



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:34 PM UTC

PDB ID : 7R97 / pdb_00007r97
Title : Crystal structure of postcleavage complex of Escherichia coli RNase III
Authors : Dharavath, S.; Shaw, G.X.; Ji, X.
Deposited on : 2021-06-28
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

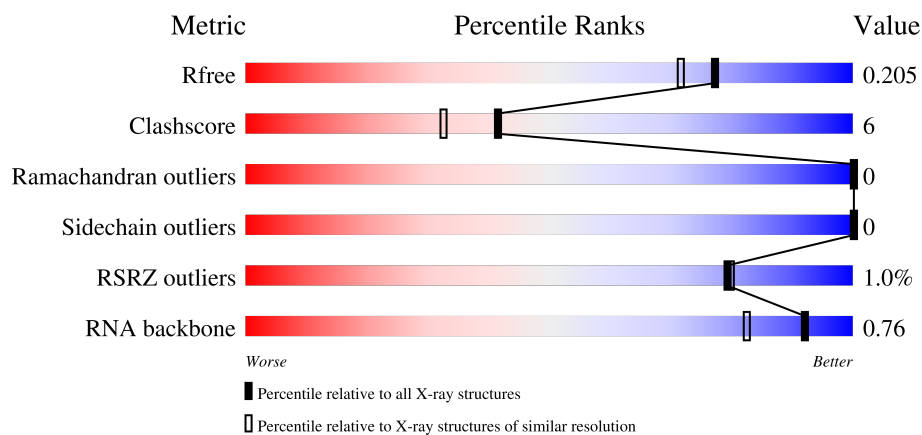
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)
RNA backbone	3983	1011 (2.20-1.40)

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	226	90% 10%
1	B	226	92% 8%
2	C	28	71% 29%
2	D	28	68% 32%

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
4	CL	A	306	-	-	X	-
5	EDO	B	308	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5402 atoms, of which 84 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 Ribonuclease 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	5	0
			1819	1137	333	344	5			
1	B	226	Total	C	N	O	S	0	2	0
			1798	1125	329	339	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ALA	GLU	engineered mutation	UNP P0A7Y0
A	65	ALA	GLU	engineered mutation	UNP P0A7Y0
A	165	ALA	GLN	engineered mutation	UNP P0A7Y0
B	38	ALA	GLU	engineered mutation	UNP P0A7Y0
B	65	ALA	GLU	engineered mutation	UNP P0A7Y0
B	165	ALA	GLN	engineered mutation	UNP P0A7Y0

- Molecule 2 is a RNA chain called RNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			598	267	106	197	28			
2	D	28	Total	C	N	O	P	0	0	0
			598	267	106	197	28			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

Continued on next page...

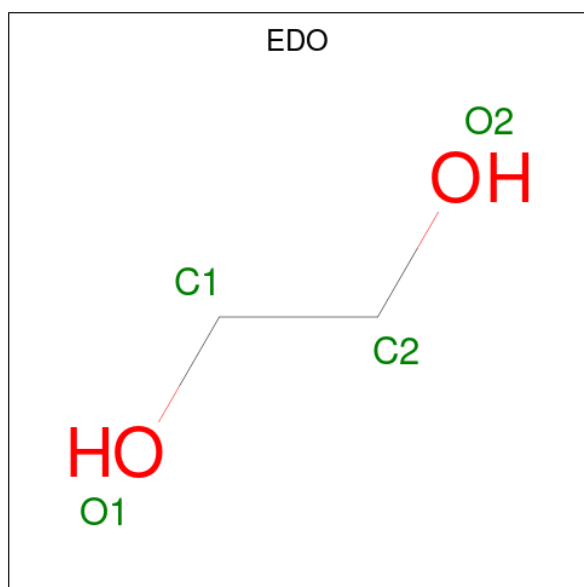
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Cl	0	0
			4	4		
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		
5	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	K	0	0
			1	1		
6	D	1	Total	K	0	0
			1	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	133	Total	O	0	0
			133	133		
8	B	112	Total	O	0	0
			112	112		
8	C	90	Total	O	0	0
			90	90		
8	D	83	Total	O	0	0
			83	83		

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.

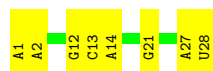
- Molecule 1: Ribonuclease 3



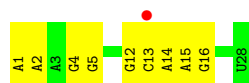
- Molecule 1: Ribonuclease 3



- Molecule 2: RNA (28-MER)



- Molecule 2: RNA (28-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.93Å 65.75Å 84.52Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	28.31 – 1.80 28.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.31-1.80) 99.2 (28.31-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.171 , 0.202 0.172 , 0.205	Depositor DCC
R_{free} test set	1000 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5402	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: K, EDO, CL, MG, TRS

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	0.41	0/1851	0.54	0/2497
1	B	0.36	0/1830	0.54	0/2468
2	C	0.48	1/668 (0.1%)	0.57	0/1037
2	D	0.49	1/668 (0.1%)	0.56	0/1037
All	All	0.41	2/5017 (0.0%)	0.55	0/7039

