



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2025 – 07:10 pm BST

PDB ID : 9GTK / pdb_00009gtk
Title : KRAS in complex with DARPin 784_F5
Authors : Kapp, J.N.; Verdurmen, W.; Schaefer, J.V.; Kopra, K.; Nagy-Davidescu, G.;
Richard, E.; Nokin, M.J.; Ernst, P.; Tamaskovic, R.; Schwill, M.; Degen, R.;
Scholl, C.; Santamaria, D.; Plueckthun, A.
Deposited on : 2024-09-18
Resolution : 2.00 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 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

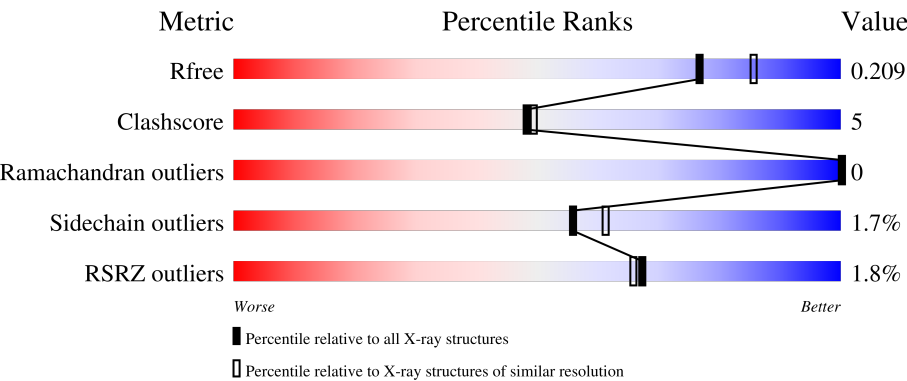
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	195	<div><div>0%</div><div>82%7%10%</div></div>
1	C	195	<div><div>2%</div><div>82%8%10%</div></div>
1	D	195	<div><div>2%</div><div>75%11%11%</div></div>
2	B	170	<div><div>3%</div><div>85%9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	170	<div> <div>%</div> <div> </div> <div>89% 6% . .</div> </div>
2	I	170	<div> <div>%</div> <div> </div> <div>85% 9% . 6%</div> </div>

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
3	EDO	B	201	-	-	X	-
7	PGE	C	212	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8908 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	6	0
			1455	907	252	287	9			
1	C	175	Total	C	N	O	S	0	7	0
			1457	908	251	288	10			
1	D	173	Total	C	N	O	S	0	5	0
			1423	886	244	284	9			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	expression tag	UNP P01116
A	188	SER	-	expression tag	UNP P01116
A	189	ALA	-	expression tag	UNP P01116
A	190	GLU	-	expression tag	UNP P01116
A	191	ASN	-	expression tag	UNP P01116
A	192	LEU	-	expression tag	UNP P01116
A	193	TYR	-	expression tag	UNP P01116
A	194	PHE	-	expression tag	UNP P01116
A	195	GLN	-	expression tag	UNP P01116
C	187	GLY	-	expression tag	UNP P01116
C	188	SER	-	expression tag	UNP P01116
C	189	ALA	-	expression tag	UNP P01116
C	190	GLU	-	expression tag	UNP P01116
C	191	ASN	-	expression tag	UNP P01116
C	192	LEU	-	expression tag	UNP P01116
C	193	TYR	-	expression tag	UNP P01116
C	194	PHE	-	expression tag	UNP P01116
C	195	GLN	-	expression tag	UNP P01116
D	187	GLY	-	expression tag	UNP P01116
D	188	SER	-	expression tag	UNP P01116
D	189	ALA	-	expression tag	UNP P01116
D	190	GLU	-	expression tag	UNP P01116
D	191	ASN	-	expression tag	UNP P01116

Continued on next page...

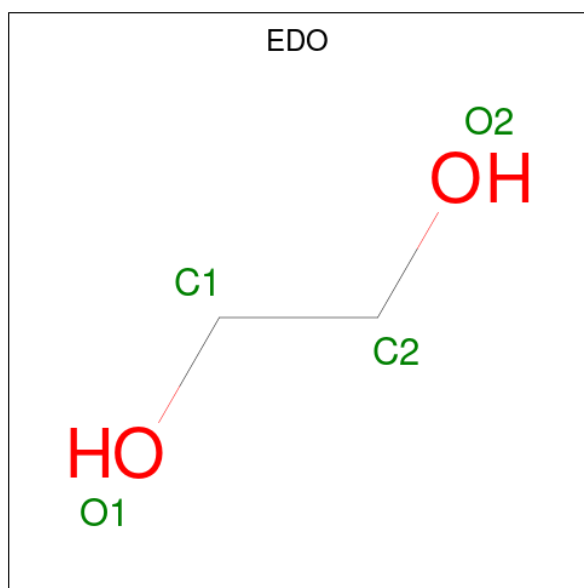
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	192	LEU	-	expression tag	UNP P01116
D	193	TYR	-	expression tag	UNP P01116
D	194	PHE	-	expression tag	UNP P01116
D	195	GLN	-	expression tag	UNP P01116

- Molecule 2 is a protein called DARPin 784_F5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	5	0
			1272	797	225	246	4			
2	H	163	Total	C	N	O	S	0	1	0
			1234	774	219	239	2			
2	I	160	Total	C	N	O	S	0	2	0
			1215	763	215	235	2			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0

Continued on next page...

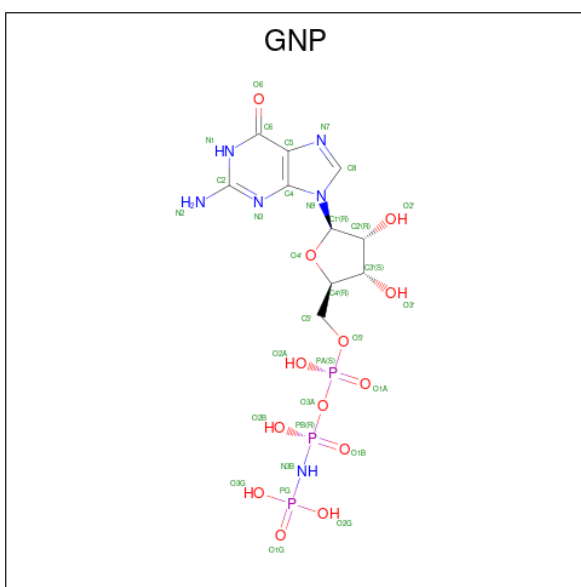
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

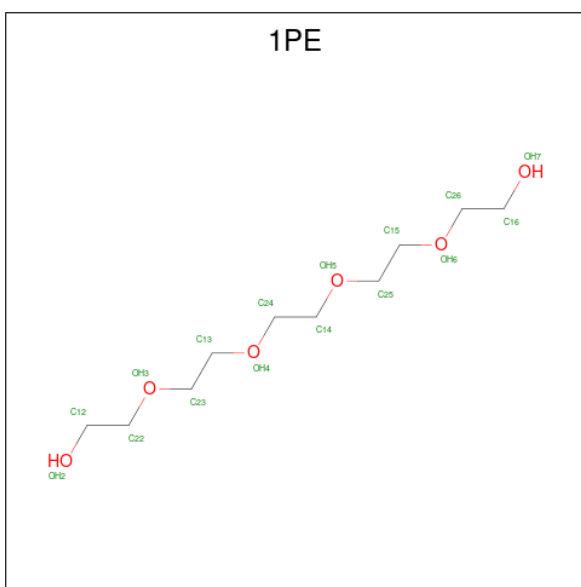
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



