



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:41 pm BST

PDB ID : 3SUA  
Title : Crystal structure of the intracellular domain of Plexin-B1 in complex with Rac1  
Authors : Bell, C.H.; Aricescu, A.R.; Jones, E.Y.; Siebold, C.  
Deposited on : 2011-07-11  
Resolution : 4.39 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

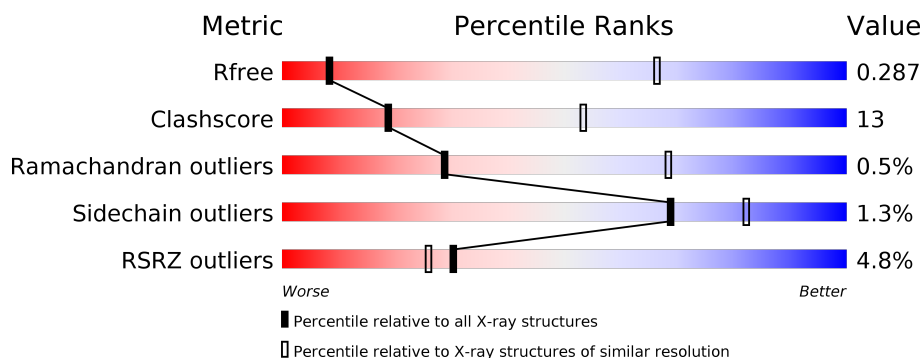
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.39 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	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1094 (5.06-3.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	184	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>••</div> </div> </div>
1	B	184	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>••</div> </div> </div>
1	C	184	<div> <div>10%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>
2	D	633	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>17%</div> <div>•</div> <div>21%</div> </div> </div>
2	E	633	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>17%</div> <div>•</div> <div>20%</div> </div> </div>
2	F	633	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>19%</div> <div>•</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16493 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 Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1392	895	230	259	8			
1	B	178	Total	C	N	O	S	0	0	0
			1392	895	230	259	8			
1	C	178	Total	C	N	O	S	0	0	0
			1392	895	230	259	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LYS	-	EXPRESSION TAG	UNP P63000
A	179	HIS	-	EXPRESSION TAG	UNP P63000
A	180	HIS	-	EXPRESSION TAG	UNP P63000
A	181	HIS	-	EXPRESSION TAG	UNP P63000
A	182	HIS	-	EXPRESSION TAG	UNP P63000
A	183	HIS	-	EXPRESSION TAG	UNP P63000
A	184	HIS	-	EXPRESSION TAG	UNP P63000
B	178	LYS	-	EXPRESSION TAG	UNP P63000
B	179	HIS	-	EXPRESSION TAG	UNP P63000
B	180	HIS	-	EXPRESSION TAG	UNP P63000
B	181	HIS	-	EXPRESSION TAG	UNP P63000
B	182	HIS	-	EXPRESSION TAG	UNP P63000
B	183	HIS	-	EXPRESSION TAG	UNP P63000
B	184	HIS	-	EXPRESSION TAG	UNP P63000
C	178	LYS	-	EXPRESSION TAG	UNP P63000
C	179	HIS	-	EXPRESSION TAG	UNP P63000
C	180	HIS	-	EXPRESSION TAG	UNP P63000
C	181	HIS	-	EXPRESSION TAG	UNP P63000
C	182	HIS	-	EXPRESSION TAG	UNP P63000
C	183	HIS	-	EXPRESSION TAG	UNP P63000
C	184	HIS	-	EXPRESSION TAG	UNP P63000

