



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2022 – 06:23 PM JST

PDB ID : 7E9R
Title : Crystal structure of Sesquisabinene B Synthase 1 mutant T313S
Authors : Singh, S.; Thulasiram, H.V.; Kulkarni, K.A.
Deposited on : 2021-03-04
Resolution : 3.41 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

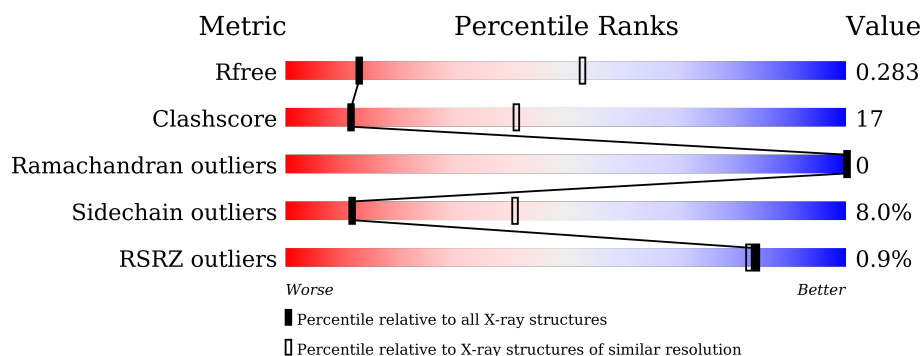
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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

Mol	Chain	Length	Quality of chain
1	A	555	<div> <div>65%</div> <div>24%</div> <div>• 8%</div> </div>
1	B	555	<div> <div>%</div> <div>63%</div> <div>27%</div> <div>• 9%</div> </div>
1	C	555	<div> <div>%</div> <div>59%</div> <div>27%</div> <div>5%</div> <div>9%</div> </div>
1	D	555	<div> <div>%</div> <div>57%</div> <div>30%</div> <div>• 9%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16432 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 Sesquisabinene B synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4129	2665	687	760	17			
1	B	506	Total	C	N	O	S	0	0	0
			4105	2652	682	754	17			
1	C	506	Total	C	N	O	S	0	0	0
			4108	2653	683	755	17			
1	D	504	Total	C	N	O	S	0	0	0
			4082	2635	679	752	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A0A0RDR2
A	13	GLU	-	expression tag	UNP A0A0A0RDR2
A	14	CYS	-	expression tag	UNP A0A0A0RDR2
A	15	GLY	-	expression tag	UNP A0A0A0RDR2
A	16	ASP	-	expression tag	UNP A0A0A0RDR2
A	17	MET	-	expression tag	UNP A0A0A0RDR2
A	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
A	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
B	12	GLY	-	expression tag	UNP A0A0A0RDR2
B	13	GLU	-	expression tag	UNP A0A0A0RDR2
B	14	CYS	-	expression tag	UNP A0A0A0RDR2
B	15	GLY	-	expression tag	UNP A0A0A0RDR2
B	16	ASP	-	expression tag	UNP A0A0A0RDR2
B	17	MET	-	expression tag	UNP A0A0A0RDR2
B	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
B	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
C	12	GLY	-	expression tag	UNP A0A0A0RDR2
C	13	GLU	-	expression tag	UNP A0A0A0RDR2
C	14	CYS	-	expression tag	UNP A0A0A0RDR2
C	15	GLY	-	expression tag	UNP A0A0A0RDR2
C	16	ASP	-	expression tag	UNP A0A0A0RDR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	MET	-	expression tag	UNP A0A0A0RDR2
C	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
C	313	SER	THR	engineered mutation	UNP A0A0A0RDR2
D	12	GLY	-	expression tag	UNP A0A0A0RDR2
D	13	GLU	-	expression tag	UNP A0A0A0RDR2
D	14	CYS	-	expression tag	UNP A0A0A0RDR2
D	15	GLY	-	expression tag	UNP A0A0A0RDR2
D	16	ASP	-	expression tag	UNP A0A0A0RDR2
D	17	MET	-	expression tag	UNP A0A0A0RDR2
D	196	LYS	GLY	cloning artifact	UNP A0A0A0RDR2
D	313	SER	THR	engineered mutation	UNP A0A0A0RDR2

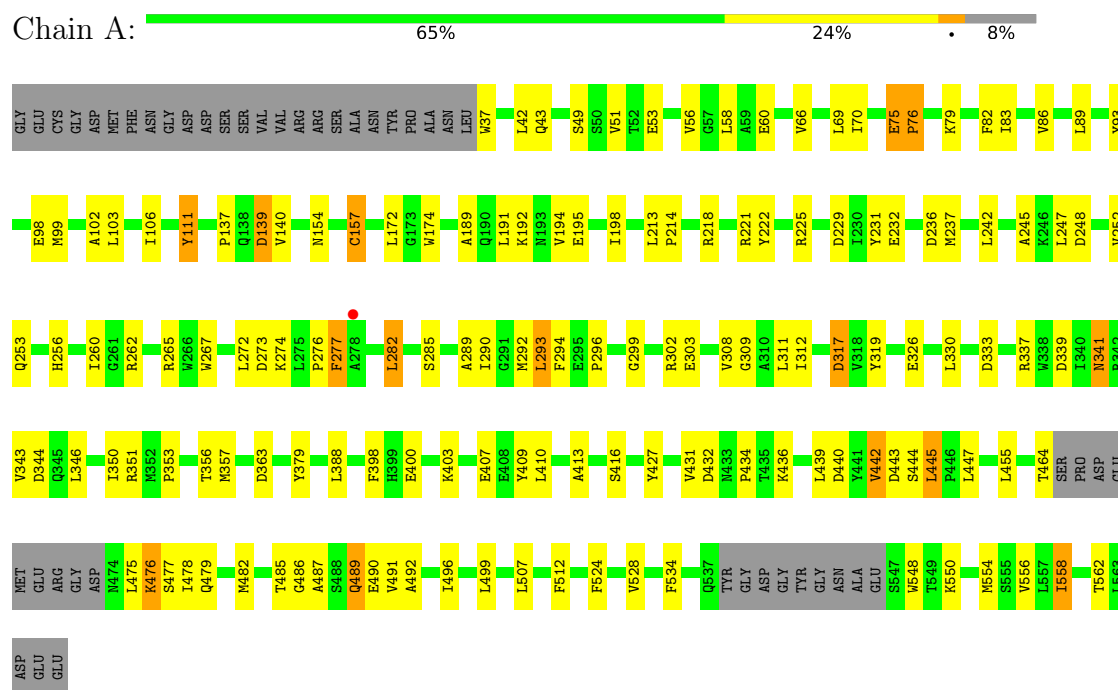
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