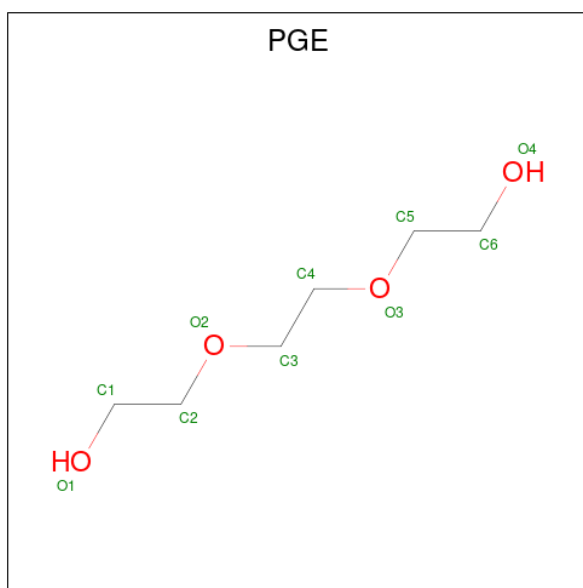
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
5	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
5	D	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



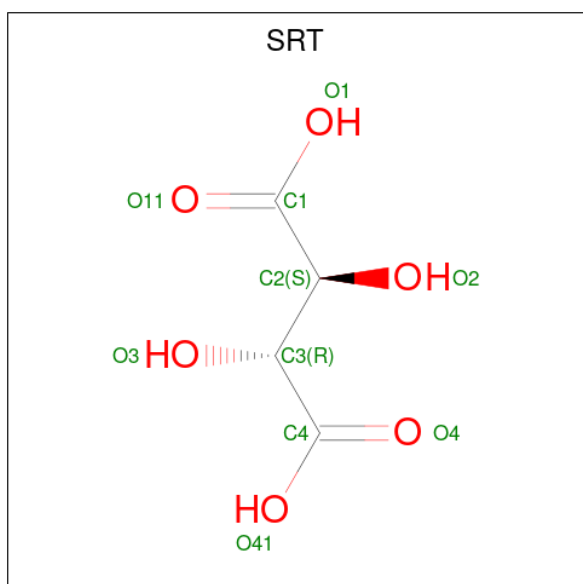
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	4	6		

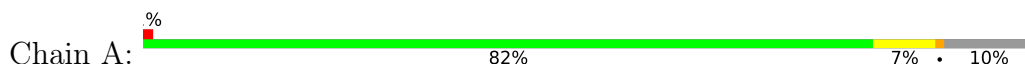
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	133	Total	O	0	0
			133	133		
9	B	133	Total	O	0	0
			133	133		
9	C	102	Total	O	0	0
			102	102		
9	D	109	Total	O	0	0
			109	109		
9	H	52	Total	O	0	0
			52	52		
9	I	35	Total	O	0	0
			35	35		

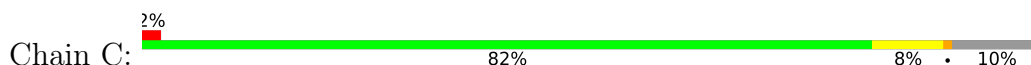
3 Residue-property plots

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

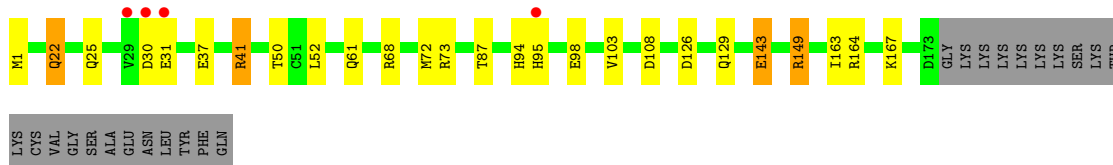
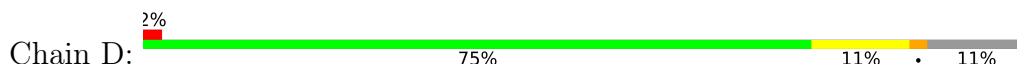
- Molecule 1: Isoform 2B of GTPase KRas



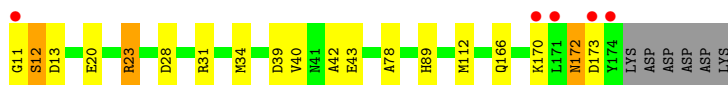
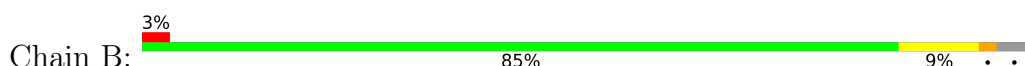
- Molecule 1: Isoform 2B of GTPase KRas



- Molecule 1: Isoform 2B of GTPase KRas



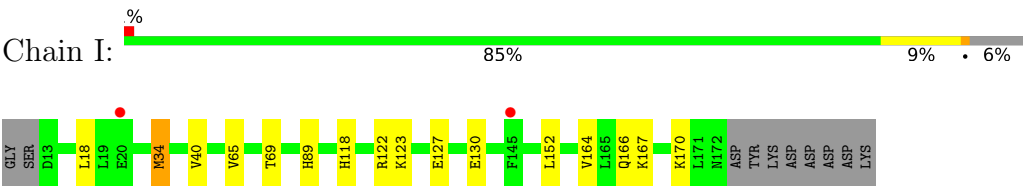
- Molecule 2: DARPin 784_F5



- Molecule 2: DARPin 784_F5



● Molecule 2: DARPin 784_F5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.32Å 152.83Å 149.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.00 47.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.28-2.00) 100.0 (47.28-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.171 , 0.201 0.182 , 0.209	Depositor DCC
R_{free} test set	4544 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8908	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, SRT, EDO, PGE, GNP, 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	0.72	0/1477	1.11	3/1985 (0.2%)
1	C	0.61	0/1479	1.05	1/1989 (0.1%)
1	D	0.65	0/1445	1.09	7/1946 (0.4%)
2	B	0.74	1/1291 (0.1%)	1.10	4/1748 (0.2%)
2	H	0.55	0/1253	1.03	2/1700 (0.1%)
2	I	0.53	0/1233	1.02	0/1672
All	All	0.64	1/8178 (0.0%)	1.07	17/11040 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	23	ARG	NE-CZ	-6.07	1.26	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CB-CA-C	7.21	121.59	109.84
1	D	108	ASP	CA-CB-CG	7.20	119.80	112.60
1	D	41	ARG	CB-CG-CD	-6.89	95.44	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	GLN	N-CA-CB	-6.53	100.52	110.12
2	H	13	ASP	CA-CB-CG	6.53	119.12	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ARG	Sidechain
1	C	123	ARG	Sidechain
1	D	164	ARG	Sidechain
1	D	41	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1455	0	1432	12	0
1	C	1457	0	1427	14	0
1	D	1423	0	1388	20	0
2	B	1272	0	1271	18	0
2	H	1234	0	1235	12	0
2	I	1215	0	1222	10	0
3	A	44	0	66	7	0
3	B	28	0	42	5	0
3	C	36	0	54	3	0
3	D	8	0	12	2	0
3	I	4	0	6	0	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
5	A	32	0	13	0	0
5	C	32	0	13	2	0
5	D	32	0	13	1	0
6	B	16	0	22	3	0
7	B	10	0	14	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	10	0	14	6	0
7	D	10	0	14	1	0
7	H	10	0	14	2	0
8	C	10	0	4	3	0
9	A	133	0	0	8	0
9	B	133	0	0	2	0
9	C	102	0	0	3	0
9	D	109	0	0	2	0
9	H	52	0	0	4	0
9	I	35	0	0	0	0
All	All	8908	0	8276	90	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 5.

