Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:22 am GMT

PDB ID	:	6GOM
Title	:	KRAS-169 Q61H GPPNHP + PPIN-1
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Deposited on	:	2018-06-01
Resolution	:	1.63 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

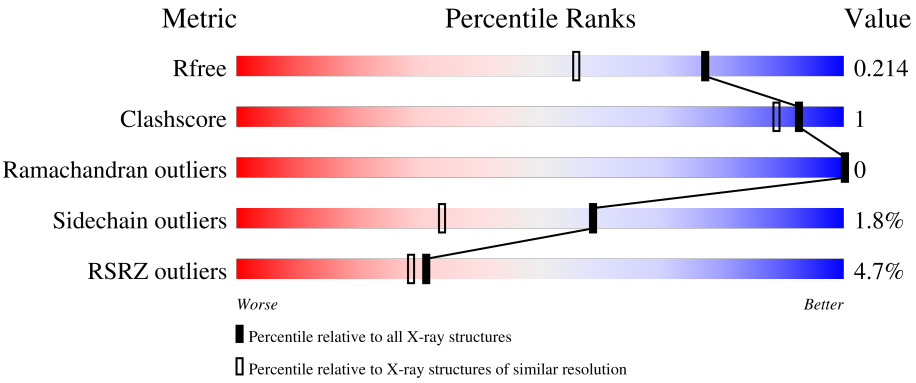
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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

Mol	Chain	Length	Quality of chain
1	A	172	88% 10%
1	B	172	92% 6%
1	C	172	5% 88% 5% 6%
1	D	172	8% 89% 6%
1	E	172	6% 88% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	172	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8808 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 GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	3	0
			1382	866	242	267	7			
1	B	169	Total	C	N	O	S	0	2	0
			1347	844	232	264	7			
1	C	161	Total	C	N	O	S	0	1	1
			1247	785	214	242	6			
1	D	161	Total	C	N	O	S	0	2	0
			1284	807	224	246	7			
1	E	163	Total	C	N	O	S	0	1	0
			1285	808	224	247	6			
1	F	160	Total	C	N	O	S	0	3	0
			1266	795	221	244	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP P01116
A	-2	PHE	-	expression tag	UNP P01116
A	-1	GLN	-	expression tag	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	61	HIS	GLN	engineered mutation	UNP P01116
B	-3	ALA	-	expression tag	UNP P01116
B	-2	PHE	-	expression tag	UNP P01116
B	-1	GLN	-	expression tag	UNP P01116
B	0	GLY	-	expression tag	UNP P01116
B	61	HIS	GLN	engineered mutation	UNP P01116
C	-3	ALA	-	expression tag	UNP P01116
C	-2	PHE	-	expression tag	UNP P01116
C	-1	GLN	-	expression tag	UNP P01116
C	0	GLY	-	expression tag	UNP P01116
C	61	HIS	GLN	engineered mutation	UNP P01116
D	-3	ALA	-	expression tag	UNP P01116
D	-2	PHE	-	expression tag	UNP P01116

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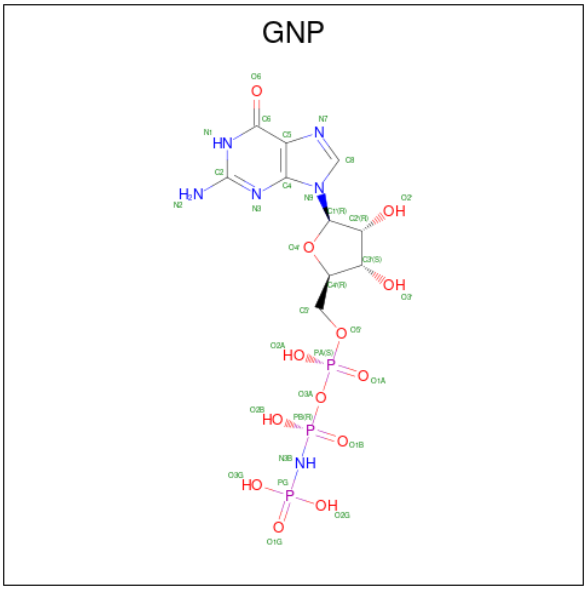
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLN	-	expression tag	UNP P01116
D	0	GLY	-	expression tag	UNP P01116
D	61	HIS	GLN	engineered mutation	UNP P01116
E	-3	ALA	-	expression tag	UNP P01116
E	-2	PHE	-	expression tag	UNP P01116
E	-1	GLN	-	expression tag	UNP P01116
E	0	GLY	-	expression tag	UNP P01116
E	61	HIS	GLN	engineered mutation	UNP P01116
F	-3	ALA	-	expression tag	UNP P01116
F	-2	PHE	-	expression tag	UNP P01116
F	-1	GLN	-	expression tag	UNP P01116
F	0	GLY	-	expression tag	UNP P01116
F	61	HIS	GLN	engineered mutation	UNP P01116

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

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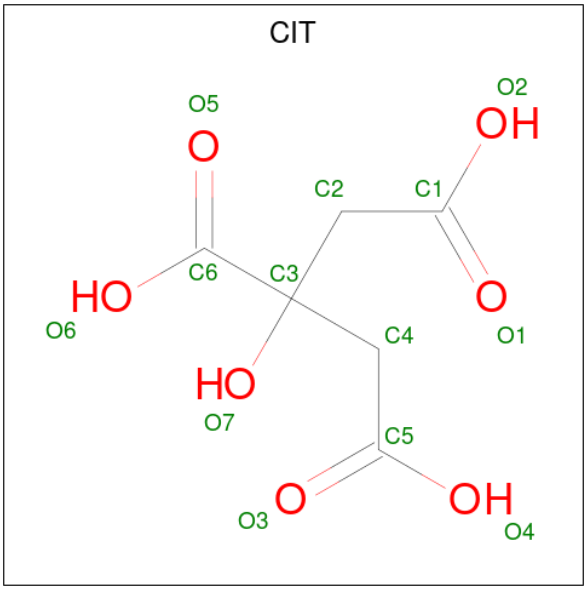
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C N O P 32 10 6 13 3	0	0
2	F	1	Total C N O P 32 10 6 13 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

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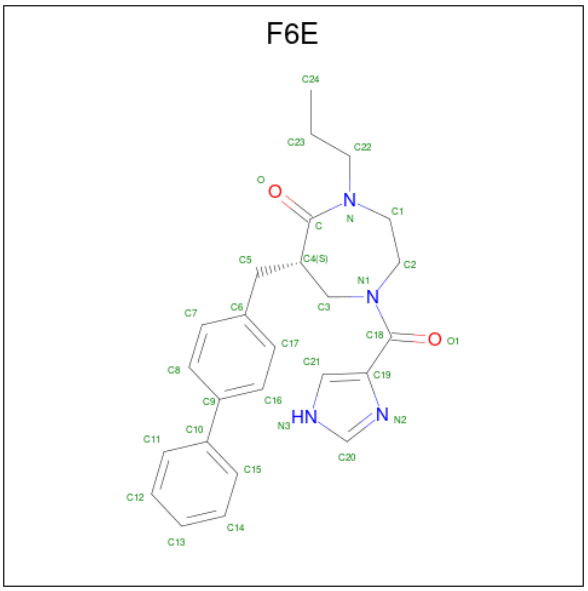
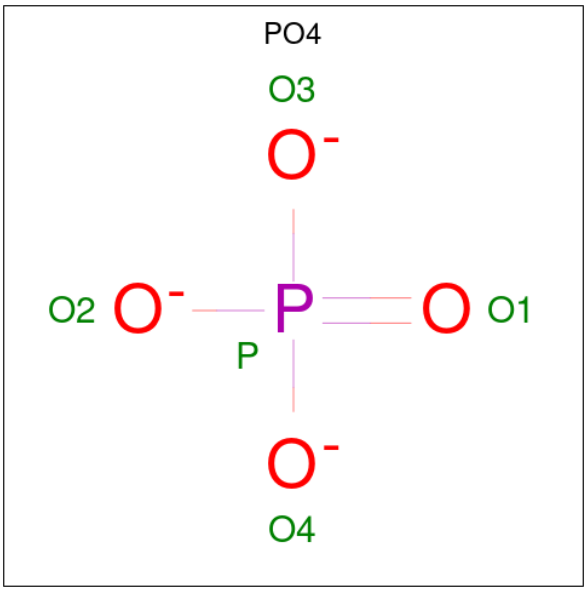
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0

- Molecule 5 is (6 {S})-1-(1 {H}-imidazol-4-ylcarbonyl)-6-[(4-phenylphenyl)methyl]-4-propyl-1,4-diazepan-5-one (three-letter code: F6E) (formula: $C_{25}H_{28}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 31 25 4 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

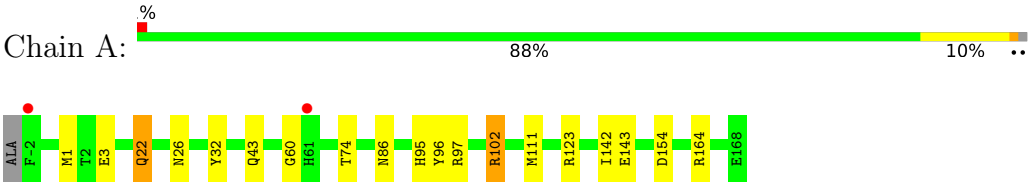
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	172	Total O 172 172	0	0
7	B	169	Total O 169 169	0	0
7	C	71	Total O 71 71	0	0
7	D	102	Total O 102 102	0	0
7	E	91	Total O 91 91	0	0
7	F	119	Total O 119 119	0	0

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.