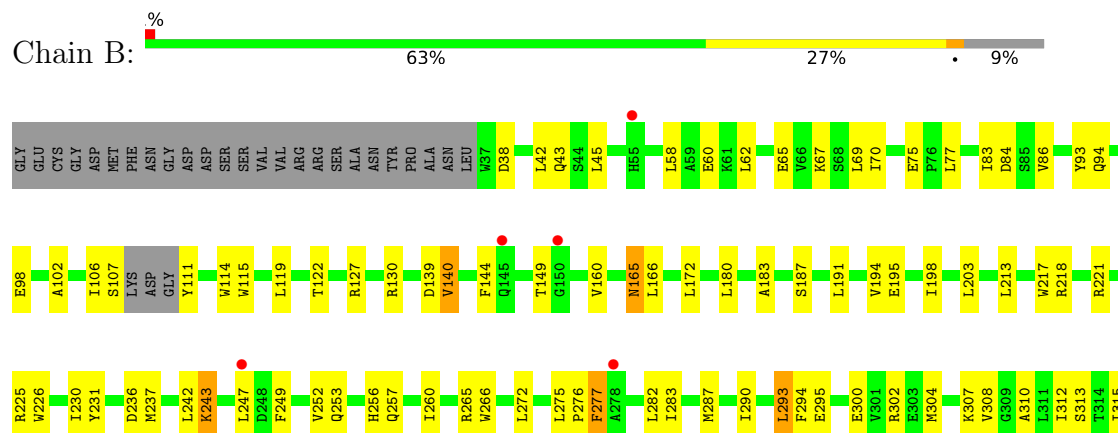
3 Residue-property plots [i](#)

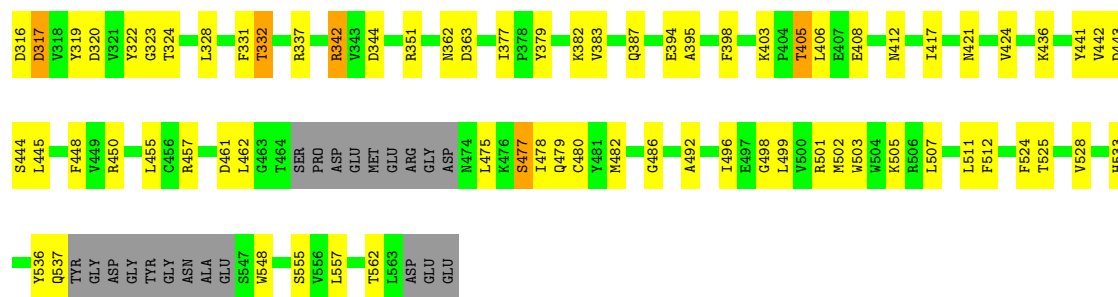
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sesquisabinene B synthase 1