The worst 5 of 90 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:204:EDO:H12	2:B:23:ARG:HD3	1.43	0.98
1:D:1:MET:HE3	1:D:50:THR:HG22	1.44	0.97
1:A:95[B]:HIS:CE1	9:A:302:HOH:O	2.20	0.95
1:C:150:GLN:HA	7:C:212:PGE:H3	1.52	0.91
1:C:97[B]:ARG:NH1	8:C:213:SRT:O2	2.12	0.82

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	180/195 (92%)	176 (98%)	4 (2%)	0	100	100
1	C	180/195 (92%)	176 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	176/195 (90%)	173 (98%)	3 (2%)	0	100	100
2	B	167/170 (98%)	165 (99%)	2 (1%)	0	100	100
2	H	162/170 (95%)	160 (99%)	2 (1%)	0	100	100
2	I	160/170 (94%)	160 (100%)	0	0	100	100
All	All	1025/1095 (94%)	1010 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/172 (94%)	157 (98%)	4 (2%)	42	45
1	C	161/172 (94%)	159 (99%)	2 (1%)	67	73
1	D	158/172 (92%)	156 (99%)	2 (1%)	65	71
2	B	131/132 (99%)	128 (98%)	3 (2%)	45	49
2	H	127/132 (96%)	125 (98%)	2 (2%)	58	64
2	I	125/132 (95%)	123 (98%)	2 (2%)	58	64
All	All	863/912 (95%)	848 (98%)	15 (2%)	56	61

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	VAL
2	I	34	MET
1	C	67	MET
2	I	65	VAL
2	H	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	99	GLN
2	H	89	HIS
2	I	89	HIS
2	H	125	HIS
2	B	59	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 6 are monoatomic - leaving 39 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	$\# Z > 2$
3	EDO	B	205	-	3,3,3	0.10	0	2,2,2	0.18	0
3	EDO	C	201	-	3,3,3	0.97	0	2,2,2	0.93	0
3	EDO	A	207	-	3,3,3	0.32	0	2,2,2	0.63	0
3	EDO	B	204	-	3,3,3	0.22	0	2,2,2	0.21	0
7	PGE	C	212	-	9,9,9	1.28	0	8,8,8	1.25	2 (25%)
7	PGE	D	205	-	9,9,9	0.30	0	8,8,8	0.09	0
7	PGE	H	202	-	9,9,9	0.53	0	8,8,8	0.37	0
8	SRT	C	213	-	9,9,9	1.10	0	12,12,12	0.93	0
3	EDO	A	206	-	3,3,3	0.31	0	2,2,2	0.59	0
3	EDO	A	208	-	3,3,3	0.27	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	210	-	3,3,3	0.65	0	2,2,2	0.51	0
3	EDO	B	206	-	3,3,3	0.20	0	2,2,2	0.24	0
5	GNP	C	211	4	29,34,34	1.72	6 (20%)	33,54,54	2.36	9 (27%)
6	1PE	B	208	-	15,15,15	0.41	0	14,14,14	0.22	0
3	EDO	A	205	-	3,3,3	0.23	0	2,2,2	0.26	0
3	EDO	C	204	-	3,3,3	0.25	0	2,2,2	0.35	0
5	GNP	A	214	4	29,34,34	1.43	4 (13%)	33,54,54	2.34	7 (21%)
3	EDO	B	201	-	3,3,3	0.54	0	2,2,2	1.00	0
3	EDO	A	201	-	3,3,3	0.48	0	2,2,2	0.73	0
3	EDO	B	207	-	3,3,3	0.23	0	2,2,2	0.22	0
3	EDO	A	209	-	3,3,3	0.51	0	2,2,2	0.51	0
3	EDO	B	203	-	3,3,3	0.51	0	2,2,2	0.61	0
3	EDO	A	203	-	3,3,3	0.32	0	2,2,2	0.19	0
3	EDO	C	203	-	3,3,3	0.52	0	2,2,2	0.49	0
3	EDO	C	206	-	3,3,3	0.14	0	2,2,2	0.25	0
5	GNP	D	204	4	29,34,34	1.54	5 (17%)	33,54,54	2.43	9 (27%)
3	EDO	C	207	-	3,3,3	0.26	0	2,2,2	0.36	0
3	EDO	C	208	-	3,3,3	0.31	0	2,2,2	0.28	0
3	EDO	A	202	-	3,3,3	0.71	0	2,2,2	0.99	0
3	EDO	D	201	-	3,3,3	0.27	0	2,2,2	0.46	0
3	EDO	A	211	-	3,3,3	0.41	0	2,2,2	0.65	0
3	EDO	C	202	-	3,3,3	0.27	0	2,2,2	0.54	0
3	EDO	I	201	-	3,3,3	0.12	0	2,2,2	0.23	0
3	EDO	A	204	-	3,3,3	0.43	0	2,2,2	0.58	0
3	EDO	D	202	-	3,3,3	0.53	0	2,2,2	0.63	0
7	PGE	B	209	-	9,9,9	0.68	0	8,8,8	0.53	0
3	EDO	C	205	-	3,3,3	0.17	0	2,2,2	0.18	0
3	EDO	C	209	-	3,3,3	0.16	0	2,2,2	0.38	0
3	EDO	B	202	-	3,3,3	0.56	0	2,2,2	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	205	-	-	1/1/1/1	-
3	EDO	C	201	-	-	0/1/1/1	-
3	EDO	A	207	-	-	1/1/1/1	-
3	EDO	B	204	-	-	0/1/1/1	-
7	PGE	C	212	-	-	4/7/7/7	-
7	PGE	D	205	-	-	4/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	H	202	-	-	4/7/7/7	-
8	SRT	C	213	-	-	6/12/12/12	-
3	EDO	A	206	-	-	1/1/1/1	-
3	EDO	A	208	-	-	1/1/1/1	-
3	EDO	A	210	-	-	0/1/1/1	-
3	EDO	B	206	-	-	0/1/1/1	-
5	GNP	C	211	4	-	3/14/38/38	0/3/3/3
6	1PE	B	208	-	-	7/13/13/13	-
3	EDO	A	205	-	-	1/1/1/1	-
3	EDO	C	204	-	-	1/1/1/1	-
5	GNP	A	214	4	-	3/14/38/38	0/3/3/3
3	EDO	B	201	-	-	1/1/1/1	-
3	EDO	A	201	-	-	1/1/1/1	-
3	EDO	B	207	-	-	1/1/1/1	-
3	EDO	A	209	-	-	1/1/1/1	-
3	EDO	B	203	-	-	1/1/1/1	-
3	EDO	A	203	-	-	1/1/1/1	-
3	EDO	C	203	-	-	1/1/1/1	-
3	EDO	C	206	-	-	1/1/1/1	-
5	GNP	D	204	4	-	4/14/38/38	0/3/3/3
3	EDO	C	207	-	-	1/1/1/1	-
3	EDO	C	208	-	-	1/1/1/1	-
3	EDO	A	202	-	-	1/1/1/1	-
3	EDO	D	201	-	-	1/1/1/1	-
3	EDO	A	211	-	-	1/1/1/1	-
3	EDO	C	202	-	-	1/1/1/1	-
3	EDO	I	201	-	-	1/1/1/1	-
3	EDO	A	204	-	-	1/1/1/1	-
3	EDO	D	202	-	-	0/1/1/1	-
7	PGE	B	209	-	-	3/7/7/7	-
3	EDO	C	205	-	-	0/1/1/1	-
3	EDO	C	209	-	-	1/1/1/1	-
3	EDO	B	202	-	-	1/1/1/1	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	214	GNP	PG-O1G	4.61	1.53	1.46
5	C	211	GNP	C6-N1	4.21	1.40	1.33
5	D	204	GNP	C6-N1	4.04	1.40	1.33
5	C	211	GNP	PB-O3A	3.92	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	214	GNP	C6-N1	3.83	1.39	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	214	GNP	C5-C6-N1	-9.03	111.08	123.43
5	D	204	GNP	C5-C6-N1	-8.70	111.53	123.43
5	C	211	GNP	C5-C6-N1	-8.58	111.70	123.43
5	A	214	GNP	C2-N1-C6	6.29	125.92	115.93
5	C	211	GNP	C2-N1-C6	5.73	125.04	115.93