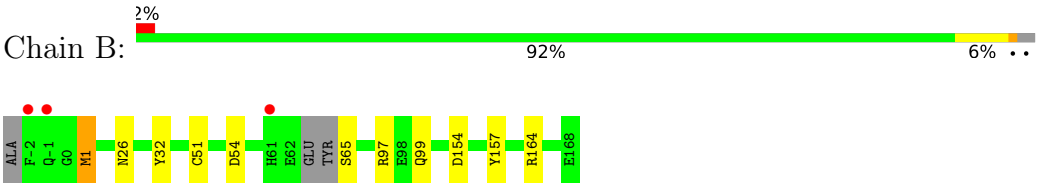
• Molecule 1: GTPase KRas

Chain A:



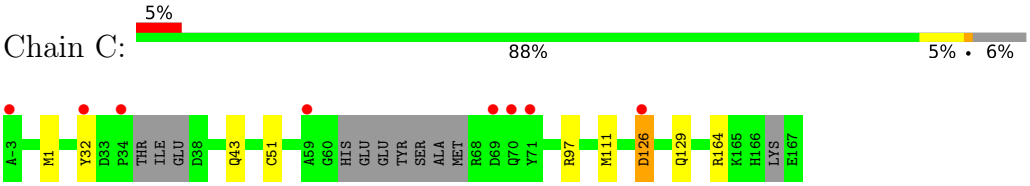
• Molecule 1: GTPase KRas

Chain B:



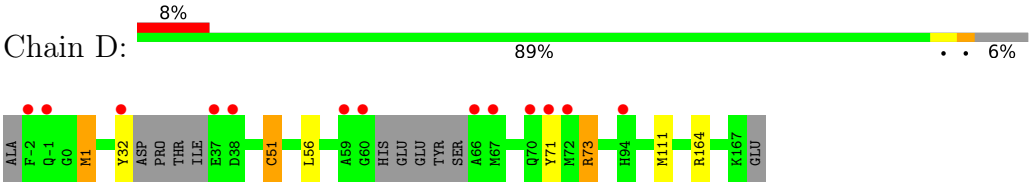
• Molecule 1: GTPase KRas

Chain C:



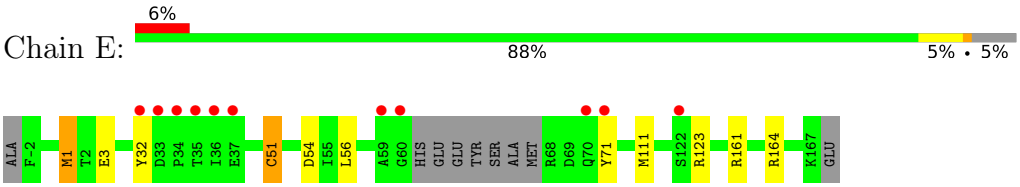
• Molecule 1: GTPase KRas

Chain D:



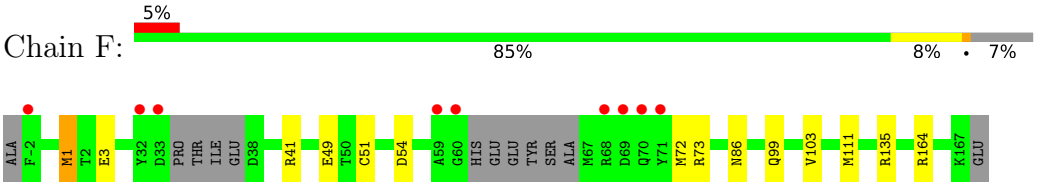
• Molecule 1: GTPase KRas

Chain E:



• Molecule 1: GTPase KRas

Chain F:


5%
85%
8%
7%
ALA
F-2
M1
T2
E3
Y32
D33
PRO
THR
ILE
GLU
D38
R41
E49
T50
C51
D54
A59
G60
HIS
GLU
GLU
TYR
SER
ALA
M67
R68
D69
Q70
Y71
M72
R73
N86
Q99
V103
M111
R135
R164
K167
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.18Å 119.84Å 158.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.13 – 1.63 66.13 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.13-1.63) 99.9 (66.13-1.63)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.186 , 0.207 0.198 , 0.214	Depositor DCC
R_{free} test set	7428 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8808	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: F6E, CIT, GNP, PO4, MG, CSO

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	1.05	4/1404 (0.3%)	1.08	12/1892 (0.6%)
1	B	0.97	0/1363	1.01	8/1836 (0.4%)
1	C	0.87	0/1256	0.93	3/1694 (0.2%)
1	D	0.86	0/1297	0.96	3/1744 (0.2%)
1	E	0.81	0/1297	0.93	5/1748 (0.3%)
1	F	0.92	0/1278	0.96	5/1720 (0.3%)
All	All	0.92	4/7895 (0.1%)	0.98	36/10634 (0.3%)

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	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	GLU	CG-CD	6.79	1.62	1.51
1	A	22	GLN	CB-CG	-5.95	1.36	1.52
1	A	60	GLY	N-CA	-5.37	1.38	1.46
1	A	164	ARG	CZ-NH1	-5.16	1.26	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97[A]	ARG	NE-CZ-NH2	-8.86	115.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	97[B]	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	97[A]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	97[B]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	97[A]	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	97[B]	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	126	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	D	73	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	111	MET	CG-SD-CE	6.87	111.19	100.20
1	B	1	MET	CB-CG-SD	6.86	132.98	112.40
1	A	123	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	F	41	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	1	MET	CB-CG-SD	6.55	132.05	112.40
1	E	1	MET	CB-CG-SD	6.55	132.05	112.40
1	F	135	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	123	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	E	123	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	143	GLU	OE1-CD-OE2	6.19	130.73	123.30
1	A	22	GLN	CA-CB-CG	5.90	126.38	113.40
1	B	54	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	F	111	MET	CG-SD-CE	-5.75	91.00	100.20
1	A	22	GLN	CG-CD-OE1	5.68	132.95	121.60
1	A	22	GLN	CG-CD-NE2	-5.62	103.20	116.70
1	C	97	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	1	MET	CB-CG-SD	5.43	128.68	112.40
1	B	157	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	22	GLN	CB-CG-CD	5.39	125.62	111.60
1	D	111	MET	CG-SD-CE	-5.38	91.59	100.20
1	A	102	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	154	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	E	123	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	111	MET	CG-SD-CE	-5.17	91.92	100.20
1	E	111	MET	CG-SD-CE	-5.14	91.97	100.20
1	F	73	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	161	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	96	TYR	CB-CG-CD1	5.09	124.05	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	86	ASN	Sidechain
1	F	86	ASN	Sidechain

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	1382	0	1354	5	0
1	B	1347	0	1315	2	0
1	C	1247	0	1210	5	0
1	D	1284	0	1267	2	0
1	E	1285	0	1262	4	0
1	F	1266	0	1239	5	0
2	A	32	0	13	0	0
2	B	32	0	13	0	0
2	C	32	0	13	0	0
2	D	32	0	13	0	0
2	E	32	0	13	0	0
2	F	32	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	26	0	10	1	0
4	D	13	0	5	0	0
5	A	31	0	0	1	0
6	B	5	0	0	0	0
7	A	172	0	0	0	0
7	B	169	0	0	1	0
7	C	71	0	0	0	0
7	D	102	0	0	0	0
7	E	91	0	0	0	0
7	F	119	0	0	0	0
All	All	8808	0	7740	23	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 1.

All (23) 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:1:MET:SD	1:C:43:GLN:NE2	2.32	1.00
1:A:1:MET:SD	1:A:43:GLN:OE1	2.43	0.76
1:C:1:MET:CE	1:C:43:GLN:NE2	2.61	0.64
1:C:1:MET:CE	1:C:43:GLN:HE21	2.17	0.57
1:A:142:ILE:HD11	1:A:154:ASP:HB3	1.87	0.56
1:F:72:MET:SD	1:F:99:GLN:HG2	2.51	0.51
1:E:56:LEU:HD21	1:E:71:TYR:CG	2.46	0.50
1:E:3:GLU:OE1	1:E:54:ASP:OD2	2.31	0.49
1:D:56:LEU:HD21	1:D:71:TYR:CG	2.47	0.48
1:A:102:ARG:NH2	4:A:205:CIT:O4	2.35	0.47
1:F:3:GLU:OE1	1:F:54:ASP:OD2	2.33	0.46
1:F:72:MET:HB2	1:F:103:VAL:HG11	1.97	0.45
1:C:126:ASP:OD1	1:C:129:GLN:HG3	2.19	0.43
1:D:51:CSO:OD	1:D:164:ARG:NH2	2.52	0.42
1:E:51:CSO:OD	1:E:164:ARG:NH2	2.51	0.42
1:A:74:THR:OG1	5:A:204:F6E:C12	2.67	0.42
1:B:51:CSO:OD	1:B:164:ARG:NH2	2.53	0.42
1:A:142:ILE:CD1	1:A:154:ASP:HB3	2.50	0.42
1:F:51:CSO:OD	1:F:164:ARG:NH2	2.54	0.41
1:F:49:GLU:OE1	1:F:164:ARG:NH2	2.53	0.41
1:B:99:GLN:OE1	7:B:301:HOH:O	2.22	0.41
1:C:51:CSO:OD	1:C:164:ARG:NH2	2.54	0.41
1:E:56:LEU:HD21	1:E:71:TYR:CD1	2.56	0.41

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	171/172 (99%)	168 (98%)	3 (2%)	0	100	100
1	B	166/172 (96%)	161 (97%)	5 (3%)	0	100	100
1	C	155/172 (90%)	152 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	156/172 (91%)	154 (99%)	2 (1%)	0	100	100
1	E	159/172 (92%)	156 (98%)	3 (2%)	0	100	100
1	F	156/172 (91%)	153 (98%)	3 (2%)	0	100	100
All	All	963/1032 (93%)	944 (98%)	19 (2%)	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	150/149 (101%)	144 (96%)	6 (4%)	31	7
1	B	146/149 (98%)	141 (97%)	5 (3%)	37	11
1	C	131/149 (88%)	130 (99%)	1 (1%)	81	68
1	D	138/149 (93%)	135 (98%)	3 (2%)	52	25
1	E	138/149 (93%)	136 (99%)	2 (1%)	67	45
1	F	135/149 (91%)	134 (99%)	1 (1%)	84	71
All	All	838/894 (94%)	820 (98%)	18 (2%)	59	26

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	26[A]	ASN
1	A	26[B]	ASN
1	A	32	TYR
1	A	95[A]	HIS
1	A	95[B]	HIS
1	B	1	MET
1	B	26[A]	ASN
1	B	26[B]	ASN
1	B	32	TYR

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Mol	Chain	Res	Type
1	B	65	SER
1	C	32	TYR
1	D	1	MET
1	D	32	TYR
1	D	73	ARG
1	E	1	MET
1	E	32	TYR
1	F	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 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	CSO	B	51	1	3,6,7	1.13	0	0,6,8	-	-
1	CSO	C	51	1	3,6,7	1.15	0	0,6,8	-	-
1	CSO	A	51	1	3,6,7	1.26	0	0,6,8	-	-
1	CSO	D	51	1	3,6,7	1.84	1 (33%)	0,6,8	-	-
1	CSO	F	51	1	3,6,7	1.22	0	0,6,8	-	-
1	CSO	E	51	1	3,6,7	1.75	1 (33%)	0,6,8	-	-

