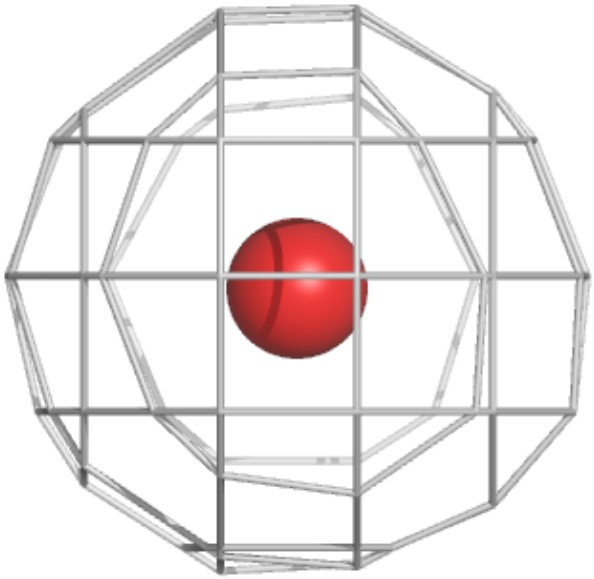


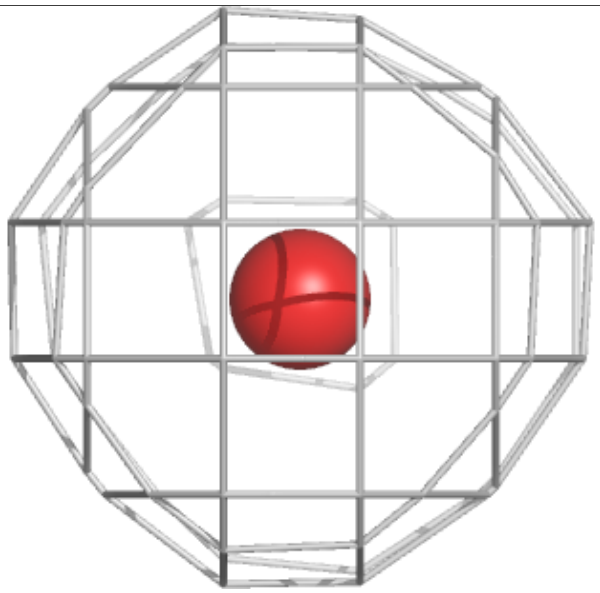


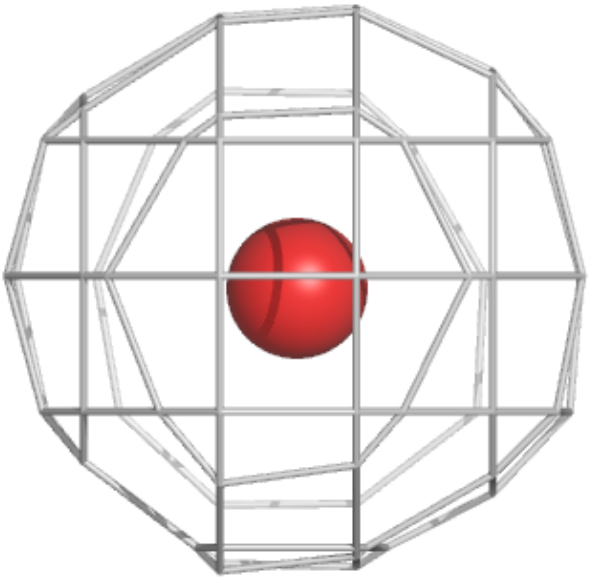


Electron density around BR CCC 603:

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

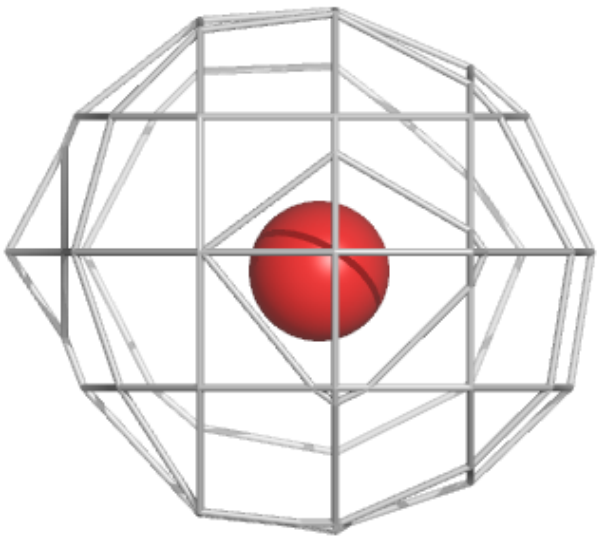


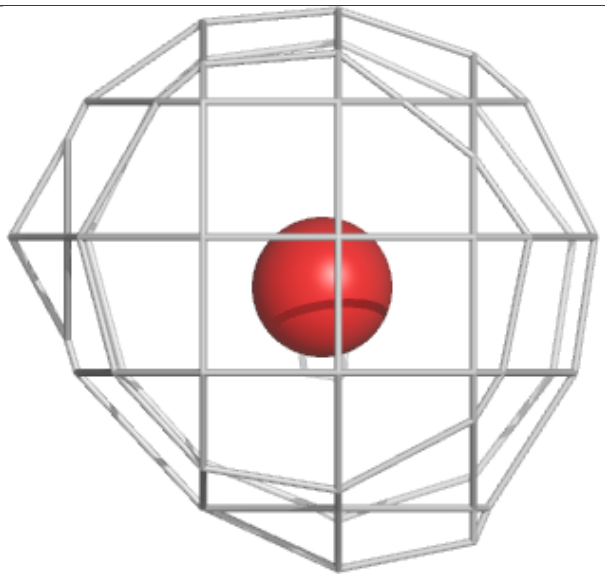


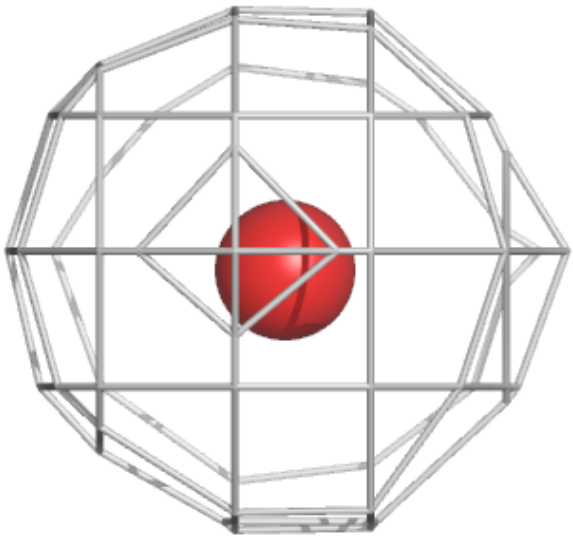


Electron density around BR CCC 605:

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

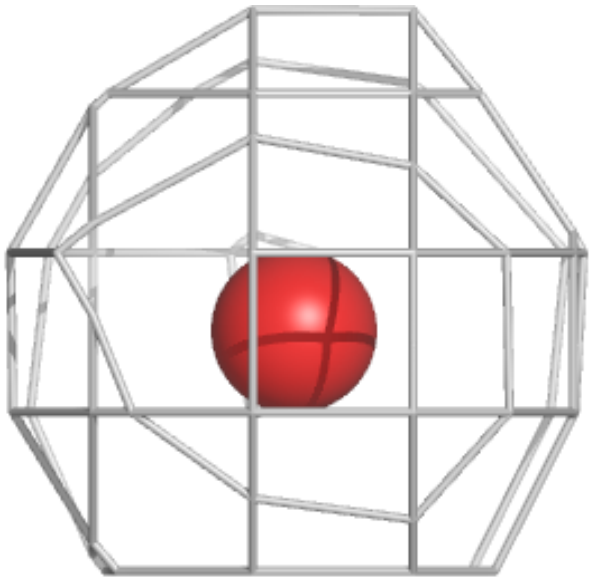


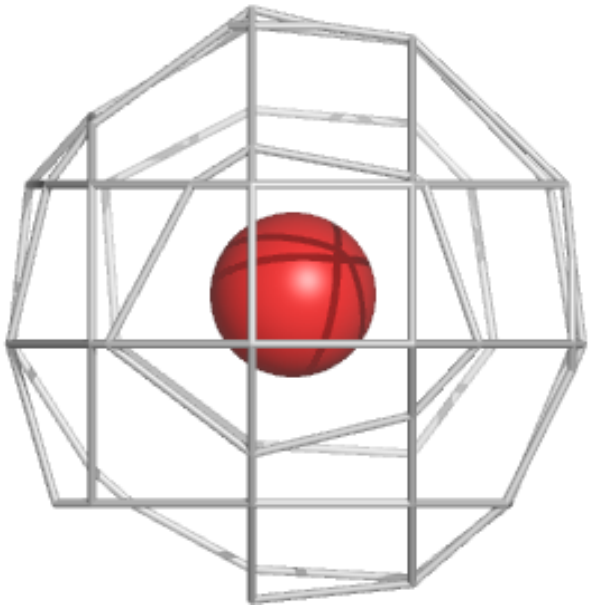


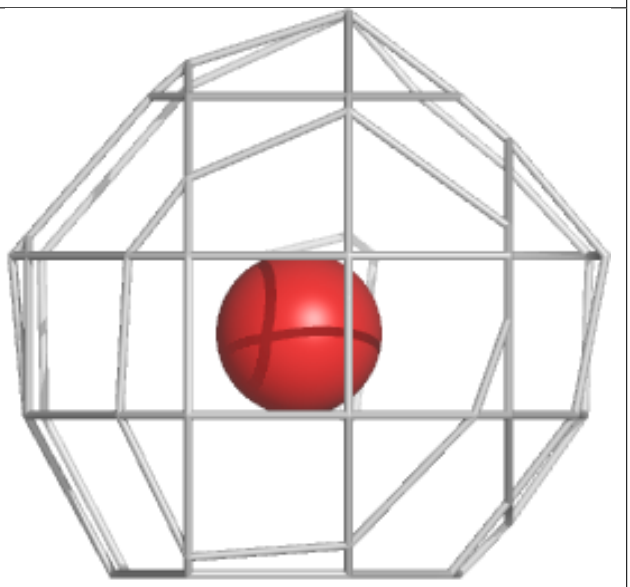


Electron density around BR CCC 611:

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

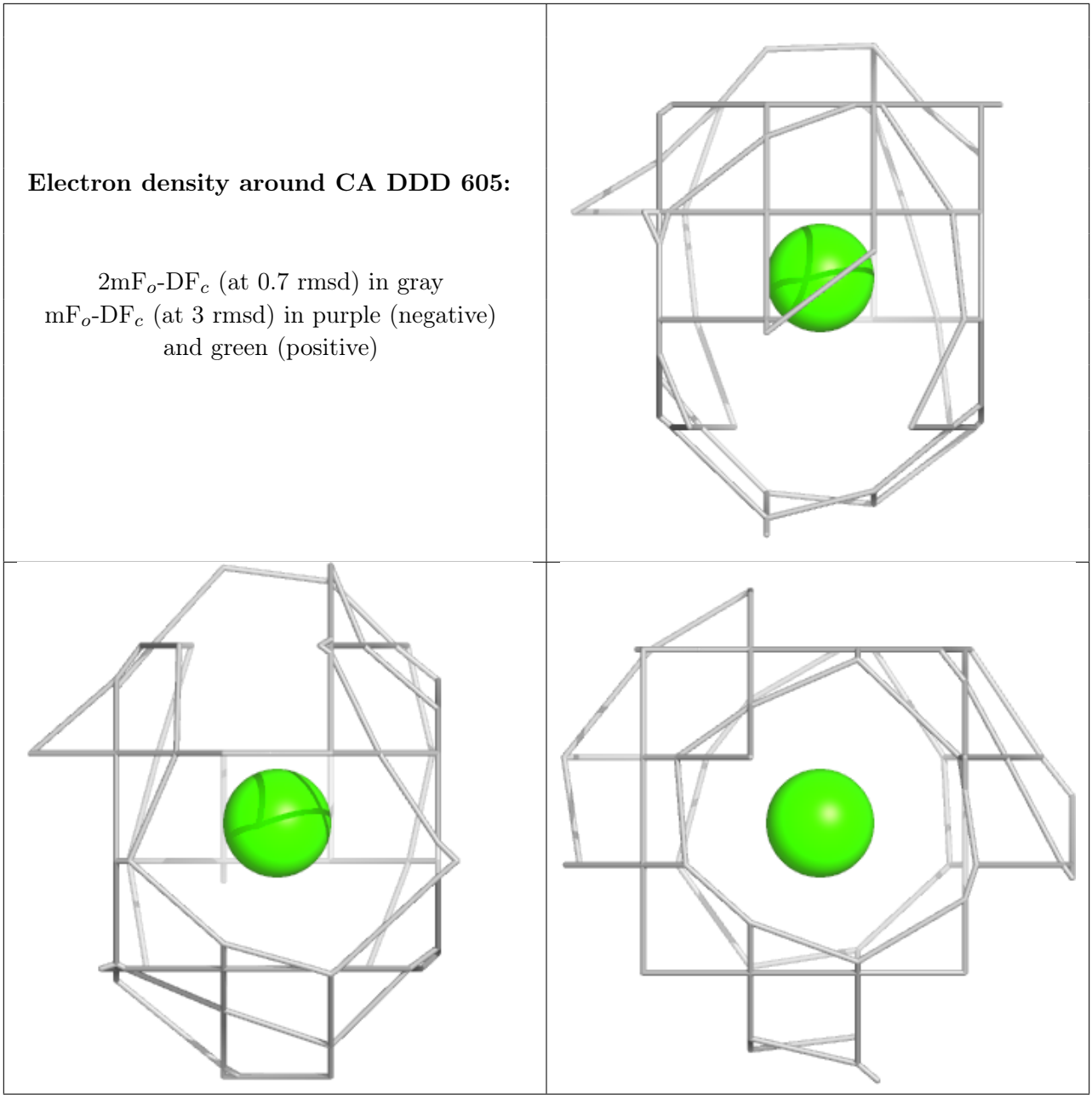






Electron density around CA DDD 605:

$2mF_o$-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.