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

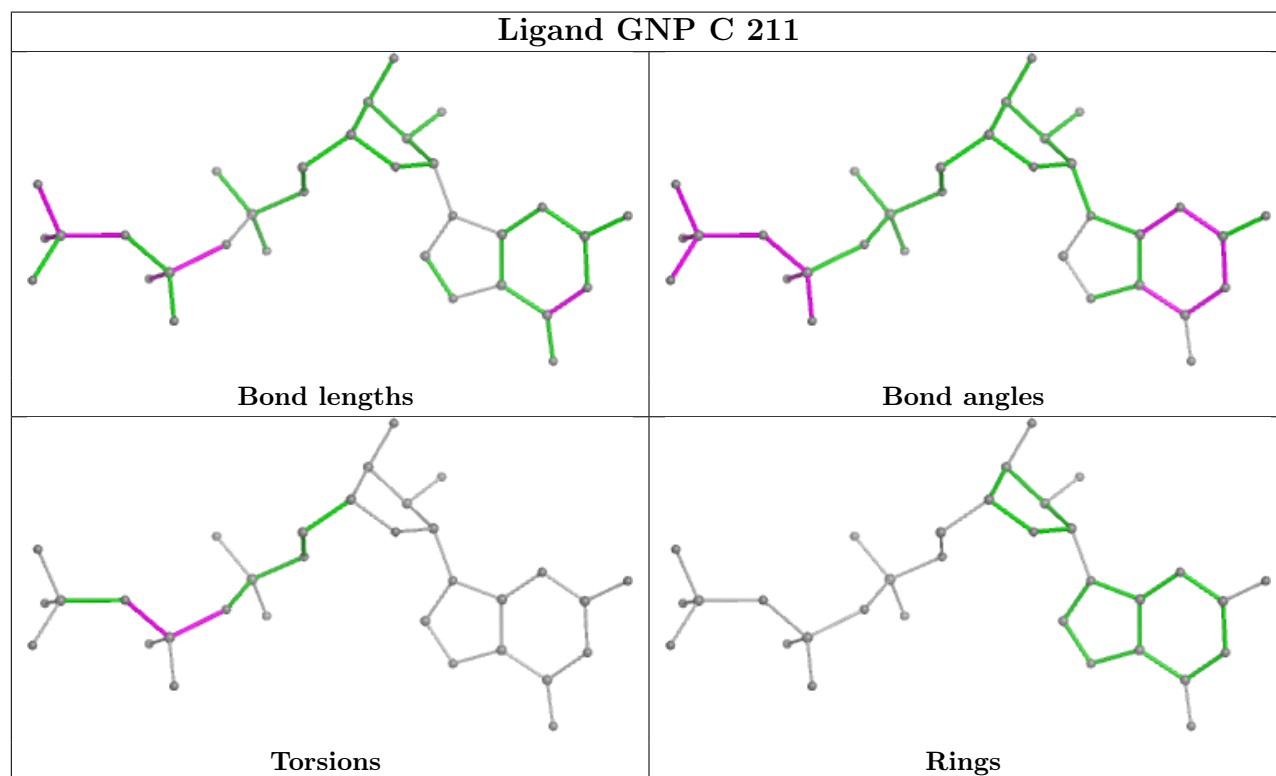
Mol	Chain	Res	Type	Atoms
5	A	214	GNP	PG-N3B-PB-O1B
5	A	214	GNP	PA-O3A-PB-O1B
5	A	214	GNP	PA-O3A-PB-O2B
5	C	211	GNP	PG-N3B-PB-O1B
5	C	211	GNP	PA-O3A-PB-O1B

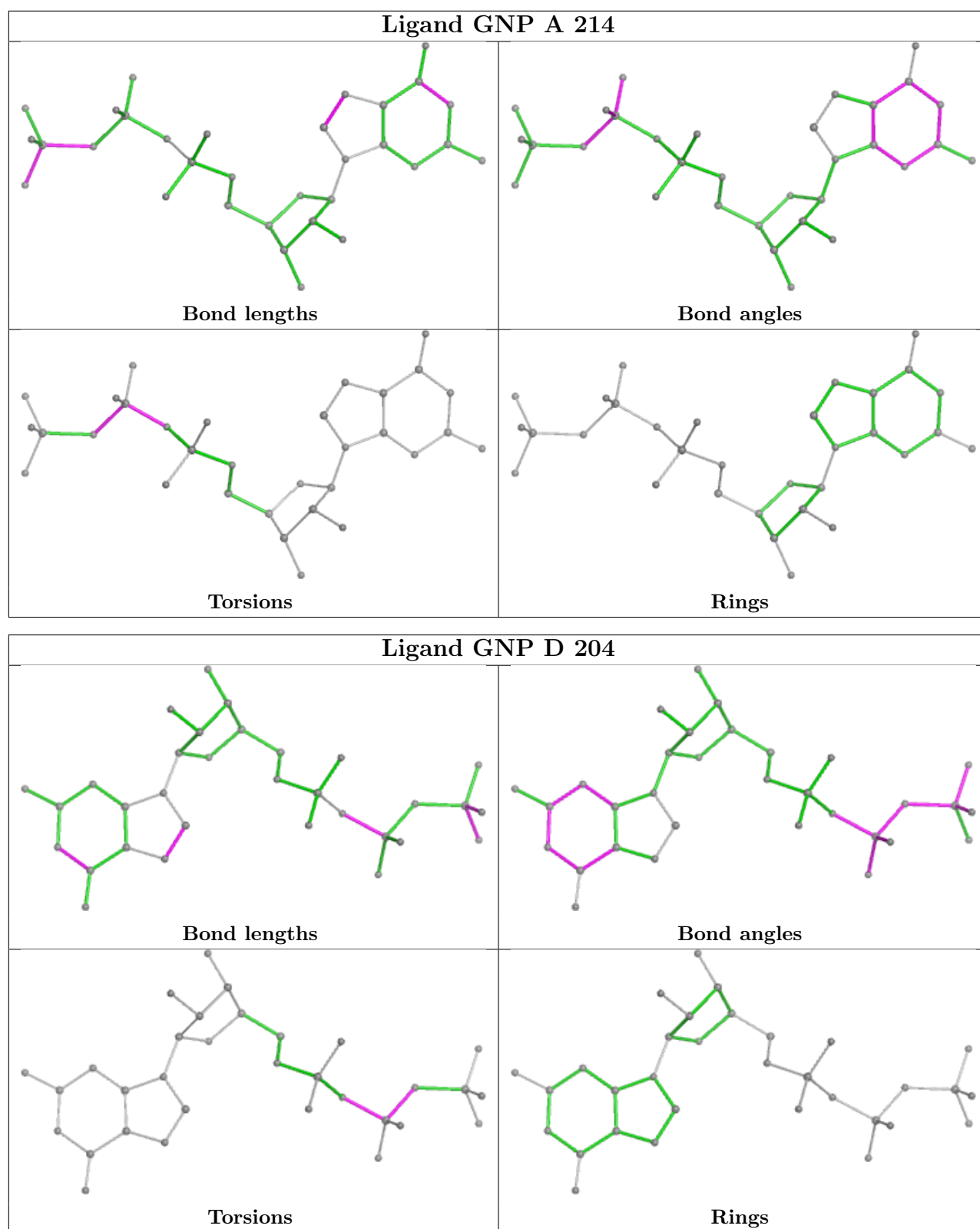
There are no ring outliers.