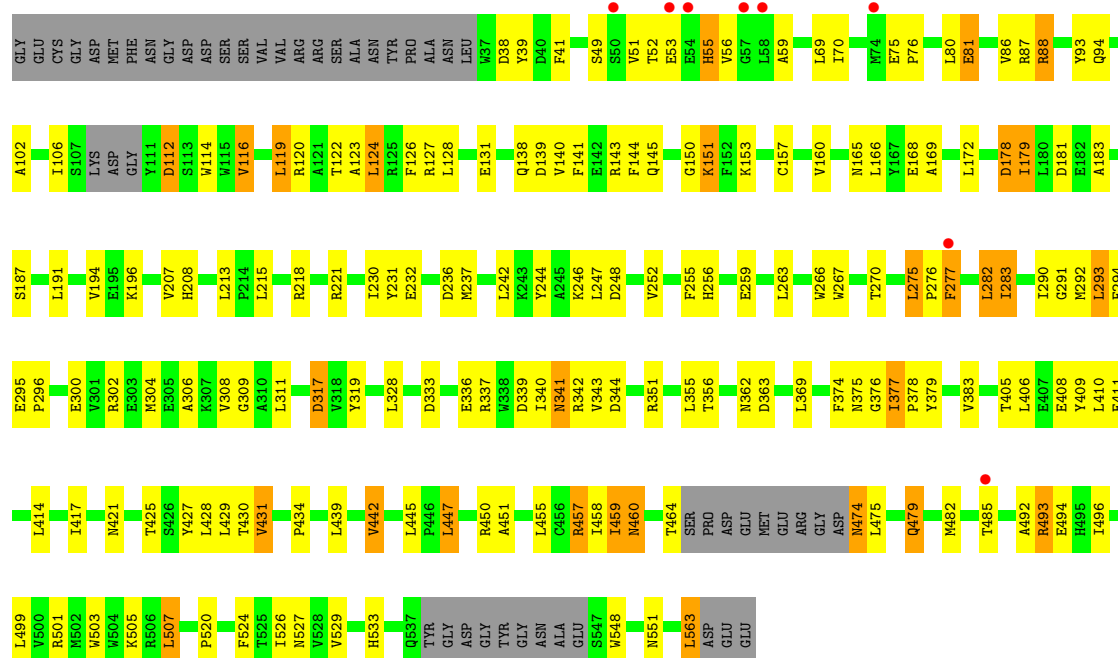


• Molecule 1: Sesquisabinene B synthase 1

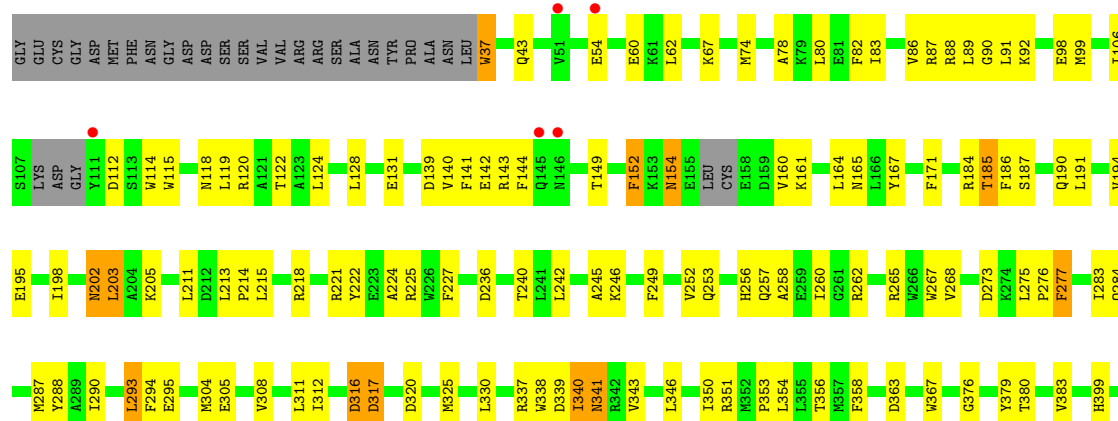




• Molecule 1: Sesquisabinene B synthase 1



• Molecule 1: Sesquisabinene B synthase 1



K403	F404	T405	E408	Y409	L410	E411	N412	I417	N421	T425	S426	Y427	L428	L429	D432	L439	D440	Y441	L445	P446	L447	L455	C456	R457	I458	I459	L462	G463	T464	SER	PRO	ASP	GLU	MET	GLU	ARG	GLY	ASP	N474	L475	K476	S477	I478	Q479	C480	Y481	M482	N483	E484	T485
G486	A492	H495	I496	L499	V500	R501	M502	W503	W504	K505	R506	L507	P516	S523	I526	N527	V528	V529	S532	H533	F534	F535	Y536	Q537	TYR	GLY	ASP	GLY	TYR	GLY	ASN	ALA	GLU	S547	W548	T549	K550	N551	Q552	G553	M554	S555	V556	L557	L558	ASP	GLU	GLU		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.88Å 82.06Å 136.83Å 99.77° 91.55° 119.78°	Depositor
Resolution (Å)	45.62 – 3.41 45.62 – 3.41	Depositor EDS
% Data completeness (in resolution range)	98.4 (45.62-3.41) 98.4 (45.62-3.41)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.219 , 0.283 0.219 , 0.283	Depositor DCC
R_{free} test set	2163 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.084 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16432	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.55	0/4232	0.69	0/5739
1	B	0.55	0/4207	0.69	0/5705
1	C	0.54	0/4210	0.72	0/5709
1	D	0.58	0/4182	0.71	0/5672
All	All	0.55	0/16831	0.70	0/22825

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4129	0	4028	100	0
1	B	4105	0	4003	110	0
1	C	4108	0	4007	198	0
1	D	4082	0	3970	161	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	16432	0	16008	567	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 17.

The worst 5 of 567 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:PHE:CD2	1:C:296:PRO:HB3	1.52	1.42
1:C:255:PHE:CE2	1:C:296:PRO:HB3	1.70	1.25
1:C:417:ILE:HD13	1:C:457:ARG:HH21	1.09	1.15
1:D:288:TYR:CE2	1:D:535:PHE:CE2	2.35	1.13
1:D:305:GLU:OE2	1:D:426:SER:HB3	1.48	1.13

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/555 (91%)	488 (97%)	15 (3%)	0	100	100
1	B	498/555 (90%)	482 (97%)	16 (3%)	0	100	100
1	C	498/555 (90%)	485 (97%)	13 (3%)	0	100	100
1	D	494/555 (89%)	478 (97%)	16 (3%)	0	100	100
All	All	1993/2220 (90%)	1933 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	441/488 (90%)	411 (93%)	30 (7%)	16	48
1	B	438/488 (90%)	409 (93%)	29 (7%)	16	49
1	C	439/488 (90%)	394 (90%)	45 (10%)	7	30
1	D	435/488 (89%)	398 (92%)	37 (8%)	10	38
All	All	1753/1952 (90%)	1612 (92%)	141 (8%)	12	41