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	A	OP3-P	5.78	1.60	1.48
2	D	1	A	OP3-P	5.20	1.58	1.48

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	1819	0	1831	18	0
1	B	1798	0	1814	22	0
2	C	598	0	300	6	0
2	D	598	0	300	9	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	2	0
4	B	3	0	0	0	0
5	A	20	30	30	4	0
5	B	16	24	24	4	0
5	C	12	18	18	1	0
5	D	8	12	12	4	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	8	0	12	4	0
7	D	8	0	12	5	0
8	A	133	0	0	0	0
8	B	112	0	0	3	0
8	C	90	0	0	1	0
8	D	83	0	0	2	0
All	All	5318	84	4353	58	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 6.

All (58) 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:B:96:LEU:H	5:B:308:EDO:H22	1.47	0.80
1:B:134:LYS:HE3	8:B:431:HOH:O	1.81	0.78
1:B:173:THR:OG1	1:B:193:GLN:HB3	1.84	0.76
1:A:154:LYS:HE2	8:D:264:HOH:O	1.87	0.73
1:B:154:LYS:HE2	8:B:499:HOH:O	1.88	0.73
1:A:1:MET:HE1	1:A:93:CYS:O	1.90	0.71
7:C:103:TRS:H21	8:C:231:HOH:O	1.92	0.68
2:C:21:G:OP1	5:C:106:EDO:H11	1.96	0.66
1:B:96:LEU:N	5:B:308:EDO:H22	2.12	0.64
1:A:143:ARG:HG3	4:A:306:CL:CL	2.34	0.64
1:B:101:LEU:HD21	5:B:308:EDO:H11	1.80	0.64
1:B:201:VAL:HG22	1:B:222:LYS:NZ	2.13	0.63
1:B:8:ARG:NH1	1:B:11:ARG:HH21	1.97	0.62
1:B:19:HIS:HB3	1:B:21:GLU:OE2	2.00	0.61
1:A:139:TRP:HA	5:A:310:EDO:H12	1.85	0.58
2:D:12:G:N7	7:D:103:TRS:H22	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ALA:CB	1:B:109[B]:GLU:HG3	2.34	0.57
2:C:12:G:N7	7:C:103:TRS:H12	2.18	0.57
1:A:2:ASN:O	1:A:5[A]:VAL:HG22	2.05	0.56
2:D:12:G:C8	7:D:103:TRS:H12	2.41	0.56
2:D:4:G:O6	5:D:105:EDO:H22	2.06	0.55
1:B:201:VAL:HG22	1:B:222:LYS:HZ2	1.71	0.55
2:D:12:G:N7	7:D:103:TRS:H12	2.23	0.54
2:D:12:G:N7	7:D:103:TRS:H31	2.23	0.53
5:D:104:EDO:H11	5:D:105:EDO:O2	2.08	0.53
7:D:103:TRS:H21	8:D:224:HOH:O	2.09	0.52
1:B:82:ALA:HB2	1:B:109[B]:GLU:HG3	1.92	0.52
1:B:96:LEU:H	5:B:308:EDO:C2	2.20	0.52
1:B:21:GLU:H	1:B:21:GLU:CD	2.17	0.51
1:B:8:ARG:HD2	1:B:11:ARG:HH21	1.77	0.50
2:C:12:G:N7	7:C:103:TRS:H22	2.25	0.50
1:B:8:ARG:HD2	1:B:11:ARG:NH2	2.26	0.49
1:A:142:THR:O	1:A:146[B]:GLU:HG2	2.13	0.49
2:D:15:A:H2'	2:D:16:G:O4'	2.12	0.49
2:D:5:G:N7	5:D:104:EDO:H12	2.27	0.49
1:B:8:ARG:HH11	1:B:11:ARG:HH21	1.59	0.49
1:B:182:GLU:O	1:B:186:GLN:HG3	2.15	0.47
2:C:12:G:C8	7:C:103:TRS:H12	2.50	0.47
1:A:12:LYS:HE2	5:A:307:EDO:O2	2.15	0.46
1:A:164:LEU:HD12	1:A:172:PRO:HD3	1.97	0.46
1:A:77:ARG:HH21	5:A:311:EDO:H11	1.81	0.45
1:B:173:THR:HG1	1:B:193:GLN:HB3	1.81	0.44
1:A:93:CYS:SG	5:A:307:EDO:H22	2.58	0.43
1:B:12:LYS:HE3	1:B:12:LYS:HB3	1.68	0.43
2:D:5:G:N7	5:D:104:EDO:C1	2.82	0.43
1:A:148:SER:OG	1:A:152:LYS:HD2	2.19	0.42
1:A:182:GLU:O	1:A:186:GLN:HG3	2.20	0.42
1:A:142:THR:OG1	4:A:306:CL:CL	2.69	0.41
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.92	0.41
1:A:208:ARG:HH11	1:A:208:ARG:HD3	1.74	0.41
1:A:90:LEU:HD21	1:A:119:LEU:HD11	2.03	0.41
1:A:164:LEU:CD1	1:A:172:PRO:HD3	2.50	0.41
2:C:13:C:H2'	2:C:14:A:O4'	2.21	0.41
2:D:13:C:C5	2:D:14:A:C4	3.08	0.41
1:A:222:LYS:HA	1:A:222:LYS:HE2	2.02	0.41
1:A:6:ILE:HG23	1:A:23:LEU:HD21	2.03	0.41