- Molecule 2 is a protein called Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	503	Total	C	N	O	S	0	0	0
			4061	2608	698	741	14			
2	E	505	Total	C	N	O	S	0	0	0
			4076	2619	700	743	14			
2	F	506	Total	C	N	O	S	0	0	0
			4081	2622	701	744	14			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1503	MET	-	EXPRESSION TAG	UNP O43157
D	1504	GLY	-	EXPRESSION TAG	UNP O43157
D	1505	HIS	-	EXPRESSION TAG	UNP O43157
D	1506	HIS	-	EXPRESSION TAG	UNP O43157
D	1507	HIS	-	EXPRESSION TAG	UNP O43157
D	1508	HIS	-	EXPRESSION TAG	UNP O43157
D	1509	HIS	-	EXPRESSION TAG	UNP O43157
D	1510	HIS	-	EXPRESSION TAG	UNP O43157
D	1625	THR	SER	SEE REMARK 999	UNP O43157
E	1503	MET	-	EXPRESSION TAG	UNP O43157
E	1504	GLY	-	EXPRESSION TAG	UNP O43157
E	1505	HIS	-	EXPRESSION TAG	UNP O43157
E	1506	HIS	-	EXPRESSION TAG	UNP O43157
E	1507	HIS	-	EXPRESSION TAG	UNP O43157
E	1508	HIS	-	EXPRESSION TAG	UNP O43157
E	1509	HIS	-	EXPRESSION TAG	UNP O43157
E	1510	HIS	-	EXPRESSION TAG	UNP O43157
E	1625	THR	SER	SEE REMARK 999	UNP O43157
F	1503	MET	-	EXPRESSION TAG	UNP O43157
F	1504	GLY	-	EXPRESSION TAG	UNP O43157
F	1505	HIS	-	EXPRESSION TAG	UNP O43157
F	1506	HIS	-	EXPRESSION TAG	UNP O43157
F	1507	HIS	-	EXPRESSION TAG	UNP O43157
F	1508	HIS	-	EXPRESSION TAG	UNP O43157
F	1509	HIS	-	EXPRESSION TAG	UNP O43157
F	1510	HIS	-	EXPRESSION TAG	UNP O43157
F	1625	THR	SER	SEE REMARK 999	UNP O43157

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

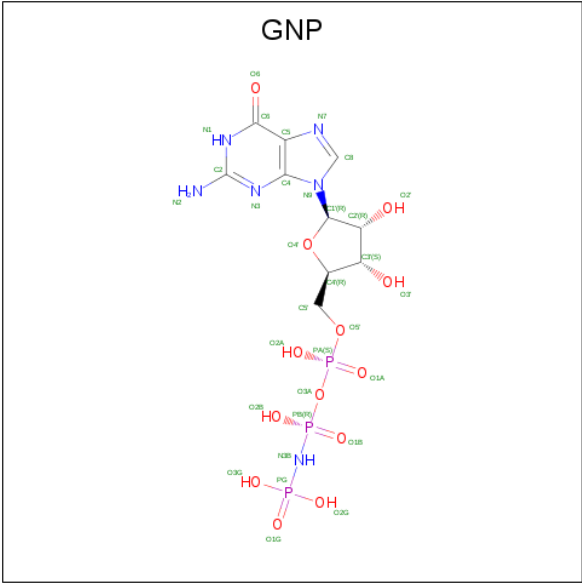
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