16 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	EDO	3	0
3	A	207	EDO	1	0
7	C	212	PGE	6	0
7	D	205	PGE	1	0
7	H	202	PGE	2	0
8	C	213	SRT	3	0
5	C	211	GNP	2	0
6	B	208	1PE	3	0
3	B	201	EDO	4	0
3	B	207	EDO	1	0
3	A	209	EDO	2	0
5	D	204	GNP	1	0
3	D	201	EDO	2	0
3	A	211	EDO	2	0
3	A	204	EDO	2	0
7	B	209	PGE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

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	176/195 (90%)	-0.33	2 (1%) 77 76	20, 45, 90, 174	6 (3%)
1	C	175/195 (89%)	-0.19	4 (2%) 61 59	24, 53, 99, 128	7 (4%)
1	D	173/195 (88%)	-0.26	4 (2%) 61 59	22, 54, 96, 139	5 (2%)
2	B	164/170 (96%)	-0.26	5 (3%) 52 51	20, 48, 81, 139	5 (3%)
2	H	163/170 (95%)	0.08	1 (0%) 85 85	36, 83, 123, 182	1 (0%)
2	I	160/170 (94%)	0.27	2 (1%) 74 73	43, 95, 148, 179	2 (1%)
All	All	1011/1095 (92%)	-0.12	18 (1%) 67 66	20, 60, 123, 182	26 (2%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	174	TYR	10.1
1	C	64[A]	TYR	5.7
2	B	173	ASP	4.8
2	B	11	GLY	4.7
1	D	29	VAL	3.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	206	4/4	0.45	0.17	108,110,112,113	0
3	EDO	B	205	4/4	0.63	0.14	102,122,126,135	0
3	EDO	C	208	4/4	0.67	0.22	88,93,107,111	0
8	SRT	C	213	10/10	0.69	0.10	97,114,121,135	0
3	EDO	A	201	4/4	0.72	0.18	73,80,98,103	0
7	PGE	H	202	10/10	0.74	0.19	68,98,120,123	0
3	EDO	C	205	4/4	0.74	0.15	72,90,93,99	0
7	PGE	B	209	10/10	0.78	0.19	59,78,90,102	0
3	EDO	A	206	4/4	0.78	0.21	73,77,88,90	0
3	EDO	B	203	4/4	0.78	0.16	78,87,87,89	0
3	EDO	C	207	4/4	0.79	0.23	86,103,107,109	0
7	PGE	C	212	10/10	0.79	0.27	41,68,88,105	0
3	EDO	C	204	4/4	0.80	0.18	82,87,89,90	0
3	EDO	A	202	4/4	0.80	0.25	68,95,100,104	0
3	EDO	D	202	4/4	0.82	0.26	80,80,82,87	0
3	EDO	I	201	4/4	0.83	0.15	95,104,104,108	0
6	1PE	B	208	16/16	0.83	0.17	65,83,94,95	0
3	EDO	B	207	4/4	0.84	0.13	64,79,79,83	0
3	EDO	B	204	4/4	0.85	0.12	75,85,86,95	0
3	EDO	A	210	4/4	0.85	0.22	73,74,88,88	0
3	EDO	A	204	4/4	0.85	0.19	58,74,82,86	0
3	EDO	B	202	4/4	0.86	0.17	65,73,80,80	0
3	EDO	C	209	4/4	0.87	0.20	88,104,111,111	0
3	EDO	A	205	4/4	0.88	0.22	86,91,93,95	0
7	PGE	D	205	10/10	0.88	0.17	64,96,110,111	0
3	EDO	D	201	4/4	0.88	0.16	76,81,85,91	0
3	EDO	C	206	4/4	0.88	0.21	99,100,103,104	0
3	EDO	A	209	4/4	0.89	0.13	61,75,76,77	0
3	EDO	A	207	4/4	0.89	0.16	65,73,74,74	0
3	EDO	C	202	4/4	0.89	0.22	65,89,92,95	0
3	EDO	C	203	4/4	0.90	0.15	80,83,89,90	0
3	EDO	A	203	4/4	0.90	0.14	49,63,66,72	0
3	EDO	C	201	4/4	0.92	0.15	58,64,66,73	0
3	EDO	A	208	4/4	0.92	0.21	90,95,104,107	0
3	EDO	A	211	4/4	0.92	0.14	54,56,57,63	0
3	EDO	B	201	4/4	0.93	0.13	38,60,65,79	0
4	MG	I	202	1/1	0.94	0.20	75,75,75,75	0

Continued on next page...

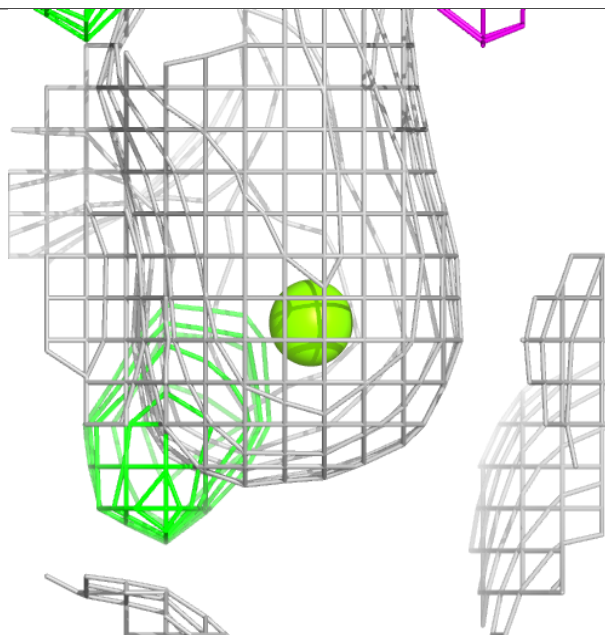
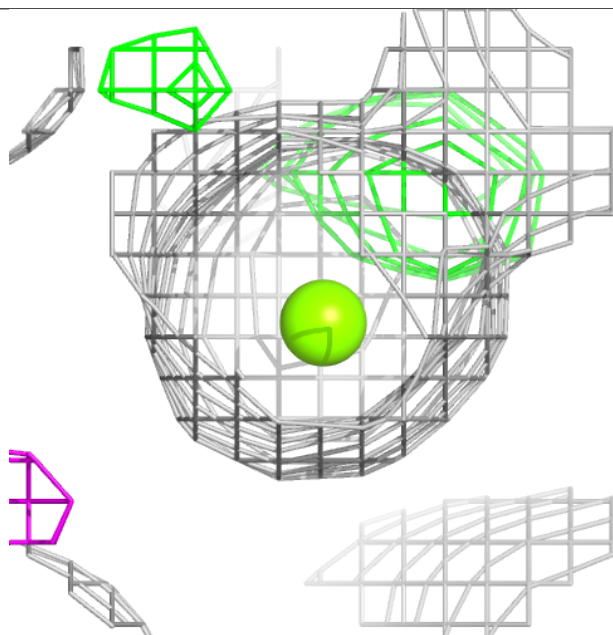
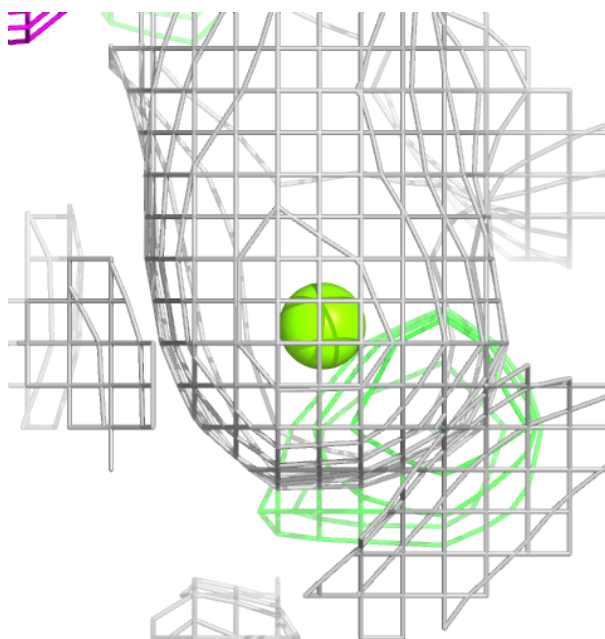
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	H	201	1/1	0.95	0.10	83,83,83,83	0
4	MG	A	213	1/1	0.95	0.18	51,51,51,51	0
5	GNP	A	214	32/32	0.98	0.05	30,38,48,54	0
5	GNP	C	211	32/32	0.98	0.05	30,47,52,57	4
5	GNP	D	204	32/32	0.98	0.04	34,40,47,49	0
4	MG	D	203	1/1	1.00	0.02	40,40,40,40	0
4	MG	A	212	1/1	1.00	0.03	34,34,34,34	0
4	MG	C	210	1/1	1.00	0.04	47,47,47,47	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.