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	CSO	B	51	1	-	0/1/5/7	-
1	CSO	C	51	1	-	0/1/5/7	-
1	CSO	A	51	1	-	0/1/5/7	-
1	CSO	D	51	1	-	0/1/5/7	-
1	CSO	F	51	1	-	0/1/5/7	-
1	CSO	E	51	1	-	0/1/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	CSO	CB-CA	-2.97	1.46	1.53
1	E	51	CSO	CB-CA	-2.74	1.46	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	51	CSO	1	0
1	C	51	CSO	1	0
1	D	51	CSO	1	0
1	F	51	CSO	1	0
1	E	51	CSO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
4	CIT	A	203	-	12,12,12	1.15	1 (8%)	17,17,17	1.42	4 (23%)
2	GNP	F	201	3	29,34,34	2.50	5 (17%)	33,54,54	1.84	8 (24%)
2	GNP	B	201	3	29,34,34	2.73	12 (41%)	33,54,54	1.92	8 (24%)
2	GNP	C	201	3	29,34,34	2.65	10 (34%)	33,54,54	1.87	7 (21%)
2	GNP	A	201	3	29,34,34	2.56	9 (31%)	33,54,54	2.36	8 (24%)
2	GNP	D	201	3	29,34,34	3.42	12 (41%)	33,54,54	2.40	9 (27%)
4	CIT	D	203	-	12,12,12	0.93	0	17,17,17	1.52	5 (29%)
5	F6E	A	204	-	30,34,34	1.16	3 (10%)	35,46,46	1.45	5 (14%)
2	GNP	E	201	3	29,34,34	2.51	6 (20%)	33,54,54	2.13	10 (30%)
4	CIT	A	205	-	12,12,12	1.32	2 (16%)	17,17,17	1.75	3 (17%)
6	PO4	B	203	-	4,4,4	1.74	1 (25%)	6,6,6	0.94	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
4	CIT	A	203	-	-	0/16/16/16	-
2	GNP	F	201	3	-	4/14/38/38	0/3/3/3
2	GNP	B	201	3	-	4/14/38/38	0/3/3/3
2	GNP	C	201	3	-	4/14/38/38	0/3/3/3
2	GNP	A	201	3	-	4/14/38/38	0/3/3/3
2	GNP	D	201	3	-	3/14/38/38	0/3/3/3
4	CIT	D	203	-	-	10/16/16/16	-
5	F6E	A	204	-	-	0/15/36/36	0/3/4/4
2	GNP	E	201	3	-	4/14/38/38	0/3/3/3
4	CIT	A	205	-	-	8/16/16/16	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	GNP	PG-O1G	12.24	1.65	1.46
2	E	201	GNP	PG-O1G	10.75	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	GNP	PG-O1G	10.10	1.62	1.46
2	F	201	GNP	PG-O1G	9.85	1.61	1.46
2	B	201	GNP	PG-O1G	8.61	1.59	1.46
2	A	201	GNP	PG-O1G	7.34	1.57	1.46
2	D	201	GNP	PB-O3A	6.95	1.67	1.59
2	A	201	GNP	PB-O1B	5.79	1.55	1.46
2	B	201	GNP	PB-O1B	5.00	1.54	1.46
2	D	201	GNP	C2'-C1'	-4.91	1.46	1.53
2	F	201	GNP	PG-N3B	4.86	1.76	1.63
2	B	201	GNP	O4'-C1'	4.67	1.47	1.41
2	B	201	GNP	C4-N3	4.53	1.42	1.35
2	D	201	GNP	PB-O1B	4.51	1.53	1.46
2	D	201	GNP	PG-N3B	4.38	1.74	1.63
2	B	201	GNP	PG-N3B	4.34	1.74	1.63
2	A	201	GNP	PG-N3B	4.32	1.74	1.63
2	D	201	GNP	PB-O2B	-4.22	1.45	1.56
2	F	201	GNP	PB-O1B	4.18	1.52	1.46
2	A	201	GNP	PB-O3A	4.13	1.64	1.59
2	C	201	GNP	PB-O3A	3.75	1.63	1.59
2	E	201	GNP	PB-N3B	3.68	1.73	1.63
2	E	201	GNP	PG-N3B	3.64	1.72	1.63
2	A	201	GNP	C5-C6	3.63	1.47	1.41
2	C	201	GNP	PB-N3B	3.55	1.72	1.63
2	D	201	GNP	C5-C4	3.45	1.50	1.40
5	A	204	F6E	C17-C16	3.44	1.45	1.38
2	A	201	GNP	PG-O3G	-3.40	1.47	1.56
6	B	203	PO4	P-O1	3.39	1.58	1.50
2	D	201	GNP	PB-N3B	3.24	1.71	1.63
2	C	201	GNP	PG-O3G	3.23	1.65	1.56
2	C	201	GNP	C2'-C1'	-3.18	1.48	1.53
2	C	201	GNP	PG-N3B	3.15	1.71	1.63
2	E	201	GNP	C5-C4	2.96	1.48	1.40
2	A	201	GNP	PB-O2B	-2.93	1.48	1.56
2	E	201	GNP	PG-O3G	2.86	1.64	1.56
2	F	201	GNP	PB-N3B	2.82	1.70	1.63
2	C	201	GNP	C5-C4	2.79	1.48	1.40
2	D	201	GNP	O3'-C3'	2.77	1.49	1.43
2	F	201	GNP	C6-N1	2.72	1.37	1.33
2	E	201	GNP	C5-C6	2.63	1.45	1.41
2	B	201	GNP	O3'-C3'	2.63	1.49	1.43
2	C	201	GNP	C5-C6	2.61	1.45	1.41
2	B	201	GNP	PB-N3B	2.52	1.69	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	GNP	PB-O3A	2.39	1.62	1.59
2	B	201	GNP	C6-N1	2.33	1.37	1.33
2	B	201	GNP	PG-O3G	-2.30	1.50	1.56
4	A	203	CIT	O6-C6	-2.29	1.21	1.30
2	A	201	GNP	C2-N2	2.27	1.38	1.33
2	D	201	GNP	C6-N1	2.27	1.37	1.33
2	C	201	GNP	O4'-C1'	2.26	1.44	1.41
5	A	204	F6E	C7-C8	2.24	1.42	1.38
2	D	201	GNP	PG-O3G	-2.22	1.50	1.56
2	D	201	GNP	O4'-C4'	-2.21	1.40	1.45
2	A	201	GNP	O4'-C4'	2.20	1.49	1.45
2	B	201	GNP	C2-N2	2.17	1.38	1.33
5	A	204	F6E	C15-C10	2.15	1.43	1.39
4	A	205	CIT	C4-C3	-2.14	1.51	1.53
2	C	201	GNP	C6-N1	2.09	1.36	1.33
2	B	201	GNP	O2'-C2'	2.05	1.47	1.43
4	A	205	CIT	O4-C5	-2.01	1.24	1.30

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201	GNP	O1G-PG-N3B	-7.93	100.10	111.77
2	A	201	GNP	C5-C6-N1	-7.31	113.44	123.43
2	A	201	GNP	C2-N1-C6	6.56	126.36	115.93
2	B	201	GNP	C5-C6-N1	-5.39	116.06	123.43
2	C	201	GNP	C5-C6-N1	-5.21	116.31	123.43
2	E	201	GNP	O2B-PB-O1B	5.00	120.39	109.92
2	F	201	GNP	C5-C6-N1	-4.92	116.71	123.43
2	D	201	GNP	C2-N1-C6	4.59	123.23	115.93
2	D	201	GNP	C5-C6-N1	-4.52	117.25	123.43
2	E	201	GNP	O1B-PB-N3B	-4.48	105.18	111.77
2	A	201	GNP	O1G-PG-N3B	-4.44	105.24	111.77
2	C	201	GNP	C2-N1-C6	4.31	122.78	115.93
2	F	201	GNP	O2G-PG-O1G	-4.26	102.75	113.45
2	E	201	GNP	C2-N3-C4	4.05	119.98	115.36
4	A	205	CIT	O6-C6-C3	4.04	120.06	113.05
2	E	201	GNP	O3G-PG-O1G	-3.97	103.46	113.45
2	E	201	GNP	C4-C5-C6	-3.82	117.15	120.80
5	A	204	F6E	C14-C15-C10	-3.81	115.77	120.56
5	A	204	F6E	C1-N-C	3.78	127.01	122.37
2	B	201	GNP	O1G-PG-N3B	-3.68	106.35	111.77
2	B	201	GNP	C2-N1-C6	3.68	121.77	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	GNP	O2B-PB-O1B	3.66	117.59	109.92
2	D	201	GNP	C4-C5-C6	-3.64	117.32	120.80
4	A	205	CIT	O7-C3-C4	-3.37	101.51	109.40
2	D	201	GNP	N3-C2-N1	-3.33	122.78	127.22
2	A	201	GNP	C4-C5-C6	-3.32	117.62	120.80
2	C	201	GNP	C4-C5-C6	-3.31	117.64	120.80
2	D	201	GNP	O2B-PB-O1B	3.29	116.82	109.92
2	E	201	GNP	C4-C5-N7	-3.27	105.99	109.40
2	C	201	GNP	O2G-PG-O3G	3.26	116.32	107.64
5	A	204	F6E	C22-N-C1	-3.21	113.20	117.53
2	B	201	GNP	O2B-PB-O1B	3.14	116.51	109.92
2	E	201	GNP	C5-C6-N1	-3.13	119.15	123.43
2	B	201	GNP	C4-C5-N7	-3.11	106.15	109.40
2	F	201	GNP	C2-N1-C6	3.08	120.83	115.93
2	C	201	GNP	O3G-PG-O1G	-3.07	105.73	113.45
2	D	201	GNP	C4-C5-N7	-3.04	106.23	109.40
2	D	201	GNP	O2G-PG-O1G	-3.01	105.89	113.45
2	D	201	GNP	C2-N3-C4	2.95	118.72	115.36
2	C	201	GNP	O1G-PG-N3B	-2.94	107.44	111.77
2	F	201	GNP	C4-C5-C6	-2.87	118.05	120.80
2	A	201	GNP	N2-C2-N1	2.87	121.72	117.25
2	E	201	GNP	C2-N1-C6	2.85	120.46	115.93
2	A	201	GNP	N3-C2-N1	-2.65	123.68	127.22
4	A	203	CIT	O4-C5-O3	2.55	129.64	123.30
4	D	203	CIT	O6-C6-C3	2.54	117.46	113.05
2	B	201	GNP	O2G-PG-O1G	-2.50	107.17	113.45
2	E	201	GNP	N3-C2-N1	-2.41	124.00	127.22
4	D	203	CIT	O3-C5-C4	-2.39	115.97	122.94
4	A	203	CIT	C4-C3-C6	2.37	115.19	110.11
4	A	203	CIT	C3-C2-C1	2.36	119.53	113.81
4	A	205	CIT	C2-C3-C6	2.33	115.11	110.11
2	F	201	GNP	C3'-C2'-C1'	2.30	104.44	100.98
4	D	203	CIT	C2-C3-C6	2.30	115.04	110.11
2	F	201	GNP	O2'-C2'-C3'	2.26	119.12	111.82
2	E	201	GNP	O2G-PG-O3G	2.25	113.62	107.64
4	A	203	CIT	O3-C5-C4	-2.20	116.52	122.94
4	D	203	CIT	C4-C3-C6	-2.16	105.47	110.11
2	B	201	GNP	O3'-C3'-C4'	-2.13	104.89	111.05
2	F	201	GNP	O1B-PB-N3B	2.10	114.86	111.77
2	C	201	GNP	N3-C2-N1	-2.08	124.44	127.22
5	A	204	F6E	C13-C14-C15	2.08	123.36	120.19
4	D	203	CIT	C3-C4-C5	-2.08	108.78	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	204	F6E	C21-N3-C20	2.05	108.99	105.78
2	F	201	GNP	O1G-PG-N3B	-2.02	108.79	111.77
2	B	201	GNP	O3A-PB-N3B	-2.02	100.98	106.59
2	A	201	GNP	PB-O3A-PA	-2.00	125.56	132.62