1:B:193:GLN:NE2	8:B:409:HOH:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:A:O2'	2:C:28:U:H5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/226 (101%)	227 (99%)	2 (1%)	0	100	100
1	B	226/226 (100%)	223 (99%)	3 (1%)	0	100	100
All	All	455/452 (101%)	450 (99%)	5 (1%)	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	196/191 (103%)	196 (100%)	0	100	100
1	B	193/191 (101%)	193 (100%)	0	100	100
All	All	389/382 (102%)	389 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	B	79	ASN
1	B	186	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	27/28 (96%)	1 (3%)	0
2	D	27/28 (96%)	1 (3%)	0
All	All	54/56 (96%)	2 (3%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	A
2	D	2	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 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
5	EDO	D	104	-	3,3,3	0.43	0	2,2,2	0.16	0
7	TRS	C	103	-	7,7,7	0.41	0	9,9,9	0.53	0
5	EDO	A	310	-	3,3,3	0.39	0	2,2,2	0.58	0
5	EDO	B	306	-	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	A	309	-	3,3,3	0.42	0	2,2,2	0.32	0
7	TRS	D	103	-	7,7,7	0.40	0	9,9,9	0.67	0
5	EDO	C	105	-	3,3,3	0.43	0	2,2,2	0.27	0
5	EDO	B	309	-	3,3,3	0.45	0	2,2,2	0.24	0
5	EDO	C	106	-	3,3,3	0.44	0	2,2,2	0.30	0
5	EDO	A	308	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	A	311	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	307	-	3,3,3	0.49	0	2,2,2	0.19	0
5	EDO	C	104	-	3,3,3	0.43	0	2,2,2	0.45	0
5	EDO	D	105	6	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	B	307	-	3,3,3	0.51	0	2,2,2	0.11	0
5	EDO	B	308	-	3,3,3	0.48	0	2,2,2	0.28	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
5	EDO	D	104	-	-	1/1/1/1	-
7	TRS	C	103	-	-	3/9/9/9	-
5	EDO	A	310	-	-	0/1/1/1	-
5	EDO	B	306	-	-	1/1/1/1	-
5	EDO	A	309	-	-	1/1/1/1	-
7	TRS	D	103	-	-	3/9/9/9	-
5	EDO	C	105	-	-	0/1/1/1	-
5	EDO	B	309	-	-	1/1/1/1	-
5	EDO	C	106	-	-	0/1/1/1	-
5	EDO	A	308	-	-	0/1/1/1	-
5	EDO	A	311	-	-	1/1/1/1	-
5	EDO	A	307	-	-	0/1/1/1	-
5	EDO	C	104	-	-	0/1/1/1	-
5	EDO	D	105	6	-	1/1/1/1	-
5	EDO	B	307	-	-	0/1/1/1	-
5	EDO	B	308	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	103	TRS	N-C-C3-O3
7	C	103	TRS	C1-C-C3-O3
5	D	104	EDO	O1-C1-C2-O2
7	D	103	TRS	N-C-C2-O2
7	D	103	TRS	C1-C-C2-O2
7	D	103	TRS	C3-C-C2-O2
5	B	308	EDO	O1-C1-C2-O2
5	A	311	EDO	O1-C1-C2-O2
5	B	306	EDO	O1-C1-C2-O2
5	A	309	EDO	O1-C1-C2-O2
5	D	105	EDO	O1-C1-C2-O2
7	C	103	TRS	C2-C-C3-O3
5	B	309	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	104	EDO	3	0
7	C	103	TRS	4	0
5	A	310	EDO	1	0
7	D	103	TRS	5	0
5	C	106	EDO	1	0
5	A	311	EDO	1	0
5	A	307	EDO	2	0
5	D	105	EDO	2	0
5	B	308	EDO	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/226 (100%)	-0.12	2 (0%) 81 81	7, 23, 40, 51	5 (2%)
1	B	226/226 (100%)	0.02	2 (0%) 81 81	8, 26, 43, 59	2 (0%)
2	C	28/28 (100%)	-0.26	0 100 100	19, 23, 55, 67	0
2	D	28/28 (100%)	-0.27	1 (3%) 46 46	19, 21, 58, 70	0
All	All	508/508 (100%)	-0.07	5 (0%) 79 80	7, 24, 43, 70	7 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	LEU	2.9
1	A	1	MET	2.8
1	A	225	LEU	2.1
1	B	173	THR	2.0
2	D	13	C	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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,