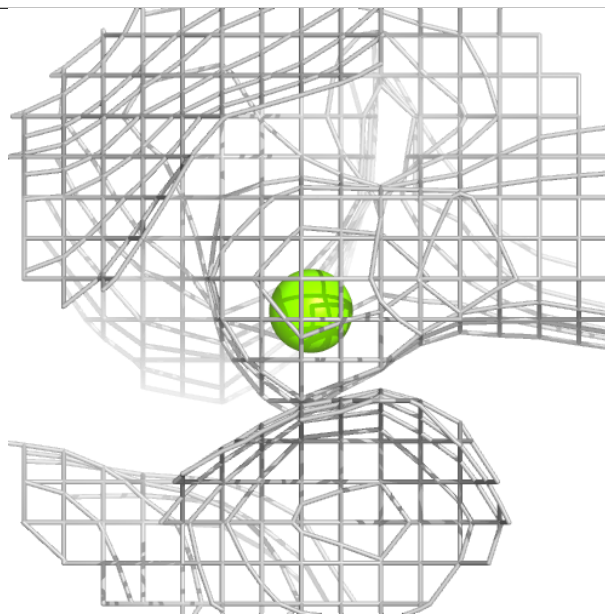
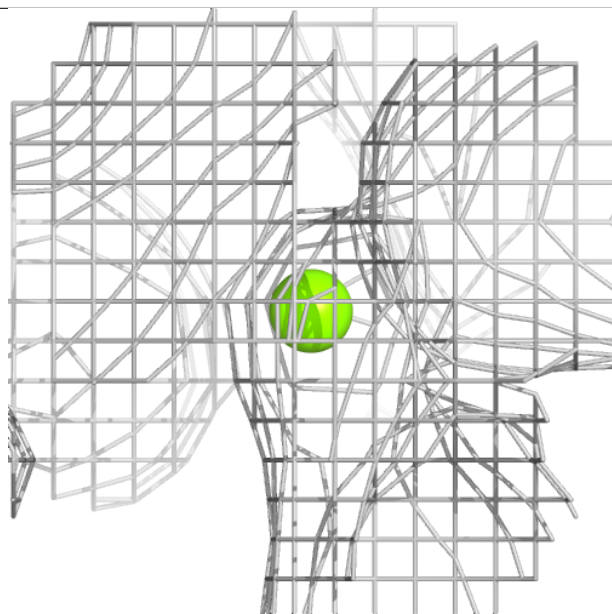
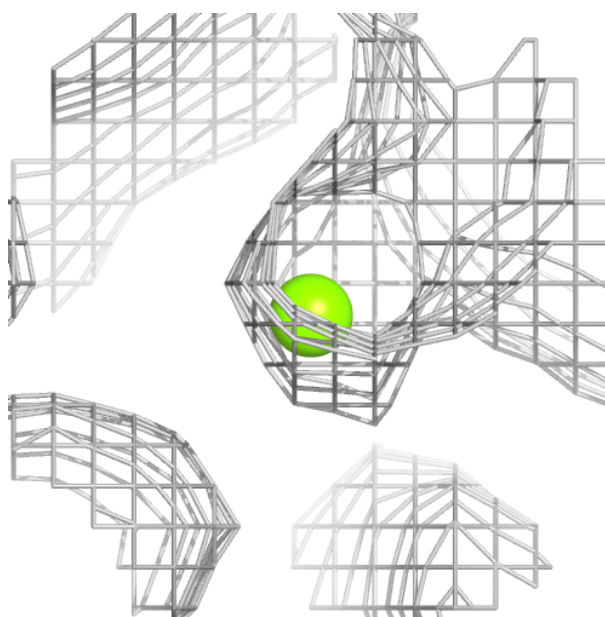
Electron density around MG I 202:

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



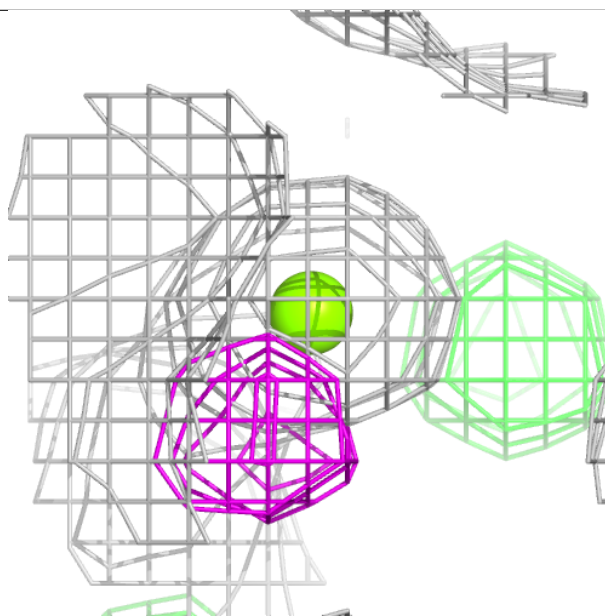
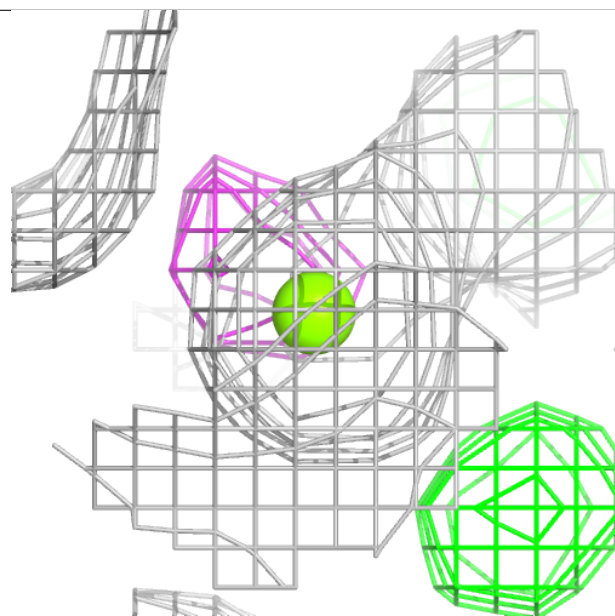
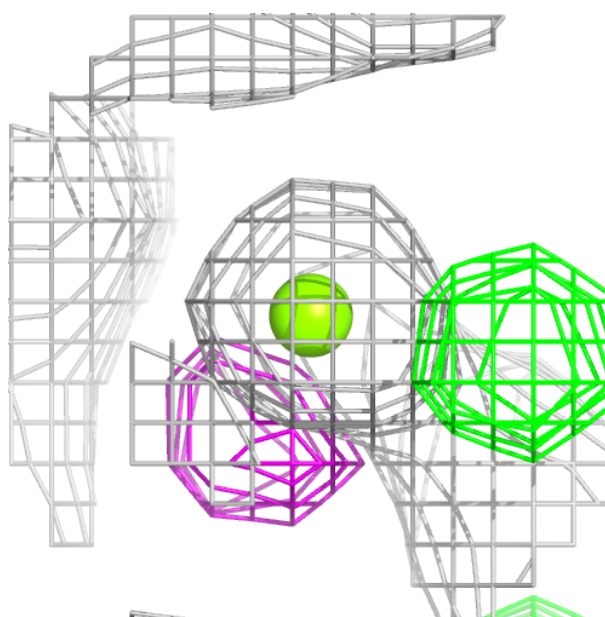
Electron density around MG H 201:

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



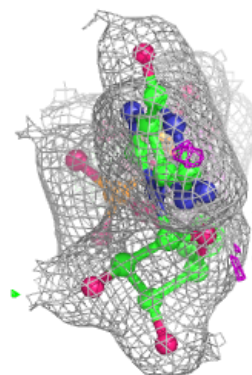
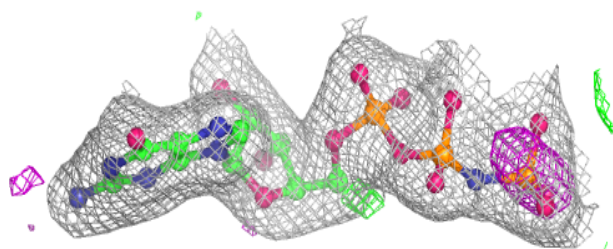
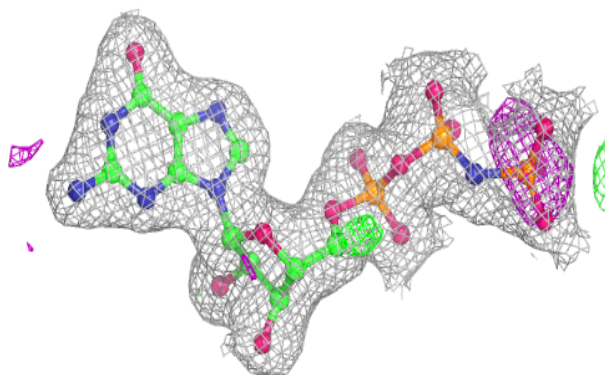
Electron density around MG A 213:

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

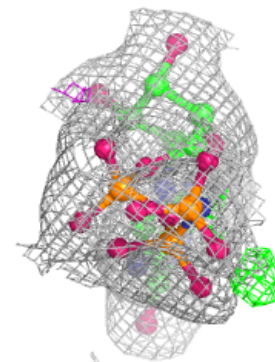
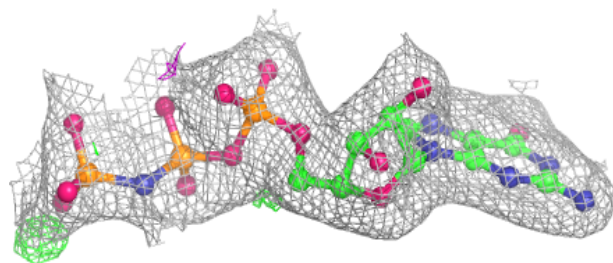
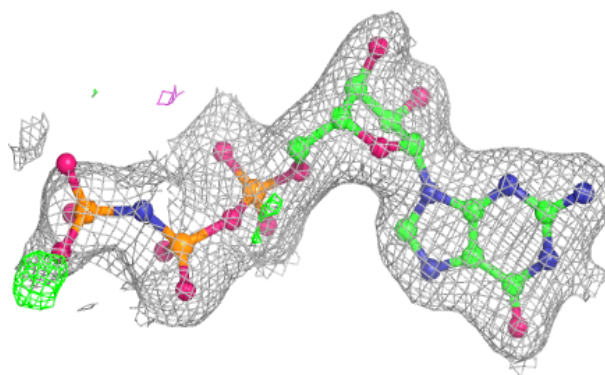


Electron density around GNP A 214:

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

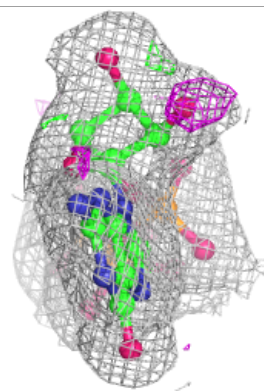
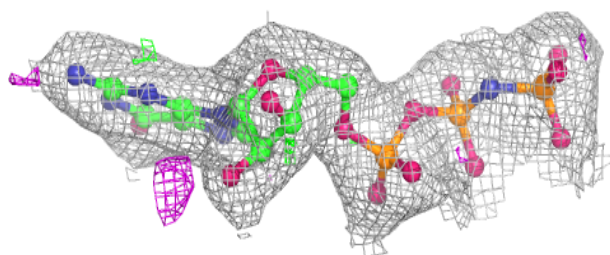
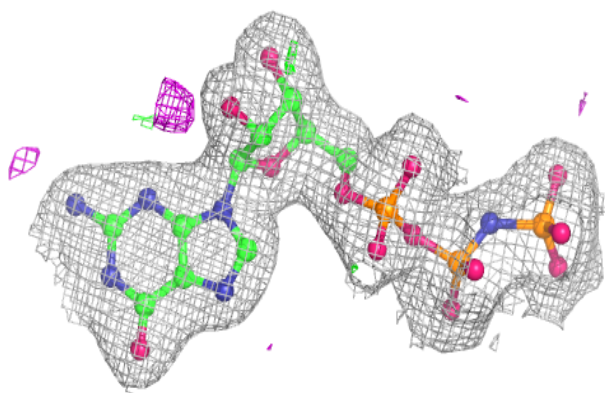
**Electron density around GNP C 211:**

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



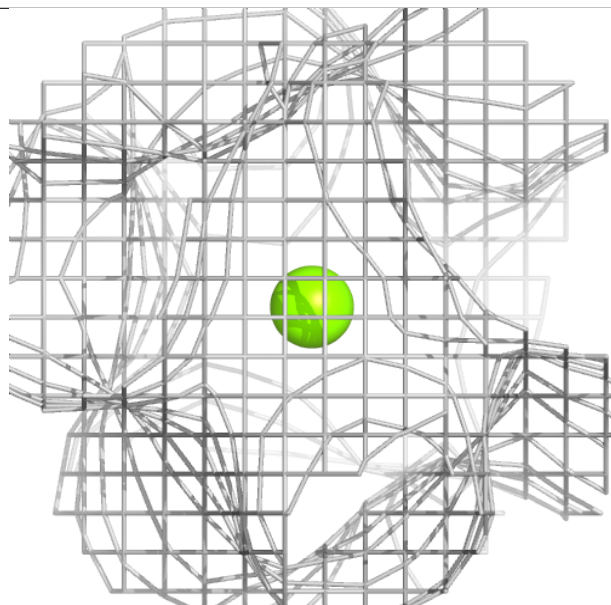
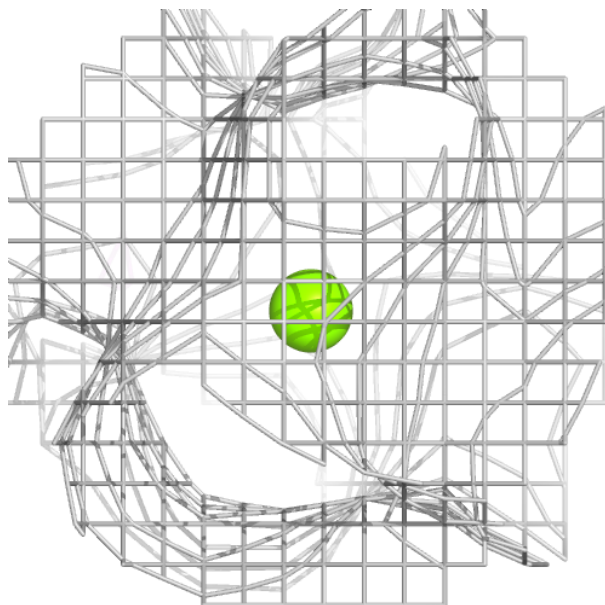
Electron density around GNP D 204:

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



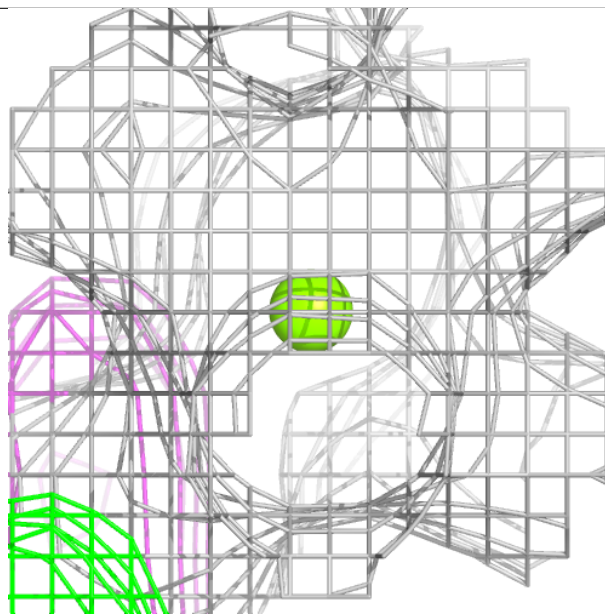
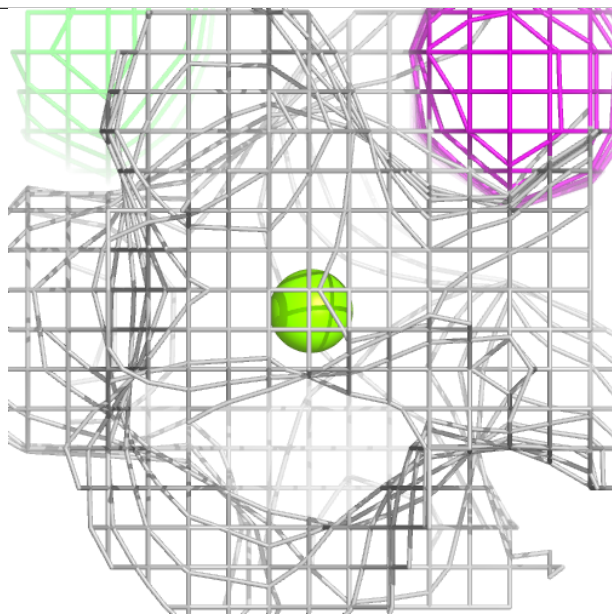
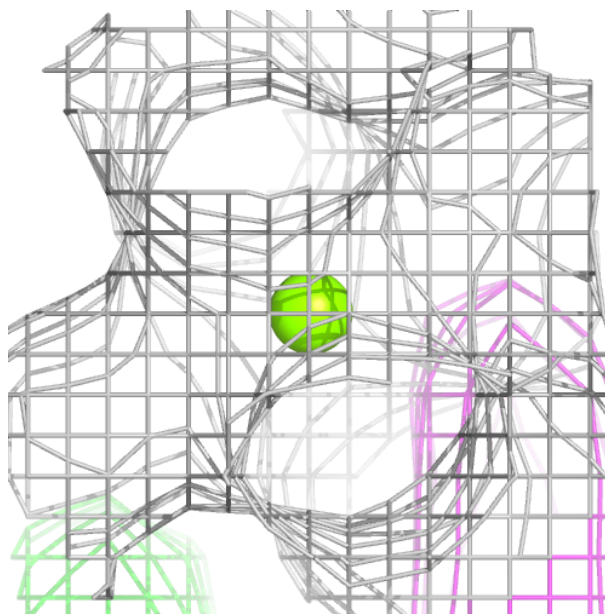
Electron density around MG D 203:

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



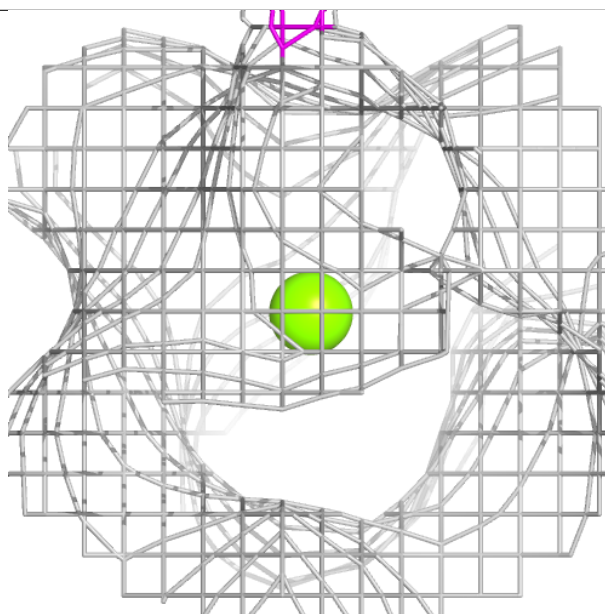
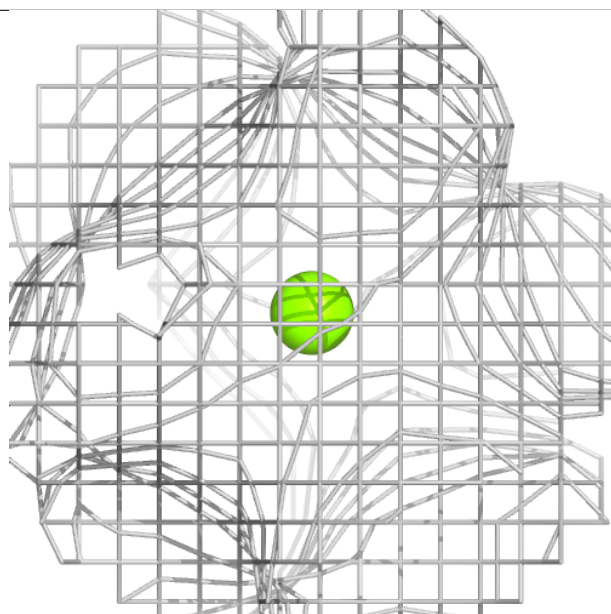
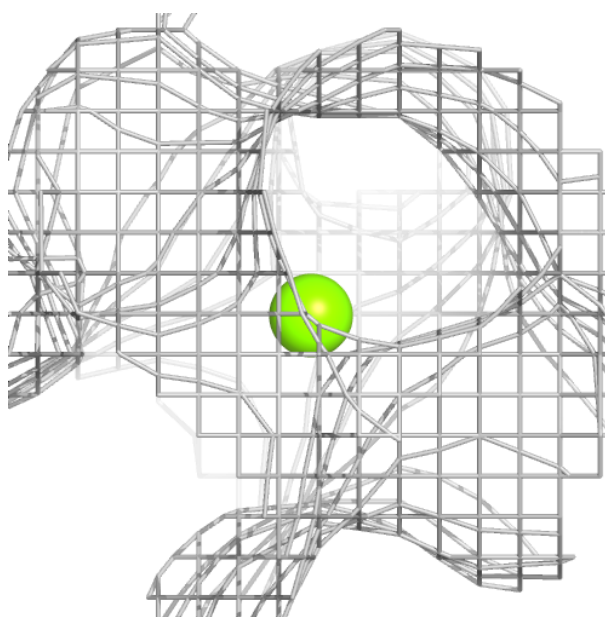
Electron density around MG A 212:

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



Electron density around MG C 210:

$2mF_o-DF_c$ (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.