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GNP	PG-N3B-PB-O1B
2	A	201	GNP	PA-O3A-PB-O1B
2	A	201	GNP	PA-O3A-PB-O2B
2	B	201	GNP	PG-N3B-PB-O1B
2	B	201	GNP	PA-O3A-PB-O1B
2	B	201	GNP	PA-O3A-PB-O2B
2	C	201	GNP	PB-N3B-PG-O1G
2	C	201	GNP	PG-N3B-PB-O1B
2	C	201	GNP	PA-O3A-PB-O1B
2	C	201	GNP	PA-O3A-PB-O2B
2	D	201	GNP	PG-N3B-PB-O1B
2	D	201	GNP	PA-O3A-PB-O1B
2	D	201	GNP	PA-O3A-PB-O2B
2	E	201	GNP	PB-N3B-PG-O1G
2	E	201	GNP	PG-N3B-PB-O1B
2	E	201	GNP	PA-O3A-PB-O1B
2	F	201	GNP	PB-N3B-PG-O1G
2	F	201	GNP	PG-N3B-PB-O1B
2	F	201	GNP	PA-O3A-PB-O2B
4	A	205	CIT	C2-C3-C6-O5
4	A	205	CIT	C2-C3-C6-O6
4	A	205	CIT	O7-C3-C6-O5
4	A	205	CIT	O7-C3-C6-O6
4	D	203	CIT	C2-C3-C4-C5
4	D	203	CIT	O7-C3-C4-C5
4	D	203	CIT	C6-C3-C4-C5
4	D	203	CIT	C2-C3-C6-O5
4	D	203	CIT	C2-C3-C6-O6
4	D	203	CIT	O7-C3-C6-O5
4	D	203	CIT	O7-C3-C6-O6
4	A	205	CIT	C1-C2-C3-C4
4	A	205	CIT	C1-C2-C3-C6
4	A	205	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
4	D	203	CIT	C1-C2-C3-C6
4	D	203	CIT	C1-C2-C3-O7
4	A	205	CIT	O7-C3-C4-C5
2	E	201	GNP	PA-O3A-PB-O2B
2	A	201	GNP	PG-N3B-PB-O3A
2	B	201	GNP	PG-N3B-PB-O3A
2	F	201	GNP	PG-N3B-PB-O3A
4	D	203	CIT	C1-C2-C3-C4

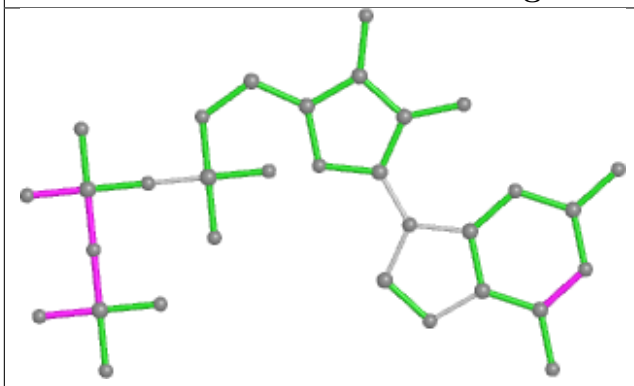
There are no ring outliers.

2 monomers are involved in 2 short contacts:

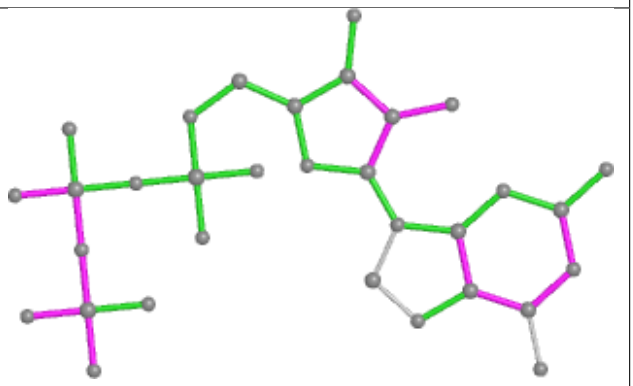
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	204	F6E	1	0
4	A	205	CIT	1	0

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.