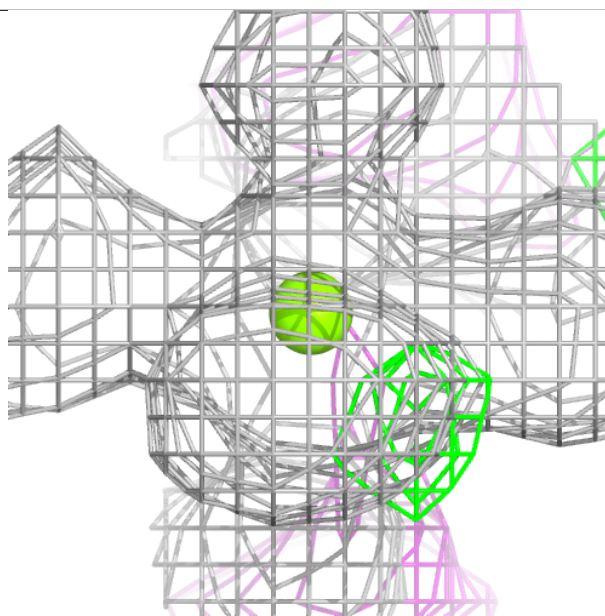
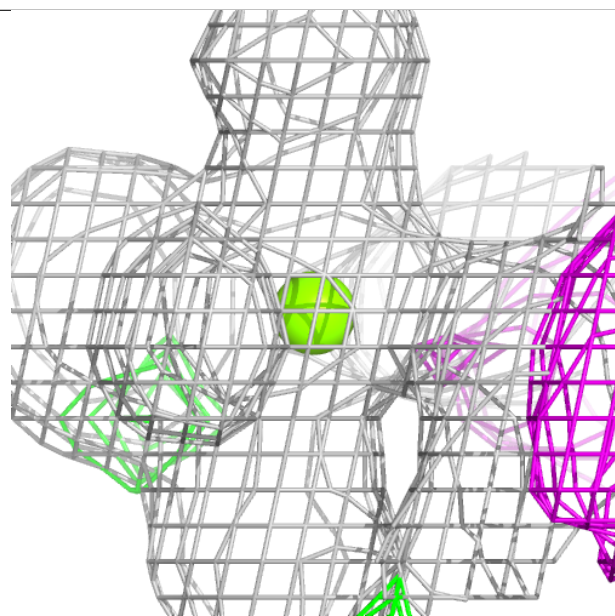
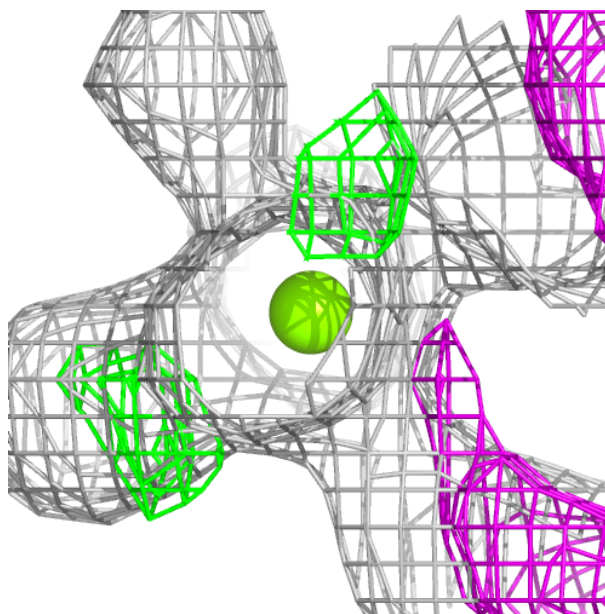
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TRS	C	103	8/8	0.73	0.17	45,52,54,66	0
7	TRS	D	103	8/8	0.77	0.15	42,45,55,57	0
5	EDO	A	310	4/4	0.82	0.12	33,41,50,58	0
5	EDO	B	309	4/4	0.83	0.18	30,39,49,52	0
5	EDO	A	307	4/4	0.84	0.12	41,54,60,67	0
5	EDO	A	309	4/4	0.85	0.11	38,50,63,65	0
5	EDO	B	308	4/4	0.86	0.12	31,38,60,63	0
5	EDO	D	105	4/4	0.86	0.16	27,36,60,60	0
5	EDO	C	106	4/4	0.88	0.14	34,43,51,61	0
5	EDO	A	311	4/4	0.88	0.13	29,48,51,57	0
5	EDO	B	306	4/4	0.89	0.14	36,43,44,48	0
5	EDO	C	105	4/4	0.89	0.11	30,36,43,43	0
5	EDO	D	104	4/4	0.90	0.12	25,33,44,53	0
3	MG	D	101	1/1	0.92	0.10	29,29,29,29	0
4	CL	A	303	1/1	0.93	0.08	55,55,55,55	0
5	EDO	B	307	4/4	0.93	0.10	29,35,44,44	0
5	EDO	A	308	4/4	0.94	0.08	27,33,47,47	0
5	EDO	C	104	4/4	0.94	0.11	22,27,31,35	0
3	MG	A	301	1/1	0.95	0.09	20,20,20,20	0
3	MG	C	101	1/1	0.95	0.05	28,28,28,28	0
3	MG	B	301	1/1	0.96	0.13	22,22,22,22	0
4	CL	A	306	1/1	0.97	0.07	29,29,29,29	1
4	CL	B	305	1/1	0.97	0.05	35,35,35,35	0
4	CL	B	304	1/1	0.98	0.14	39,39,39,39	0
3	MG	B	302	1/1	0.98	0.06	20,20,20,20	0
3	MG	A	302	1/1	0.99	0.05	18,18,18,18	0
4	CL	B	303	1/1	0.99	0.02	28,28,28,28	0
6	K	C	102	1/1	0.99	0.04	26,26,26,26	0
6	K	D	102	1/1	0.99	0.07	24,24,24,24	0
4	CL	A	304	1/1	0.99	0.03	32,32,32,32	0
4	CL	A	305	1/1	0.99	0.03	31,31,31,31	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.