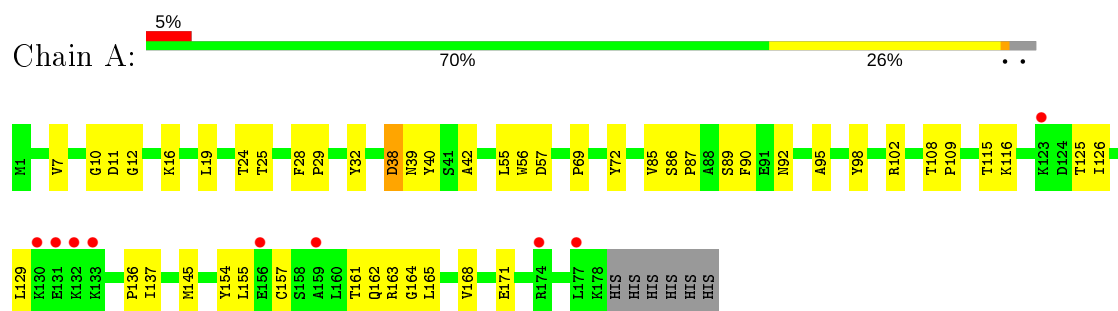


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

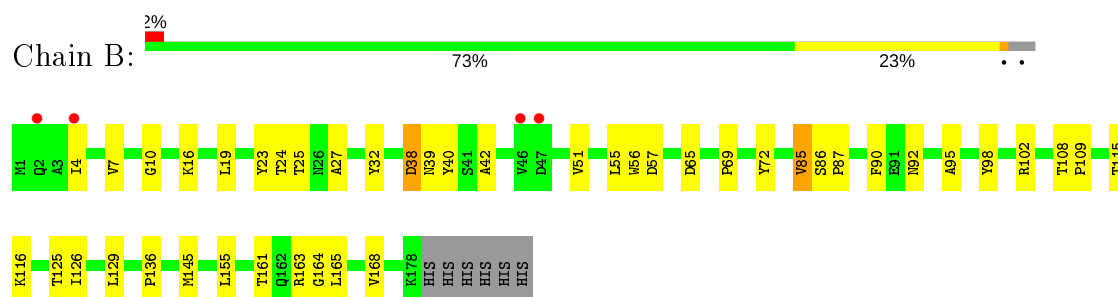
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

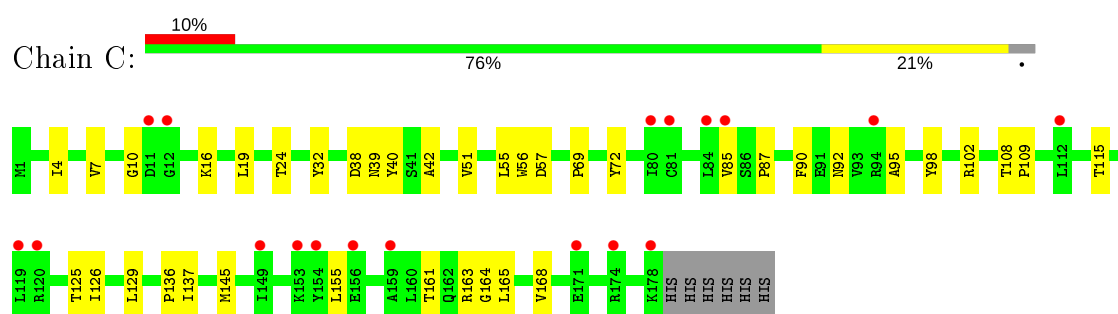
- Molecule 1: Ras-related C3 botulinum toxin substrate 1



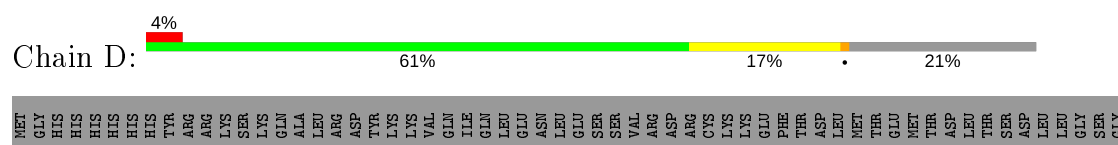
- Molecule 1: Ras-related C3 botulinum toxin substrate 1