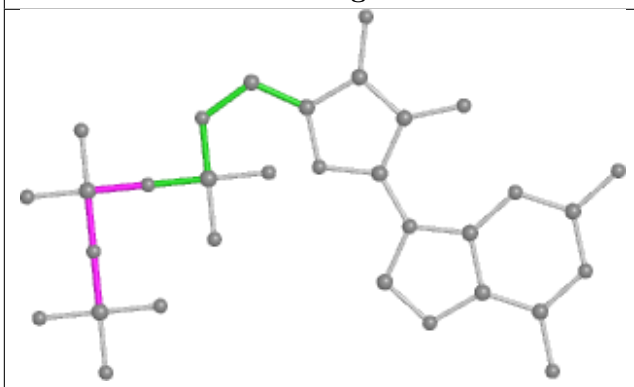
Ligand GNP F 201



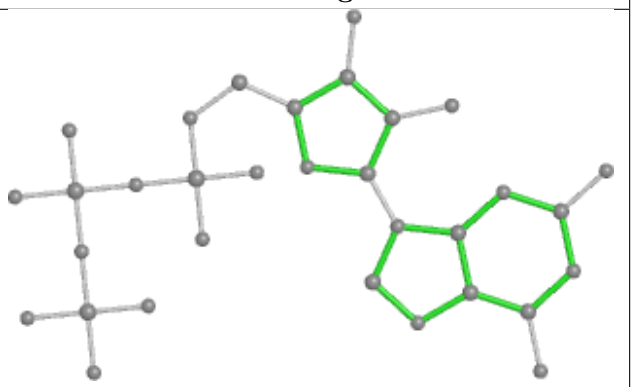
Bond lengths



Bond angles

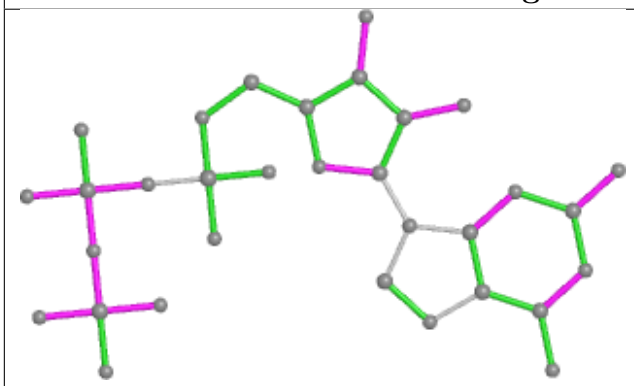


Torsions

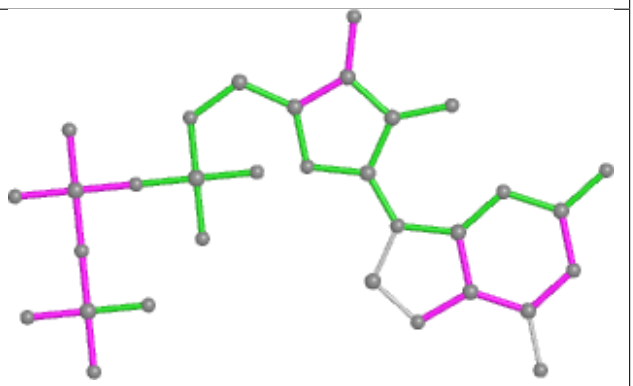


Rings

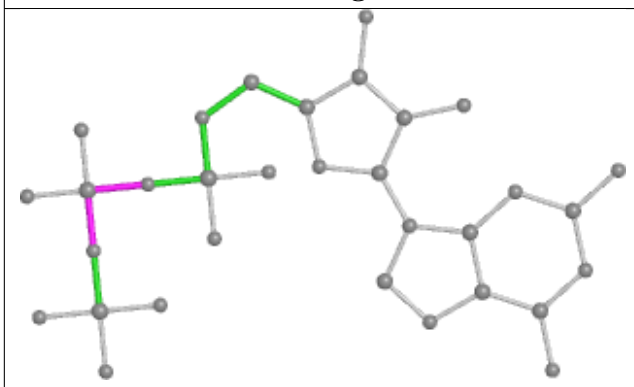
Ligand GNP B 201



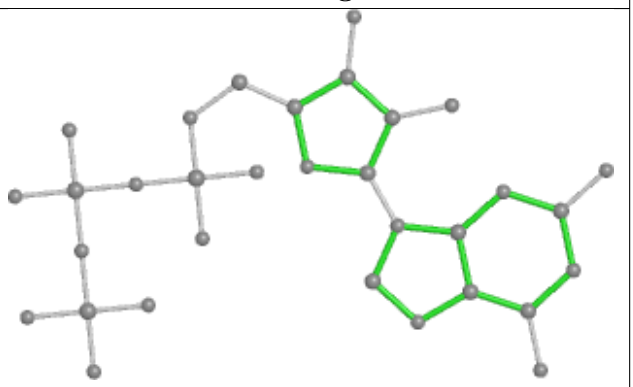
Bond lengths



Bond angles

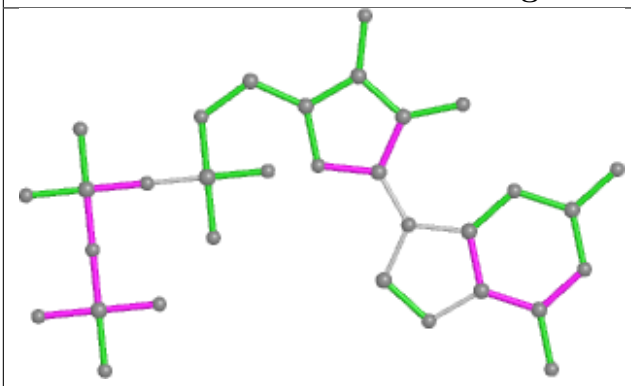


Torsions

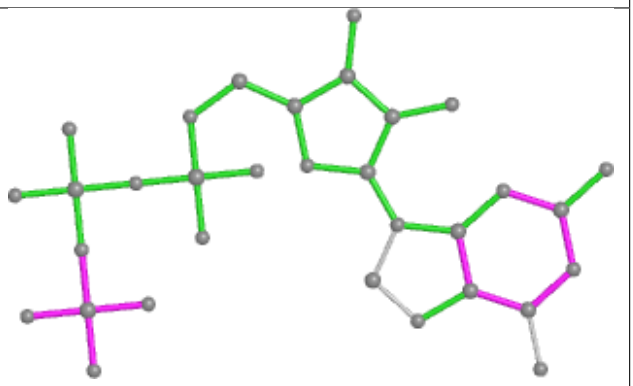


Rings

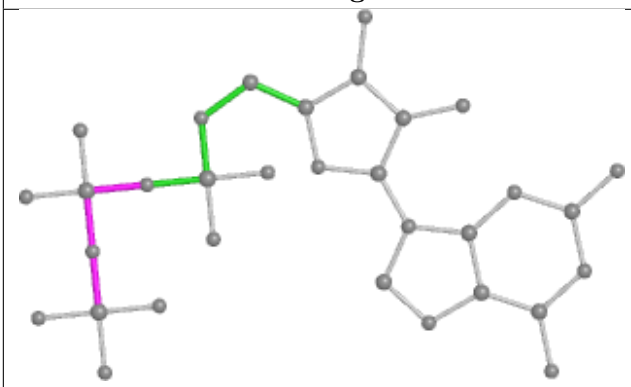
Ligand GNP C 201



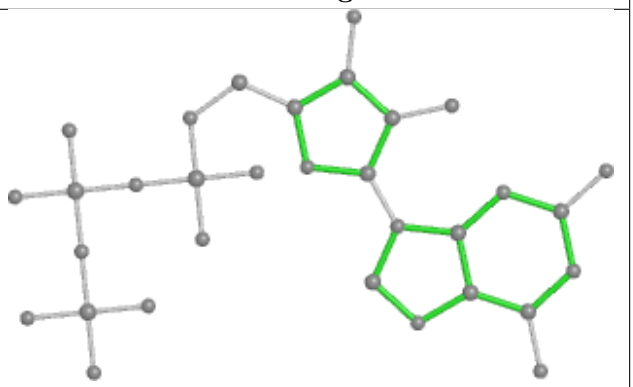
Bond lengths



Bond angles

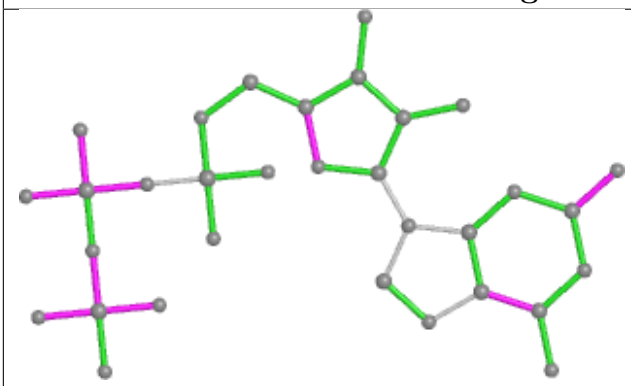


Torsions

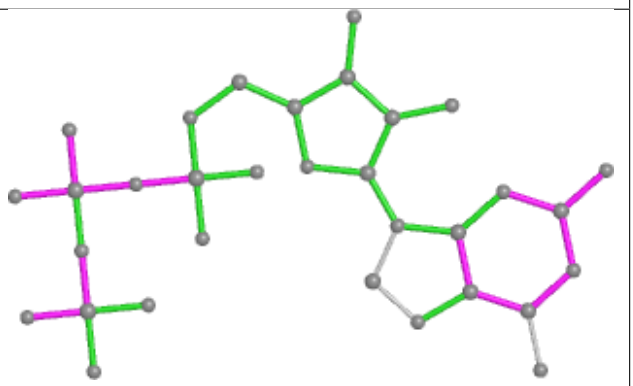


Rings

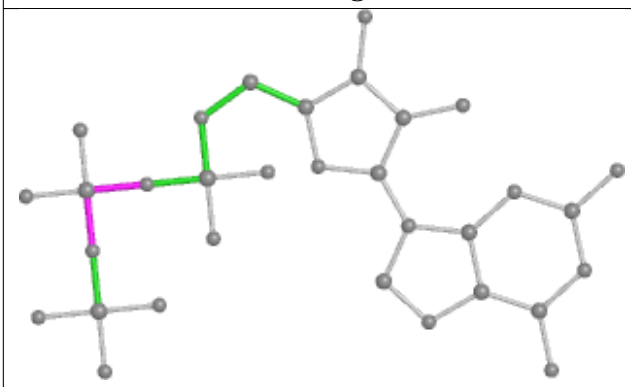
Ligand GNP A 201



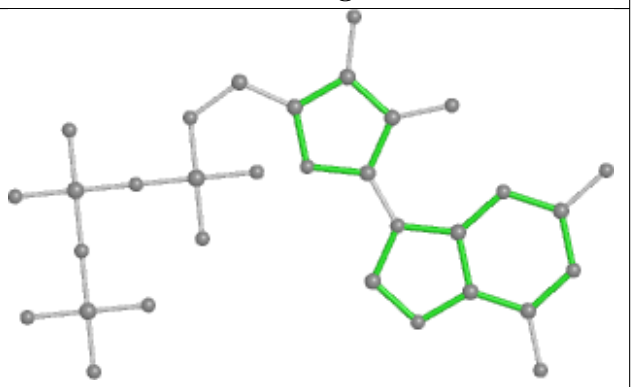
Bond lengths



Bond angles

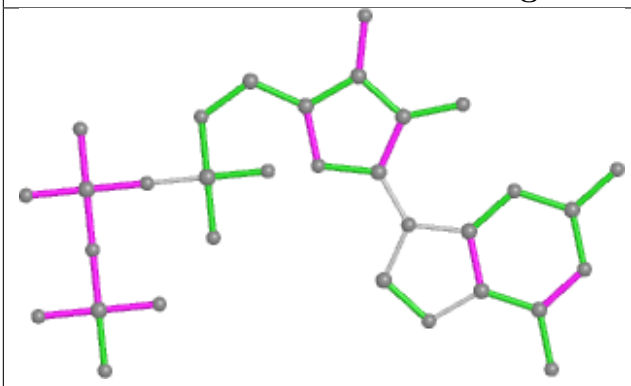


Torsions

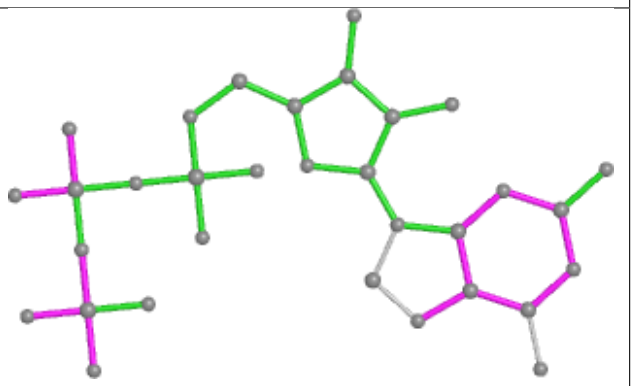


Rings

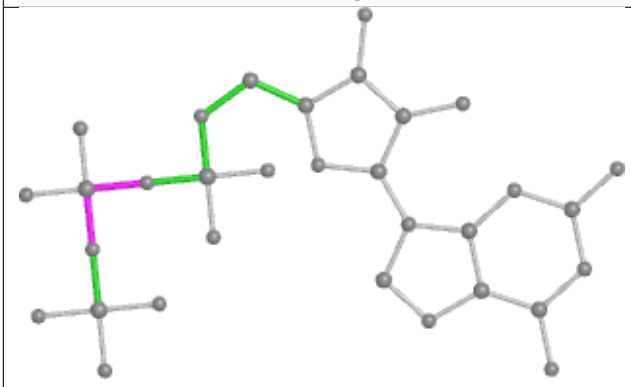
Ligand GNP D 201



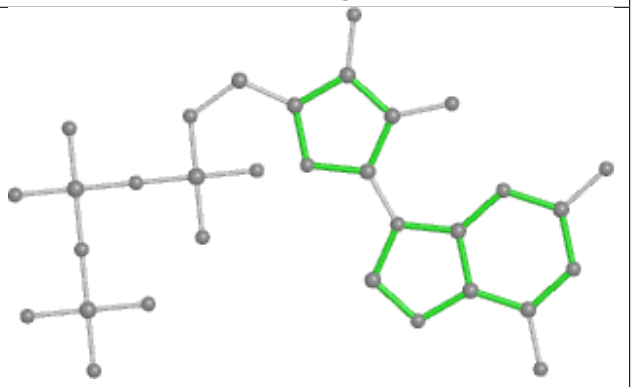
Bond lengths



Bond angles

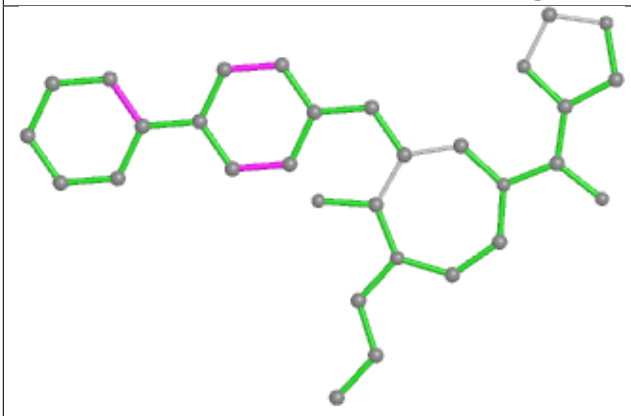


Torsions

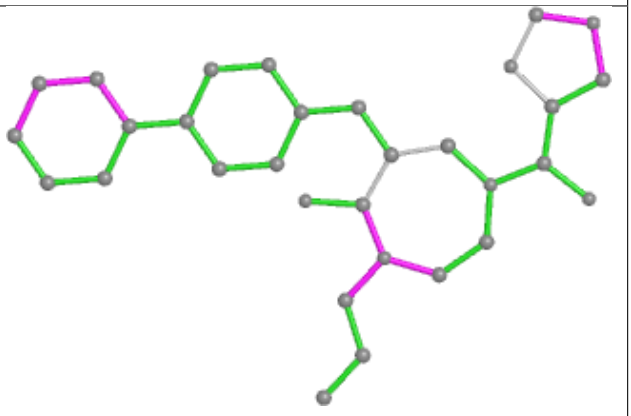


Rings

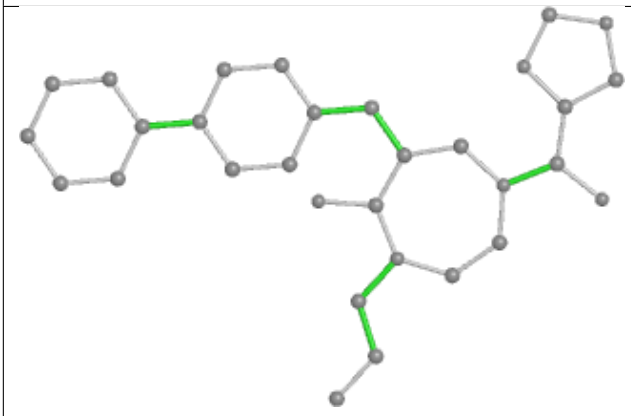
Ligand F6E A 204



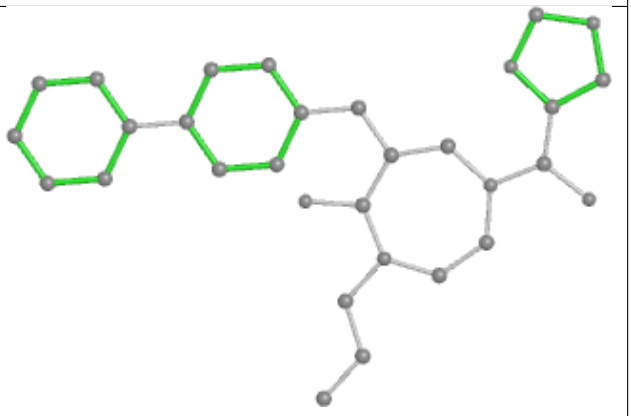
Bond lengths



Bond angles

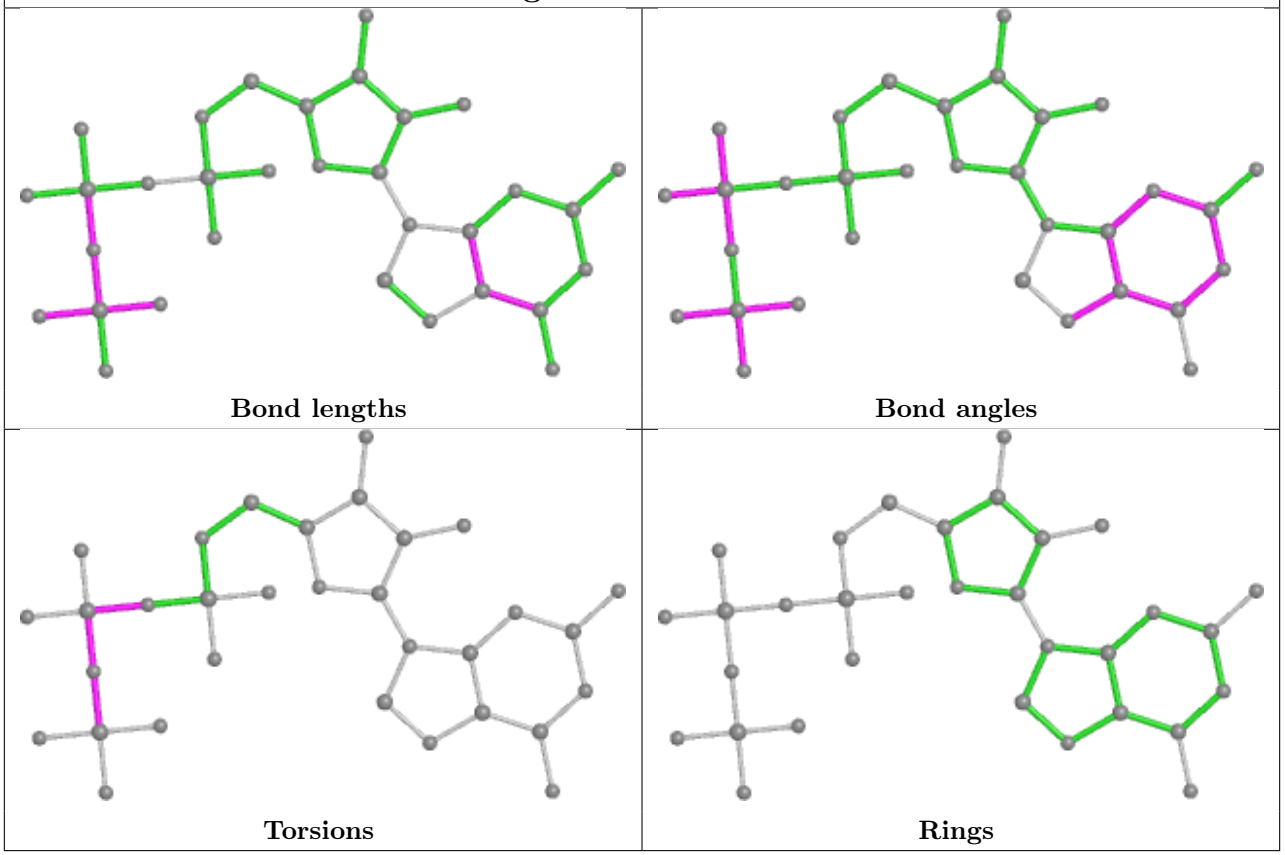


Torsions



Rings

Ligand GNP E 201



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	170/172 (98%)	0.05	2 (1%)	79	79	14, 22, 47, 62	0