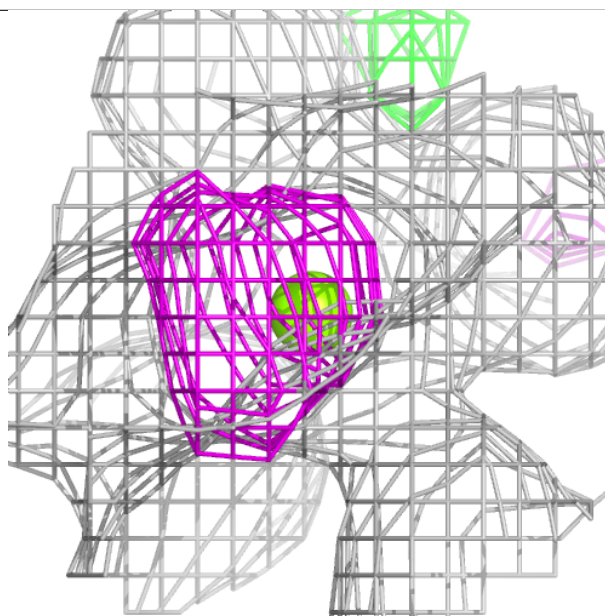
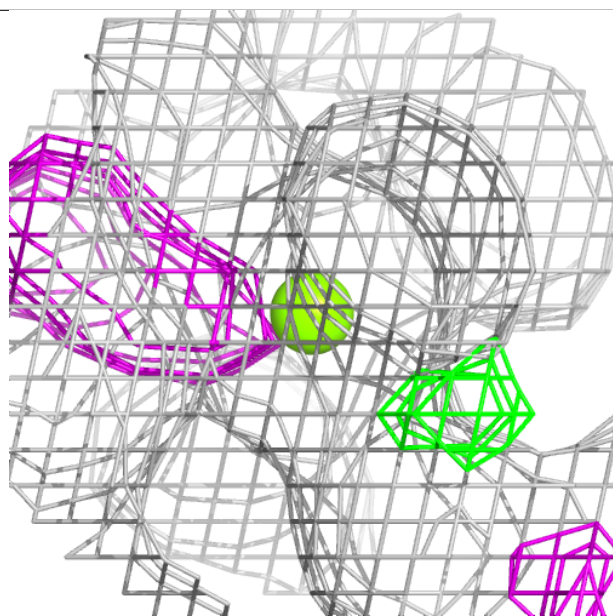
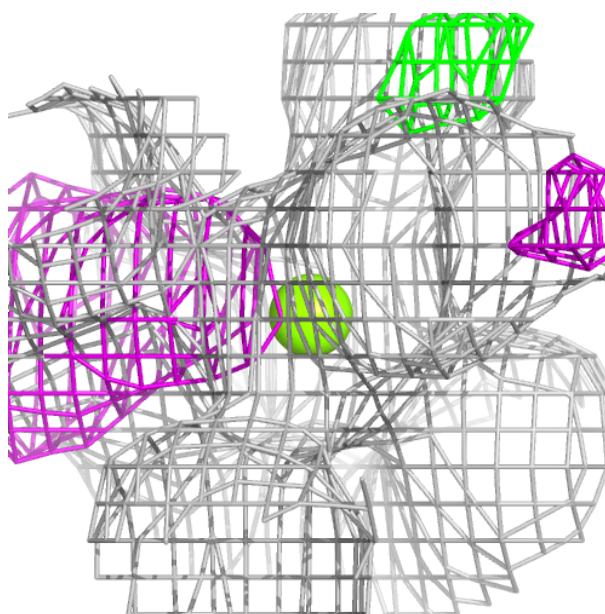
Electron density around MG D 101:

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



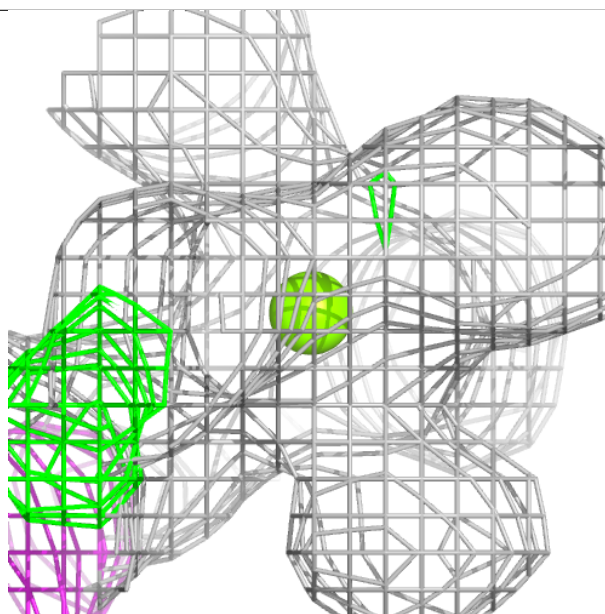
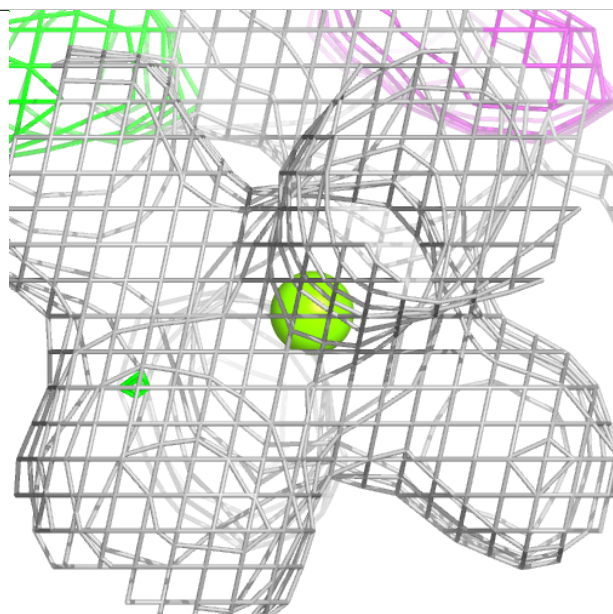
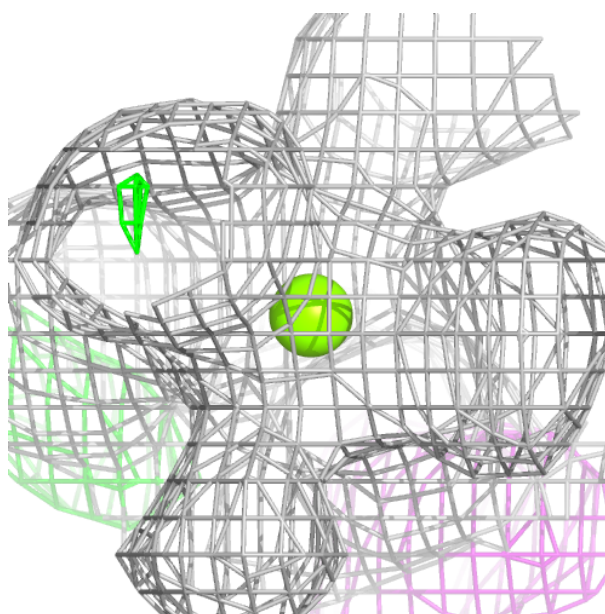
Electron density around MG A 301:

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



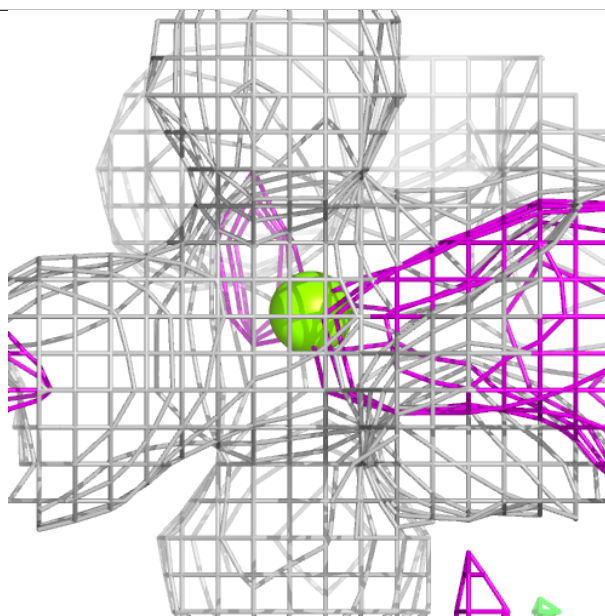
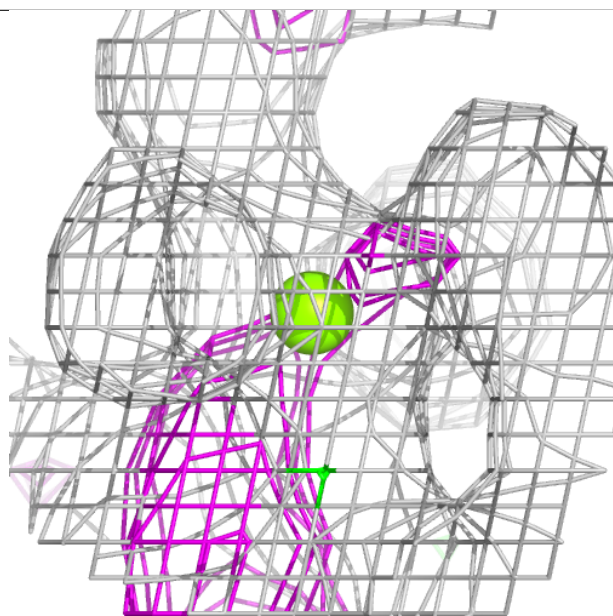
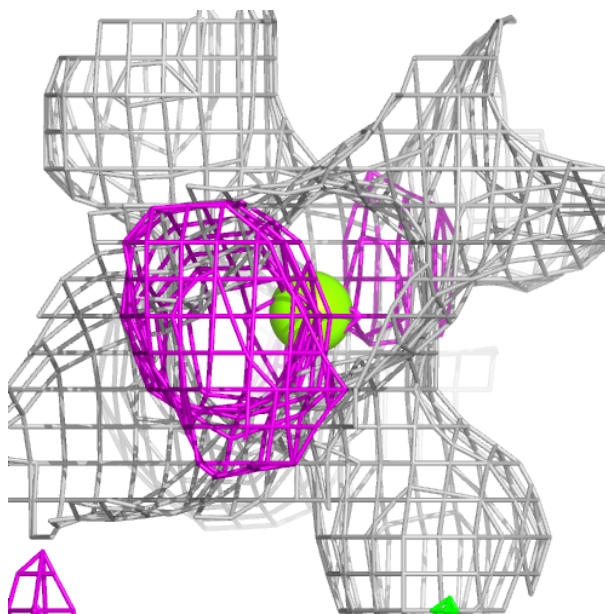
Electron density around MG C 101:

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



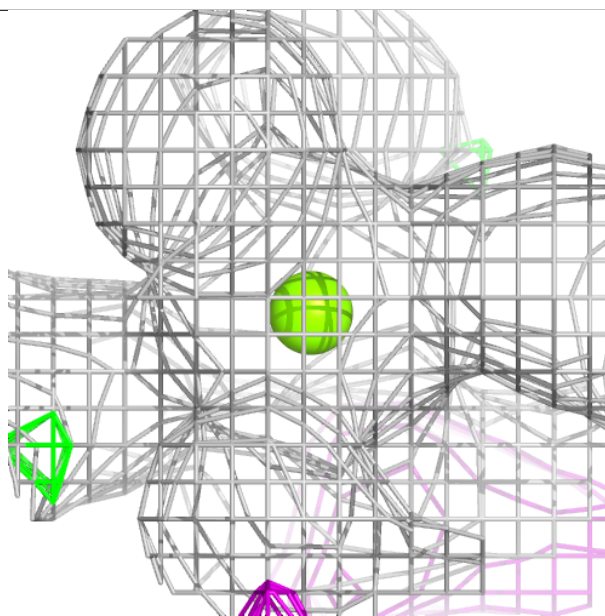
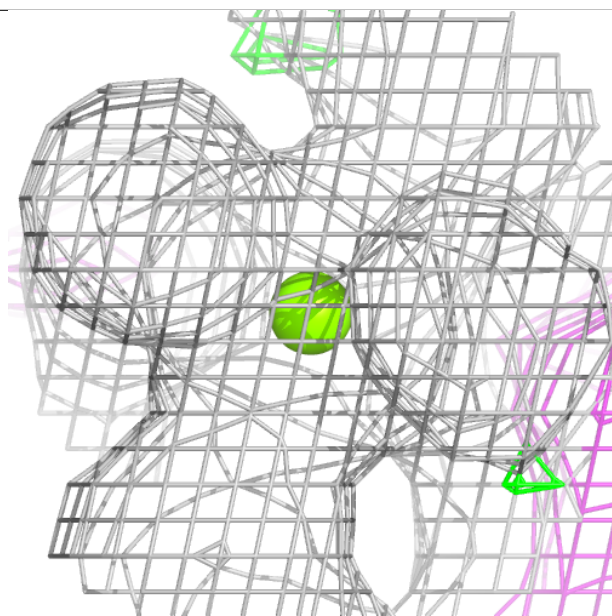
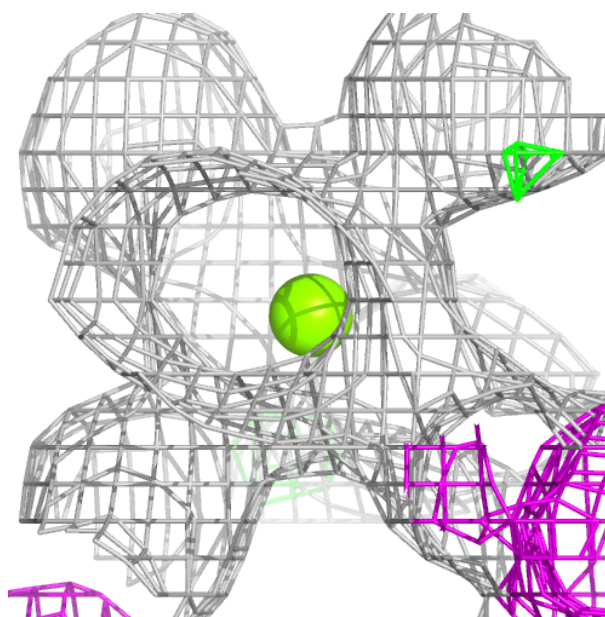
Electron density around MG B 301:

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



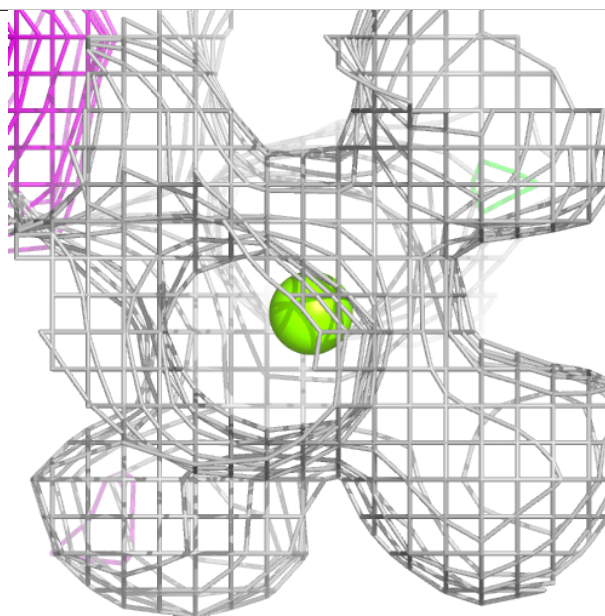
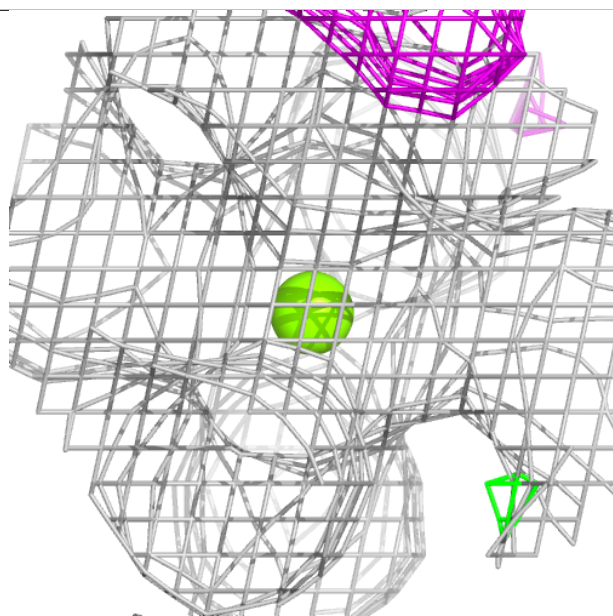
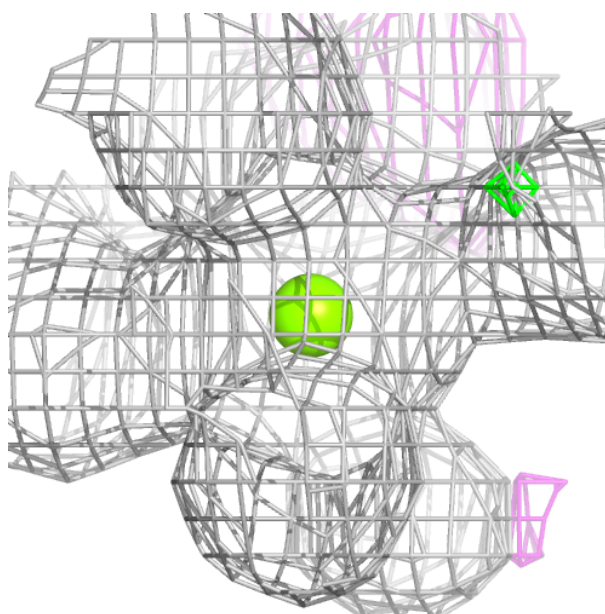
Electron density around MG B 302:

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



Electron density around MG A 302:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.