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	205	LYS
1	D	295	GLU
1	D	411	GLU
1	B	332	THR
1	B	331	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	HIS
1	C	460	ASN
1	D	257	GLN
1	C	533	HIS
1	B	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	509/555 (91%)	-0.21	1 (0%) 95 95	23, 32, 54, 76	0
1	B	506/555 (91%)	-0.06	5 (0%) 82 81	21, 36, 57, 78	0
1	C	506/555 (91%)	0.02	8 (1%) 72 71	24, 43, 78, 102	0
1	D	504/555 (90%)	-0.12	5 (0%) 82 81	19, 38, 72, 89	0
All	All	2025/2220 (91%)	-0.09	19 (0%) 84 83	19, 37, 67, 102	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	GLN	3.2
1	C	50	SER	2.9
1	C	74	MET	2.7
1	D	146	ASN	2.6
1	C	485	THR	2.6

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](#)

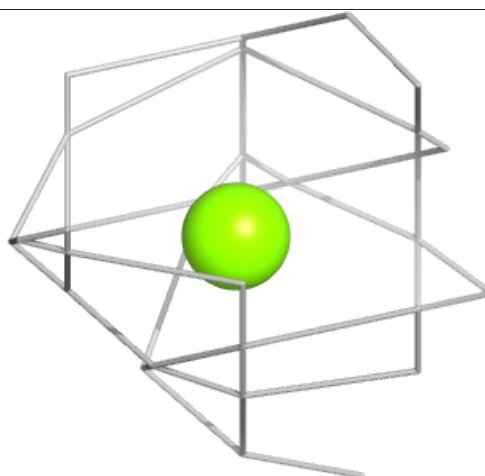
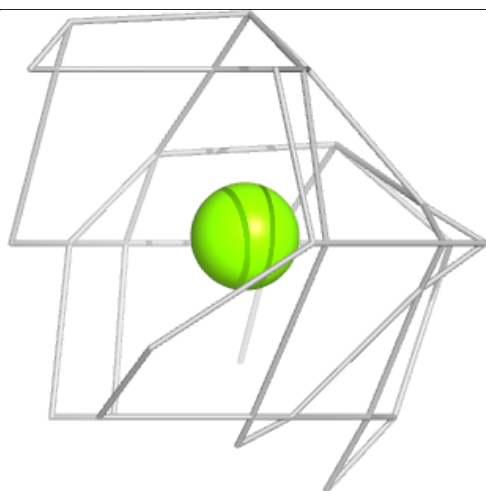
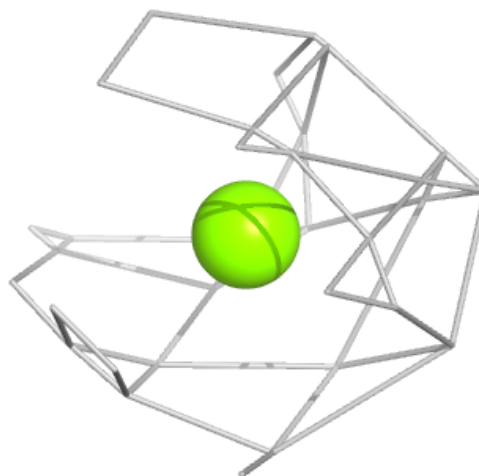
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	602	1/1	0.88	0.15	19,19,19,19	0
2	MG	B	601	1/1	0.91	0.19	25,25,25,25	0
2	MG	A	601	1/1	0.93	0.23	19,19,19,19	0
2	MG	C	601	1/1	0.95	0.15	28,28,28,28	0
2	MG	C	602	1/1	0.95	0.23	20,20,20,20	0
2	MG	A	602	1/1	0.96	0.24	18,18,18,18	0
2	MG	D	602	1/1	0.96	0.12	9,9,9,9	0
2	MG	D	601	1/1	0.98	0.20	16,16,16,16	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.