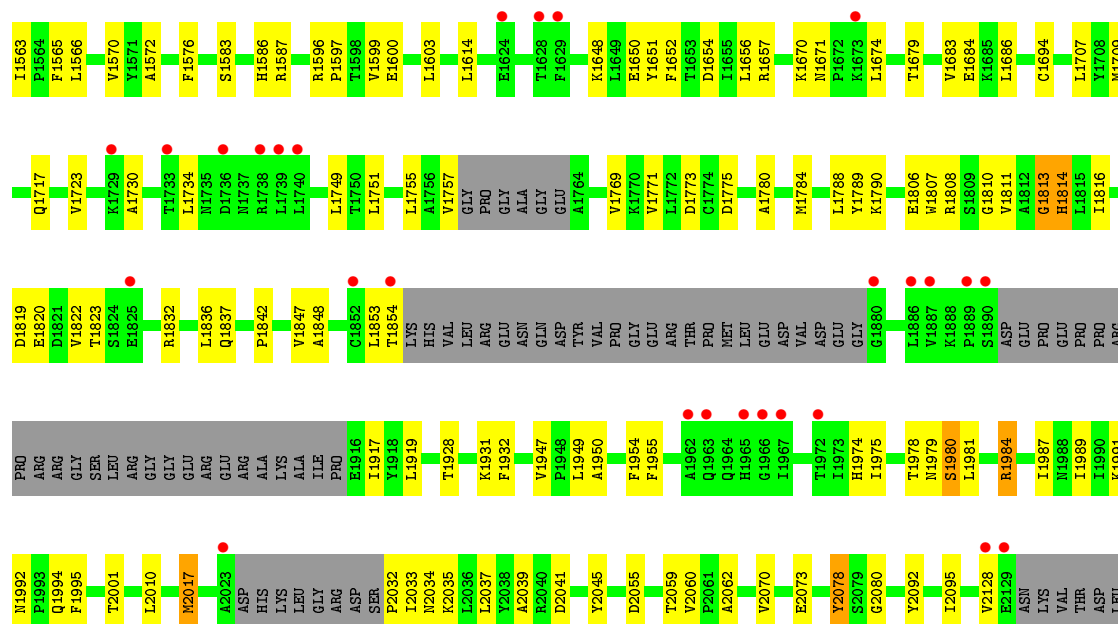


- Molecule 1: Ras-related C3 botulinum toxin substrate 1

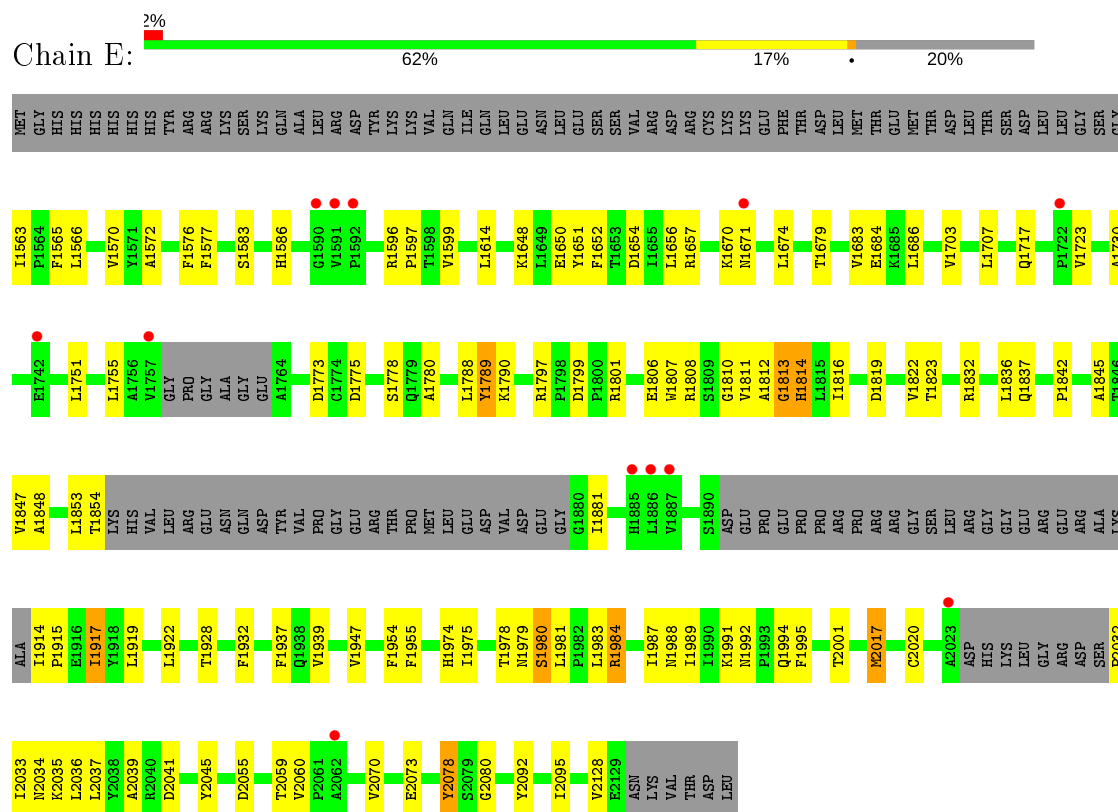


- Molecule 2: Plexin-B1

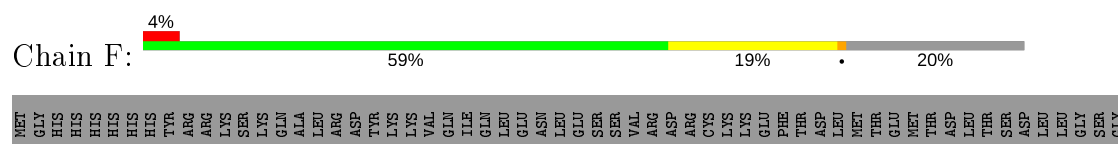




### • Molecule 2: Plexin-B1



### • Molecule 2: Plexin-B1



V2070	T1978	L1886	E1806	L1707	I1563
E2073	M1979	V1887	M1807	Q1717	P1564
Y2078	S1980	K1888	R1808	P1722	F1565
S2079	L1981	P1889	V1811	V1723	L1566
G2080	L1982	S1890	A1812	A1730	K1569
D2081	L1983	ASP	G1813	L1734	V1570
L2082	R1984	GLU	H1814	L1735	Y1571
Y2092	I1987	PRQ	L1815	D1736	A1572
I2095	H1988	GLU	I1816	N1737	F1576
M2115	I1989	PRQ	D1819	D1737	F1577
V2128	I1990	PRQ	V1822	A1738	S1583
E2129	K1991	ARG	T1823	E1742	H1586
ASN	M1992	ARG	S1824	D1743	R1587
LYS	P1993	GLY	E1825	V1744	D1588
VAL	Q1994	SER	R1832	F1745	L1589
THR	F1995	LEU	L1836	V1746	R1596
ASP	T2001	ARG	Q1837	L1749	P1597
LEU	M2004	GLY	L1837	T1750	T1598
	L2009	GLU	P1842	L1751	V1599
	L2010	ARG	V1847	L1755	L1614
	V2011	ARG	A1848	A1756	F1629
	L2012	ALA	L1852	V1757	R1634
	M2017	LYS	C1852	GLY	K1648
	C2020	A1913	L1853	PRO	L1649
	A2023	I1914	T1854	GLY	E1650
ASP	ASP	P1915	LYS	ALA	Y1651
HIS	HIS	E1916	HIS	GLY	D1654
LEU	LEU	I1917	VAL	GLU	L1655
LEU	LYS	Y1918	LEU	D1772	R1657
GLY	LEU	L1919	ARG	D1773	V1668
GLY	LEU	T1928	GLU	C1774	A1669
ARG	GLY	F1932	ASN	D1775	K1670
ASP	ASP	V1939	GLN	S1778	N1671
SER	SER	V1947	ASP	Q1779	P1672
P2032	P2032	P1948	TYR	A1780	K1673
I2033	I2033	L1949	VAL	M1784	L1674
N2034	N2034	F1954	PRO		M1675