1	B	168/172 (97%)	0.05	3 (1%)	68	69	15, 25, 54, 83	0
1	C	160/172 (93%)	0.08	8 (5%)	28	26	21, 36, 61, 87	0
1	D	160/172 (93%)	0.36	13 (8%)	12	10	19, 33, 80, 122	0
1	E	162/172 (94%)	0.19	11 (6%)	17	15	23, 35, 72, 119	0
1	F	159/172 (92%)	0.12	9 (5%)	23	21	17, 26, 69, 107	0
All	All	979/1032 (94%)	0.14	46 (4%)	31	29	14, 29, 64, 122	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	71	TYR	10.8
1	D	66	ALA	10.2
1	D	71	TYR	9.6
1	D	70	GLN	6.2
1	E	32	TYR	6.2
1	E	33	ASP	6.1
1	D	32	TYR	5.9
1	E	35	THR	5.7
1	E	36	ILE	5.5
1	D	67	MET	5.1
1	F	32	TYR	4.8
1	C	32	TYR	4.6
1	F	33	ASP	4.3
1	C	70	GLN	4.3
1	E	34	PRO	4.2
1	F	71	TYR	4.1
1	D	-2	PHE	4.0
1	B	-2	PHE	3.8
1	E	37	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	61	HIS	3.6
1	D	59	ALA	3.6
1	D	38	ASP	3.4
1	F	-2	PHE	3.3
1	D	37	GLU	3.3
1	E	70	GLN	3.1
1	F	69	ASP	3.1
1	C	-3	ALA	3.1
1	D	72	MET	3.0
1	C	71	TYR	3.0
1	D	60	GLY	2.9
1	F	68	ARG	2.8
1	F	59	ALA	2.8
1	C	69	ASP	2.7
1	D	-1	GLN	2.6
1	E	60	GLY	2.5
1	C	34	PRO	2.5
1	C	126	ASP	2.4
1	A	-2	PHE	2.3
1	F	70	GLN	2.3
1	C	59	ALA	2.2
1	B	61	HIS	2.2
1	B	-1	GLN	2.1
1	E	122	SER	2.0
1	D	94	HIS	2.0
1	E	59	ALA	2.0
1	F	60	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	D	51	7/8	0.94	0.09	23,24,28,33	0
1	CSO	A	51	7/8	0.95	0.10	19,23,26,29	0
1	CSO	E	51	7/8	0.95	0.08	24,25,32,39	0
1	CSO	F	51	7/8	0.96	0.07	24,26,32,37	0
1	CSO	C	51	7/8	0.97	0.07	23,26,31,32	0
1	CSO	B	51	7/8	0.98	0.07	23,26,32,32	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