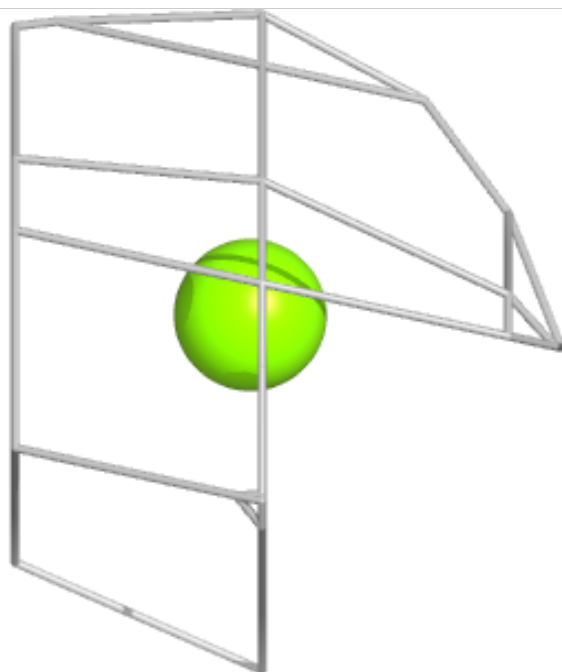
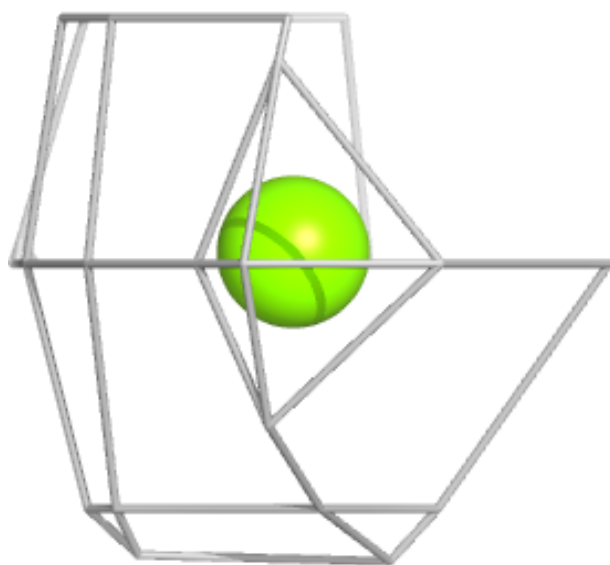
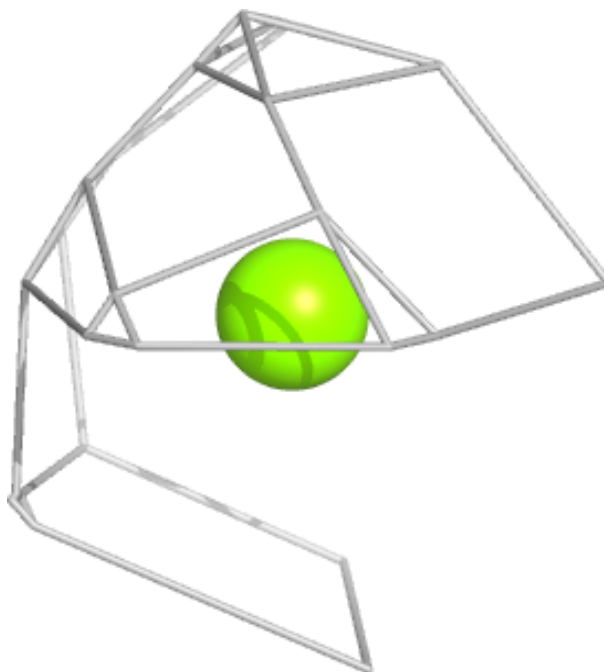
Electron density around MG B 602:

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



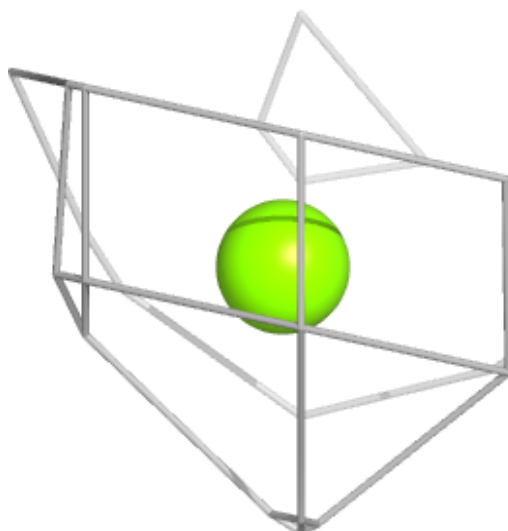
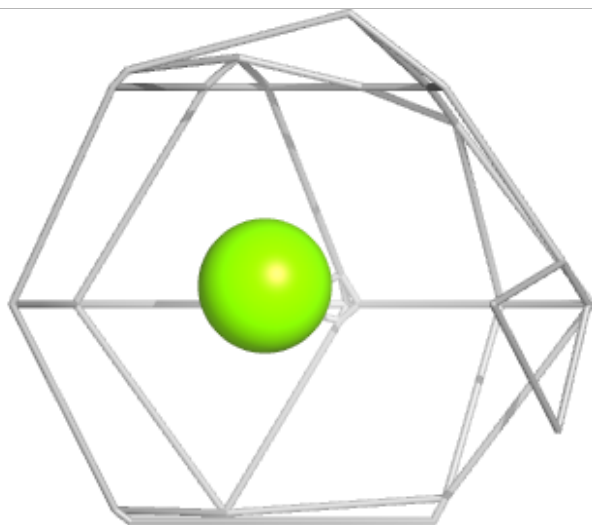
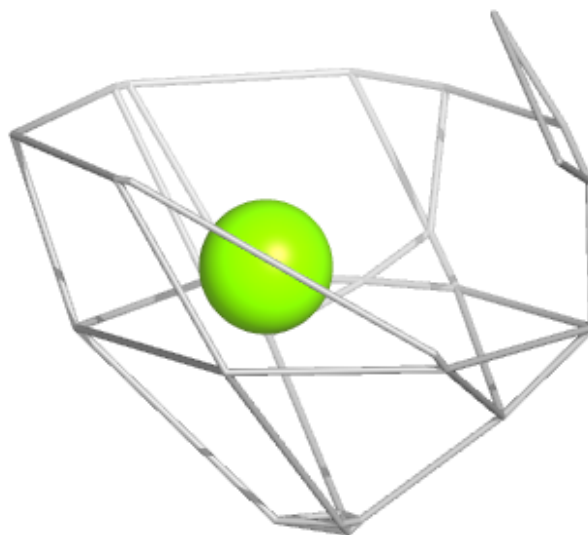
Electron density around MG B 601:

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



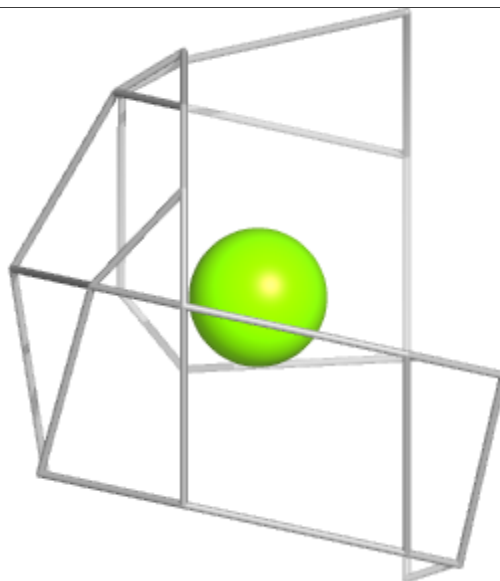
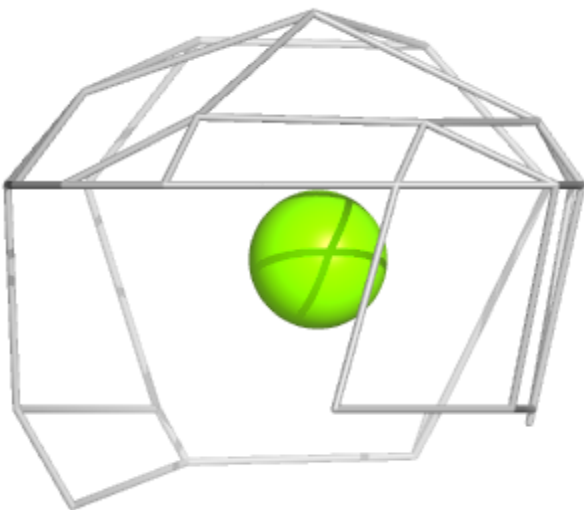
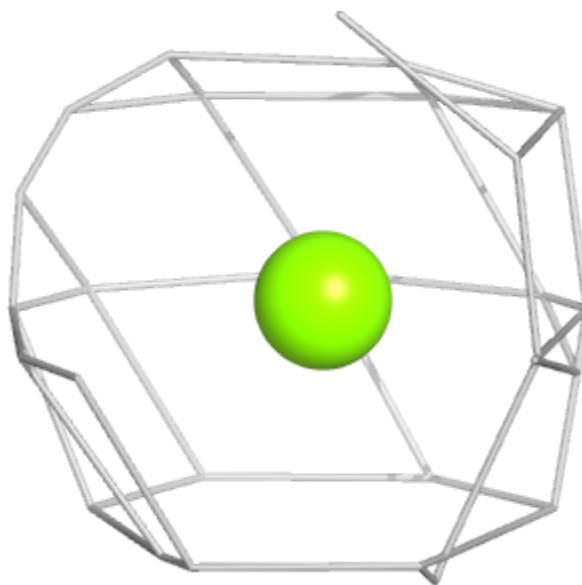
Electron density around MG A 601:

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



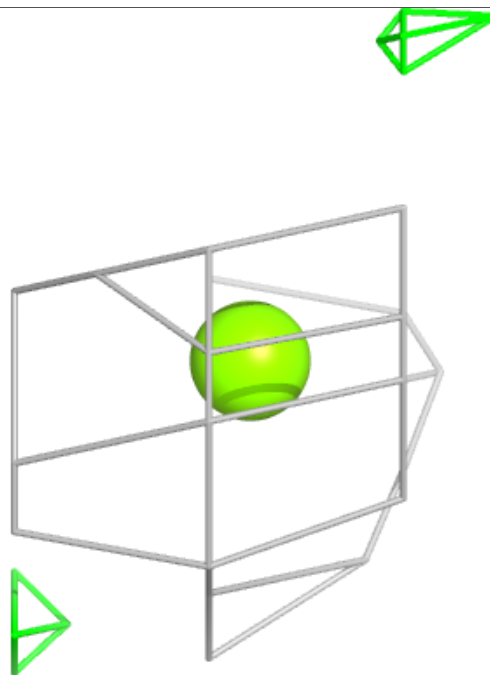
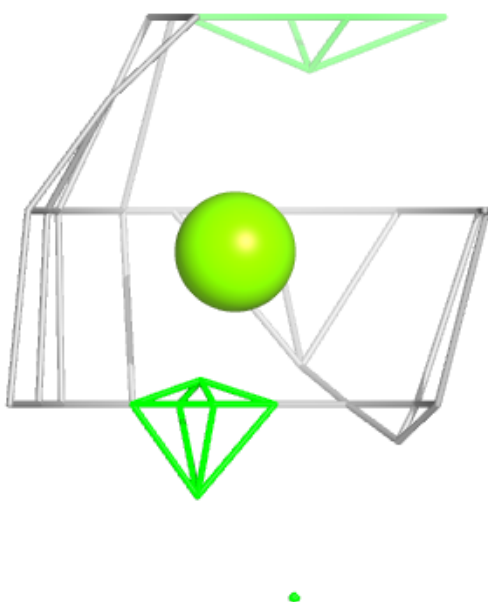
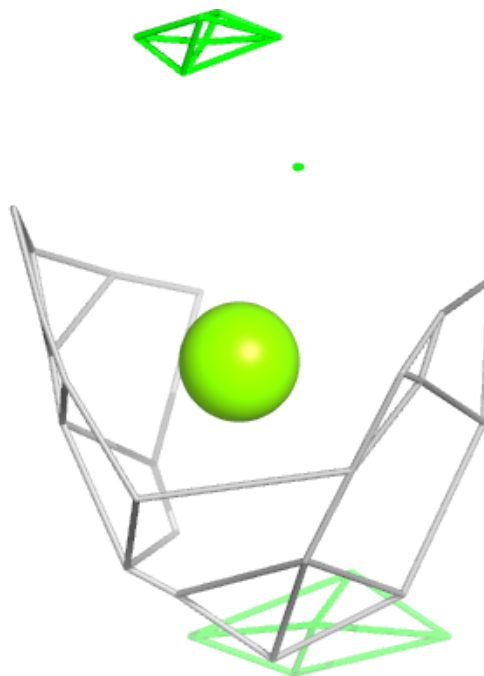
Electron density around MG C 601:

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



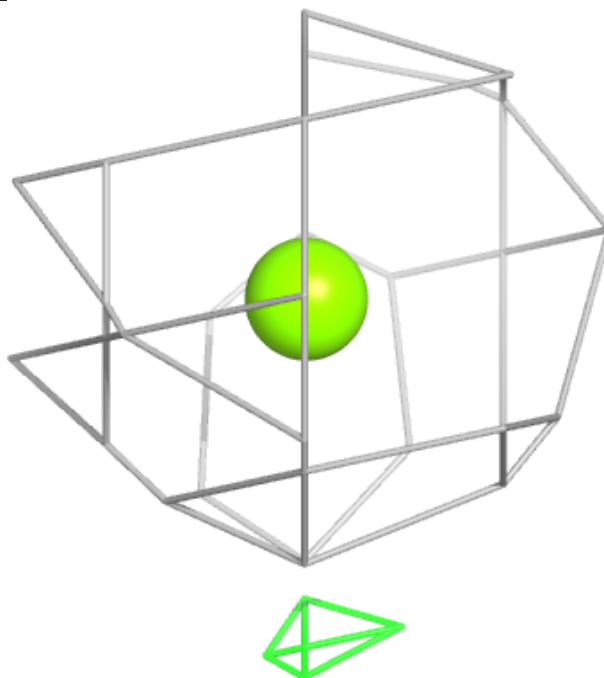
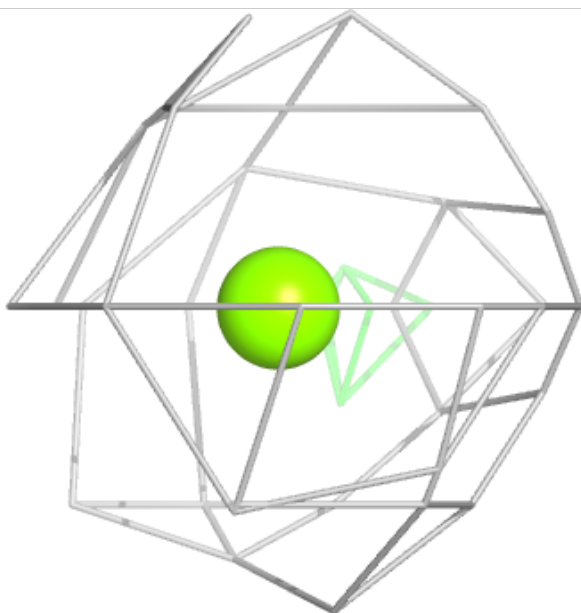
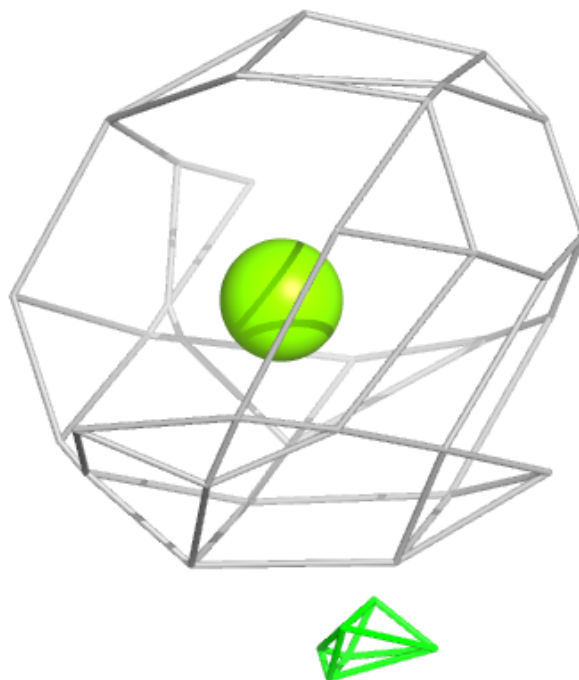
Electron density around MG C 602:

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



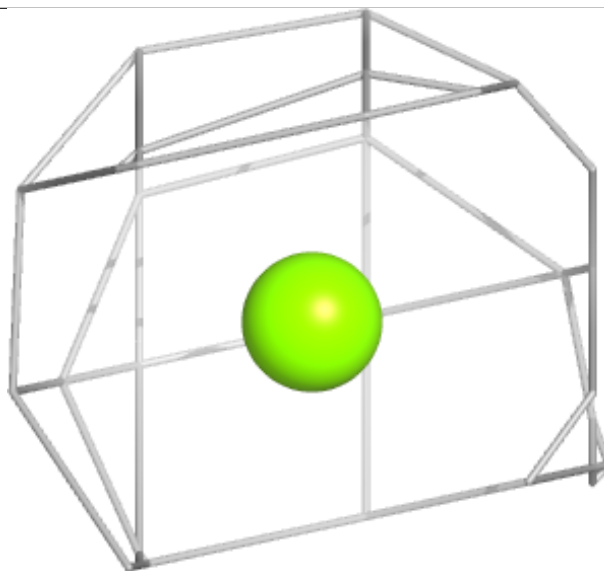
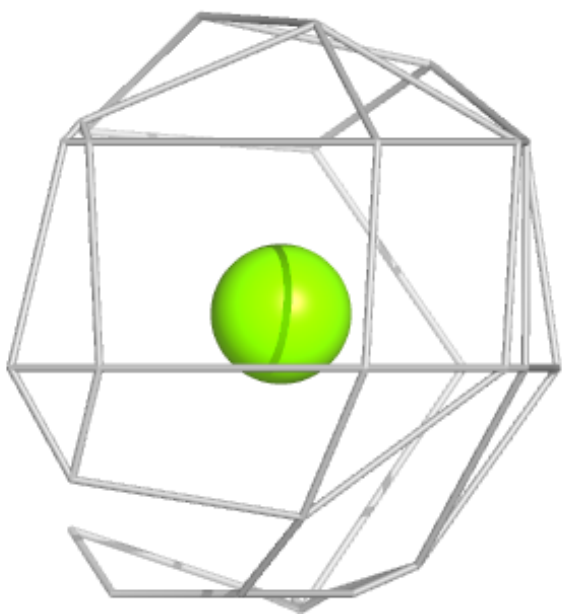
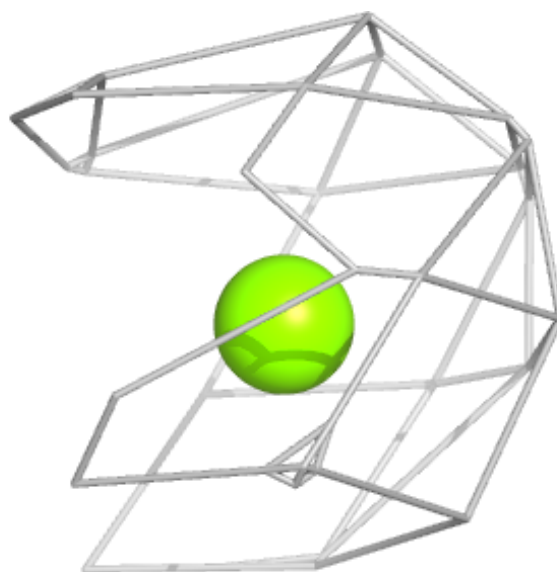
Electron density around MG A 602:

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



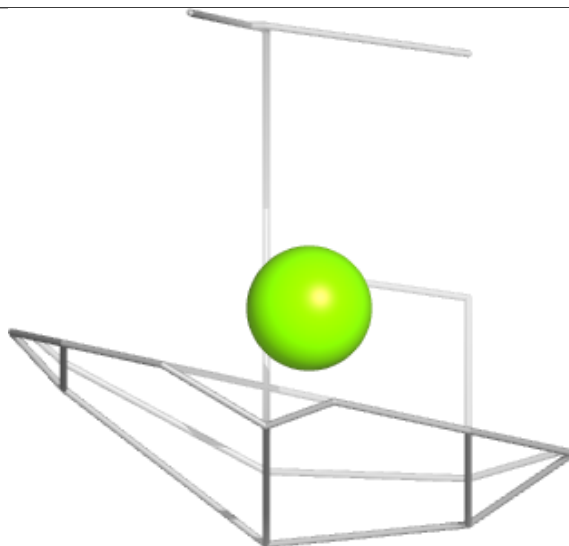
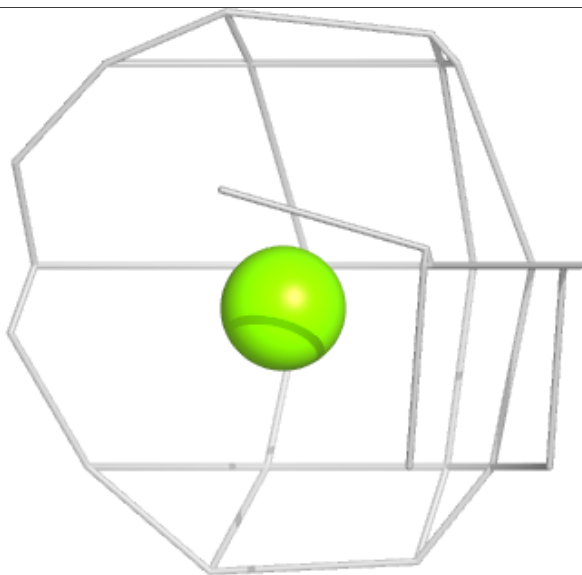
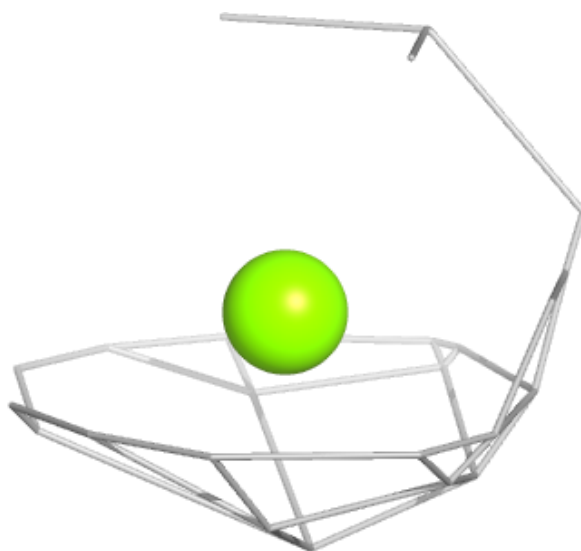
Electron density around MG D 602:

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



Electron density around MG D 601:

$2mF_o-DF_c$ (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.