K2035	K2035	F1955	GLY		L1676
L2036	L2036	D1959	GLU		T1679
L2037	L2037	E1960	ARG		V1683
Y2038	Y2038	Q1961	THR		E1684
A2039	A2039	A1962	PRO		K1685
K2040	K2040	Q1963	MET		L1686
D2041	D2041	Q1964	LEU		V1703
Y2045	Y2045	S1968	GLY		
D2055	D2055	H1974	GLU		
T2059	T2059	I1975	ASP		
V2060	V2060		VAL		
P2061	P2061		ASP		
A2062	A2062		GLY		
			G1880		
			I1881		
			R1882		
			P1883		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.34Å 224.25Å 258.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 4.39 47.81 – 4.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.81-4.39) 95.6 (47.81-4.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 4.45Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.234 , 0.264 0.256 , 0.287	Depositor DCC
$R_{free}$ test set	1318 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	186.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 205.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.43	0/1422	0.74	2/1933 (0.1%)
1	B	0.45	0/1422	0.72	1/1933 (0.1%)
1	C	0.43	0/1422	0.71	0/1933
2	D	0.48	0/4145	0.75	5/5626 (0.1%)
2	E	0.46	0/4161	0.75	6/5649 (0.1%)
2	F	0.48	0/4166	0.75	6/5656 (0.1%)
All	All	0.47	0/16738	0.74	20/22730 (0.1%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1980	SER	N-CA-C	-8.45	88.18	111.00
2	F	1980	SER	N-CA-C	-7.89	89.71	111.00
2	E	1980	SER	N-CA-C	-7.71	90.20	111.00
2	F	1980	SER	CB-CA-C	7.57	124.49	110.10
2	D	1980	SER	CB-CA-C	7.27	123.91	110.10