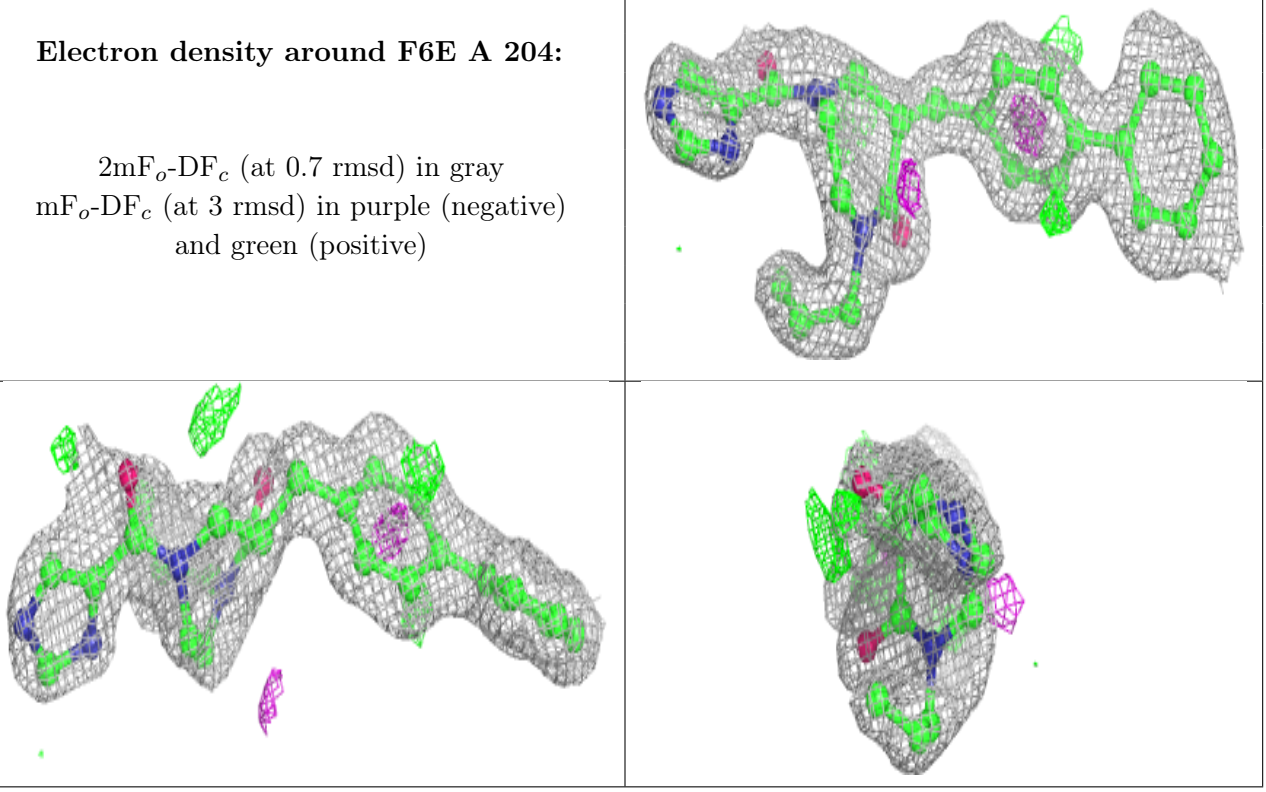
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CIT	A	205	13/13	0.68	0.26	50,69,87,91	0
4	CIT	D	203	13/13	0.70	0.30	66,84,98,102	0
6	PO4	B	203	5/5	0.79	0.24	44,47,58,65	0
3	MG	D	202	1/1	0.85	0.45	71,71,71,71	0
5	F6E	A	204	31/31	0.87	0.16	27,36,65,66	0
3	MG	F	202	1/1	0.87	0.24	48,48,48,48	0
4	CIT	A	203	13/13	0.90	0.12	24,32,37,38	0
3	MG	C	202	1/1	0.93	0.20	51,51,51,51	0
2	GNP	C	201	32/32	0.94	0.09	26,31,50,55	0
2	GNP	D	201	32/32	0.95	0.08	23,30,58,62	0
2	GNP	E	201	32/32	0.96	0.08	25,30,46,46	0
2	GNP	F	201	32/32	0.96	0.08	18,24,40,42	0
3	MG	E	202	1/1	0.97	0.28	44,44,44,44	0
2	GNP	A	201	32/32	0.99	0.08	15,16,19,20	0
2	GNP	B	201	32/32	0.99	0.09	14,17,23,23	0
3	MG	A	202	1/1	0.99	0.08	16,16,16,16	0
3	MG	B	202	1/1	1.00	0.04	20,20,20,20	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.

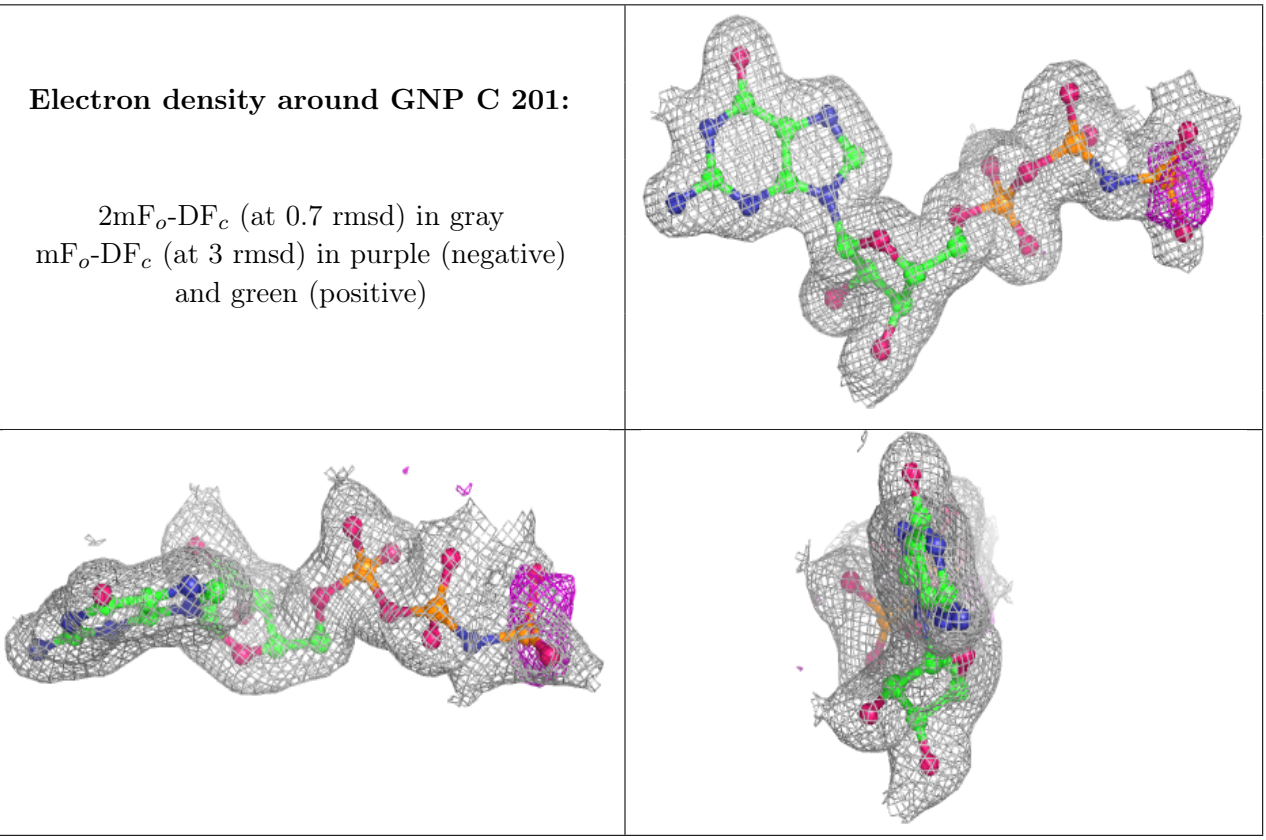
Electron density around F6E A 204:

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



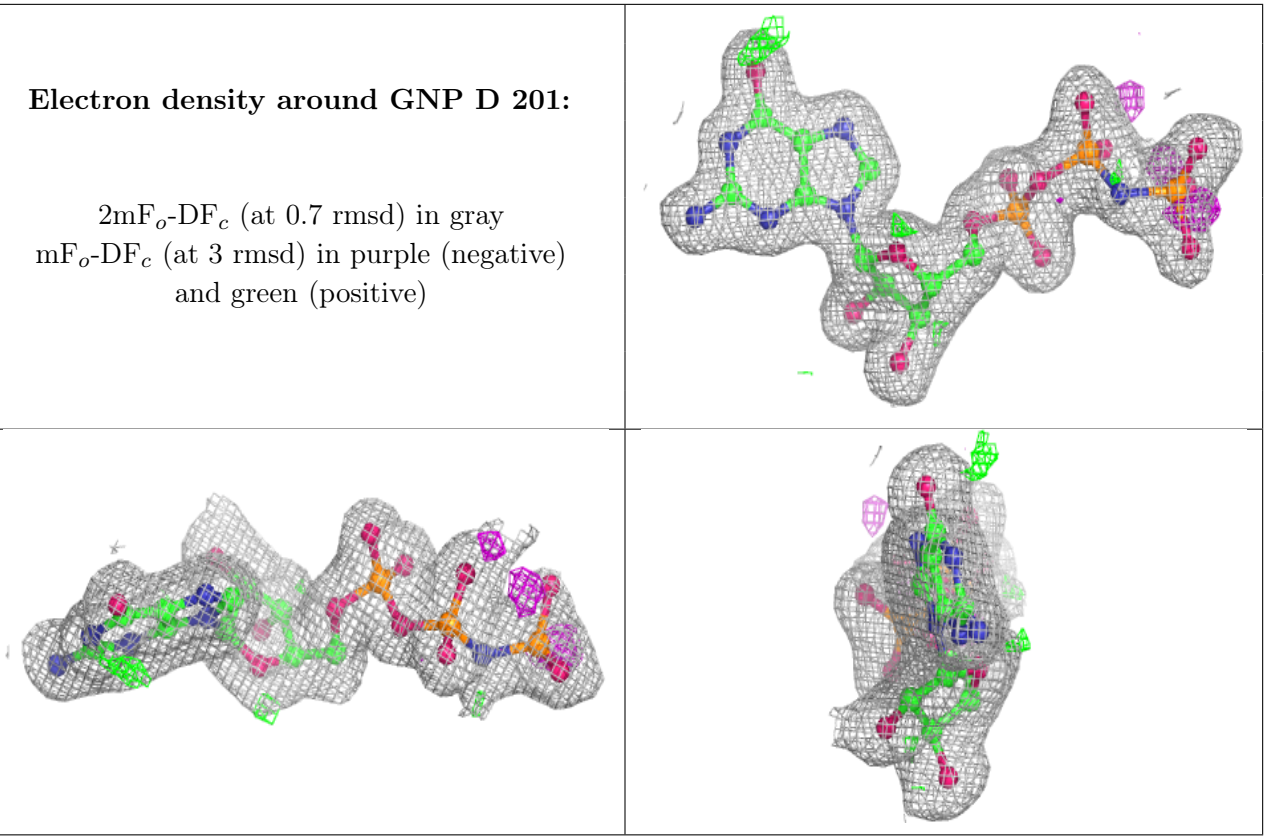
Electron density around GNP C 201:

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



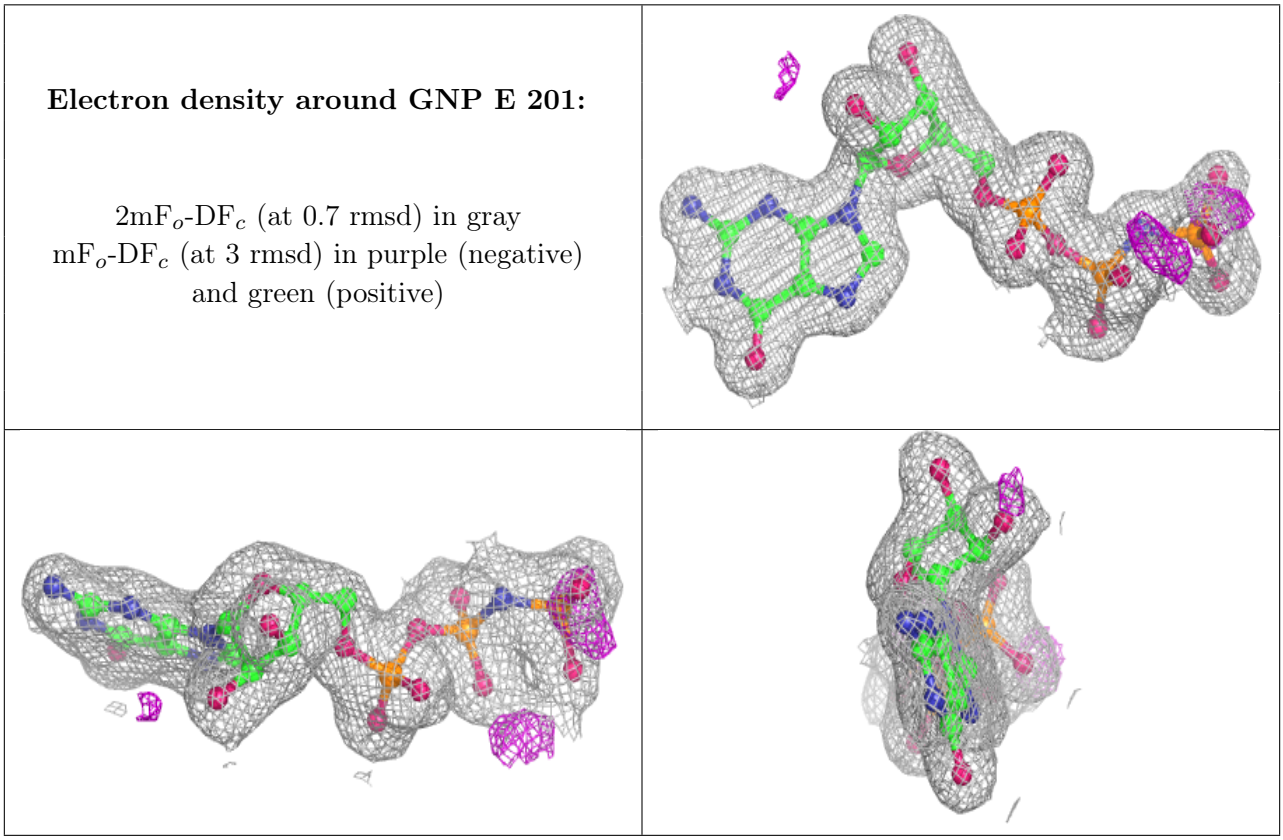
Electron density around GNP D 201:

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



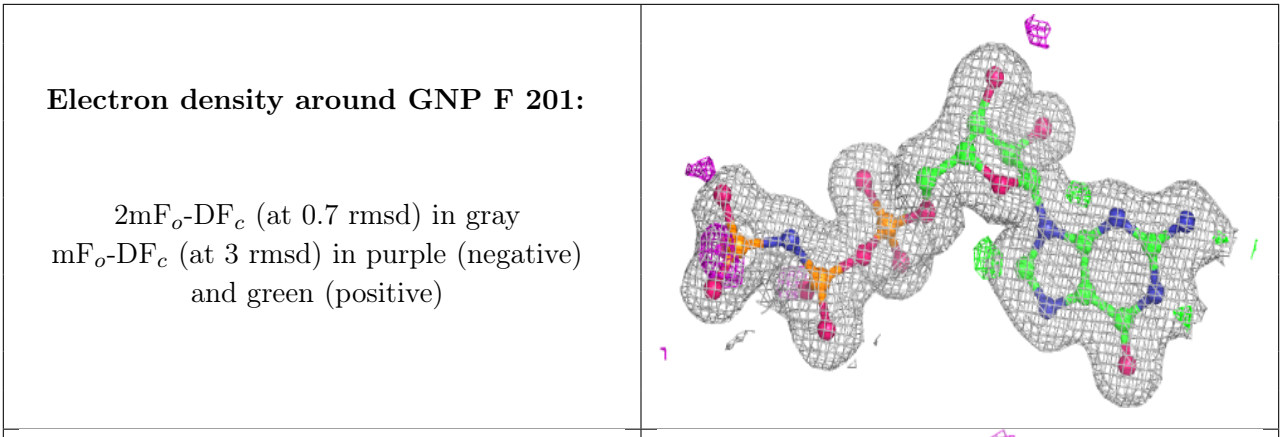
Electron density around GNP E 201:

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



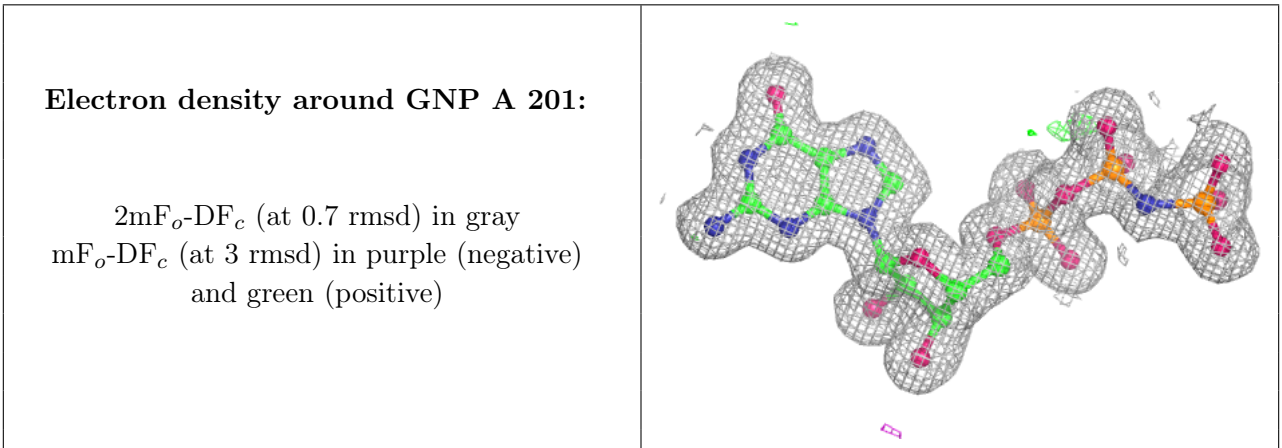
Electron density around GNP F 201:

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



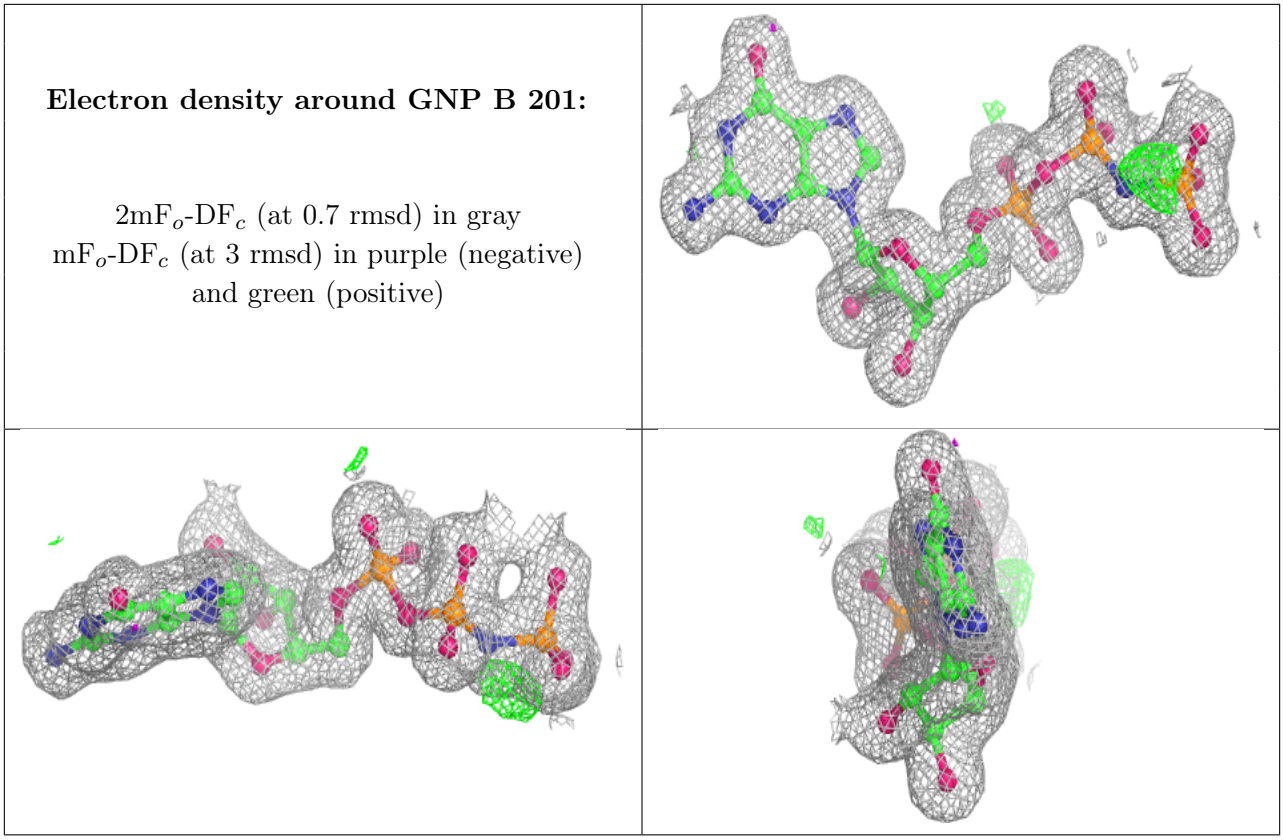
Electron density around GNP A 201:

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



Electron density around GNP B 201:

$2mF_o$-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.