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	1392	0	1418	44	0
1	B	1392	0	1418	40	0
1	C	1392	0	1418	41	0
2	D	4061	0	4121	98	0
2	E	4076	0	4139	113	0
2	F	4081	0	4144	118	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	3	0
4	B	32	0	13	3	0
4	C	32	0	13	3	0
All	All	16493	0	16697	436	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 13.

The worst 5 of 436 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:19:LEU:CD1	1:C:165:LEU:HD13	1.35	1.53
1:C:19:LEU:HD11	1:C:165:LEU:CD1	1.45	1.42
1:C:19:LEU:CD1	1:C:165:LEU:CD1	1.94	1.41
1:C:19:LEU:HD12	1:C:165:LEU:CD1	1.74	1.14
2:E:1922:LEU:CD1	2:E:2033:ILE:HD11	1.77	1.14

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	176/184 (96%)	162 (92%)	14 (8%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	176/184 (96%)	163 (93%)	13 (7%)	0	100	100
1	C	176/184 (96%)	161 (92%)	15 (8%)	0	100	100
2	D	493/633 (78%)	430 (87%)	59 (12%)	4 (1%)	19	60
2	E	495/633 (78%)	431 (87%)	61 (12%)	3 (1%)	25	65
2	F	496/633 (78%)	430 (87%)	63 (13%)	3 (1%)	25	65
All	All	2012/2451 (82%)	1777 (88%)	225 (11%)	10 (0%)	29	68

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2039	ALA
2	E	1670	LYS
2	E	2039	ALA
2	F	2039	ALA
2	D	1670	LYS

### 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	154/160 (96%)	154 (100%)	0	100	100
1	B	154/160 (96%)	152 (99%)	2 (1%)	69	82
1	C	154/160 (96%)	154 (100%)	0	100	100
2	D	448/563 (80%)	443 (99%)	5 (1%)	73	85
2	E	450/563 (80%)	443 (98%)	7 (2%)	62	79
2	F	450/563 (80%)	441 (98%)	9 (2%)	55	74
All	All	1810/2169 (83%)	1787 (99%)	23 (1%)	69	82

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	1932	PHE

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Mol	Chain	Res	Type
2	E	2017	MET
2	F	2017	MET
2	E	1984	ARG
2	E	2078	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1611	ASN
2	E	1930	GLN
2	F	1992	ASN
2	E	1671	ASN
2	E	1961	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	GNP	B	200	3	28,34,34	1.98	5 (17%)	30,54,54	2.16	10 (33%)
4	GNP	C	200	3	28,34,34	1.97	5 (17%)	30,54,54	2.11	9 (30%)
4	GNP	A	200	3	28,34,34	2.07	5 (17%)	30,54,54	2.10	11 (36%)

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	GNP	B	200	3	-	7/17/38/38	0/3/3/3
4	GNP	C	200	3	-	8/17/38/38	0/3/3/3
4	GNP	A	200	3	-	7/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	200	GNP	C4-N9	-7.09	1.38	1.47
4	C	200	GNP	C4-N9	-6.77	1.38	1.47
4	B	200	GNP	C4-N9	-6.41	1.39	1.47
4	C	200	GNP	C5-C6	-4.34	1.45	1.52
4	A	200	GNP	C5-C6	-4.30	1.45	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	200	GNP	PA-O3A-PB	-6.00	111.50	132.62
4	C	200	GNP	PA-O3A-PB	-5.95	111.68	132.62
4	A	200	GNP	PA-O3A-PB	-5.80	112.18	132.62
4	B	200	GNP	C4-C5-N7	4.09	107.88	102.46
4	A	200	GNP	C4-C5-N7	3.77	107.46	102.46

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	200	GNP	PB-N3B-PG-O1G
4	C	200	GNP	PG-N3B-PB-O1B
4	C	200	GNP	PG-N3B-PB-O3A
4	C	200	GNP	C5'-O5'-PA-O3A

*Continued on next page...*

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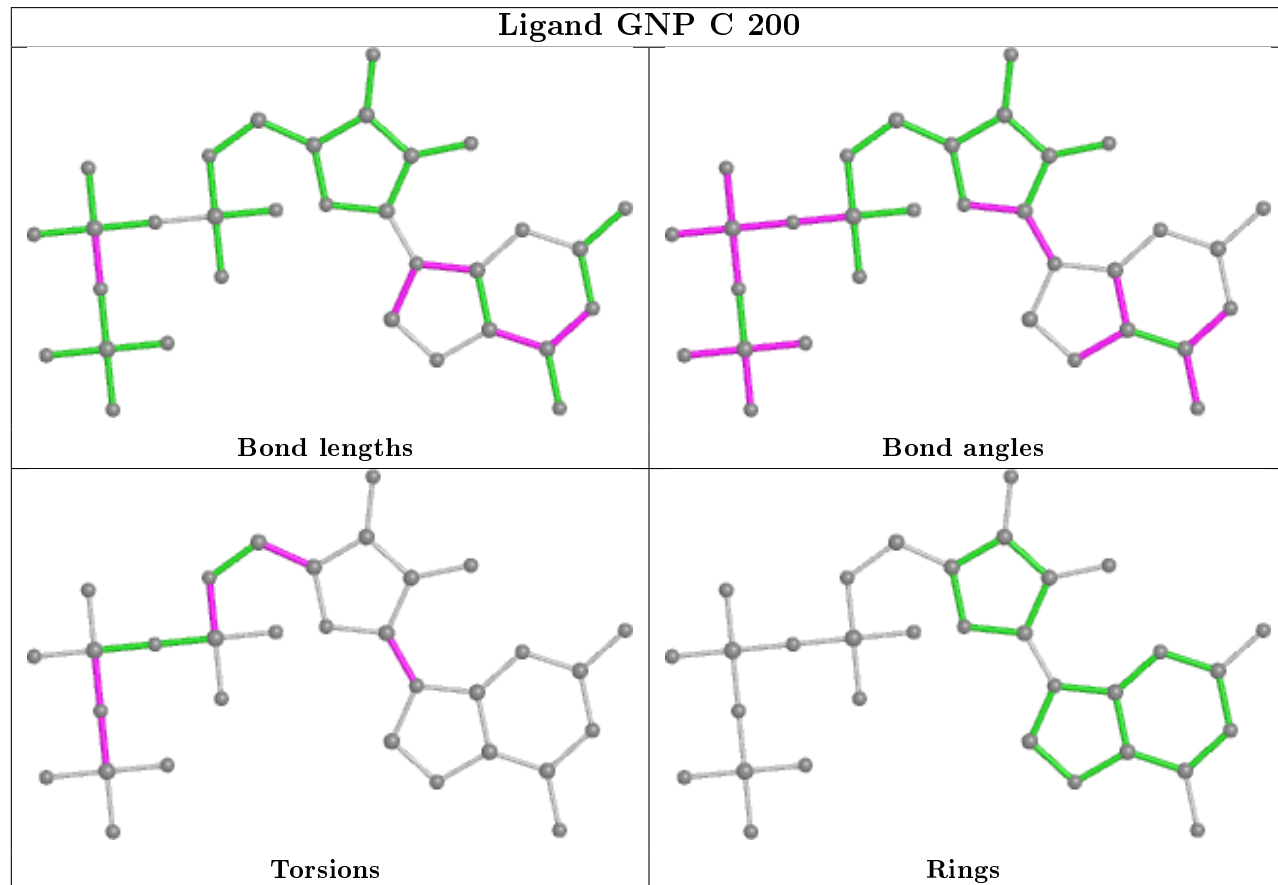
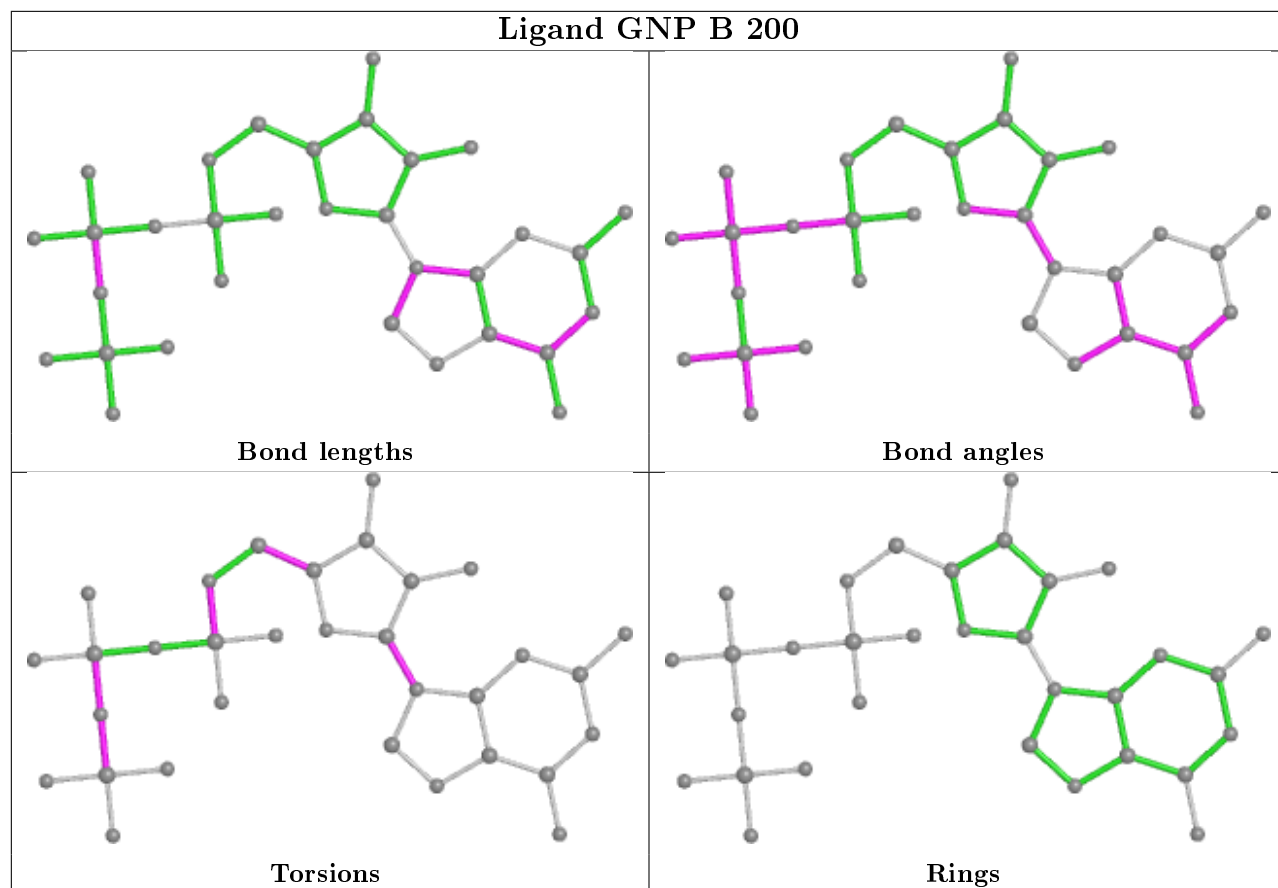
Mol	Chain	Res	Type	Atoms
4	C	200	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

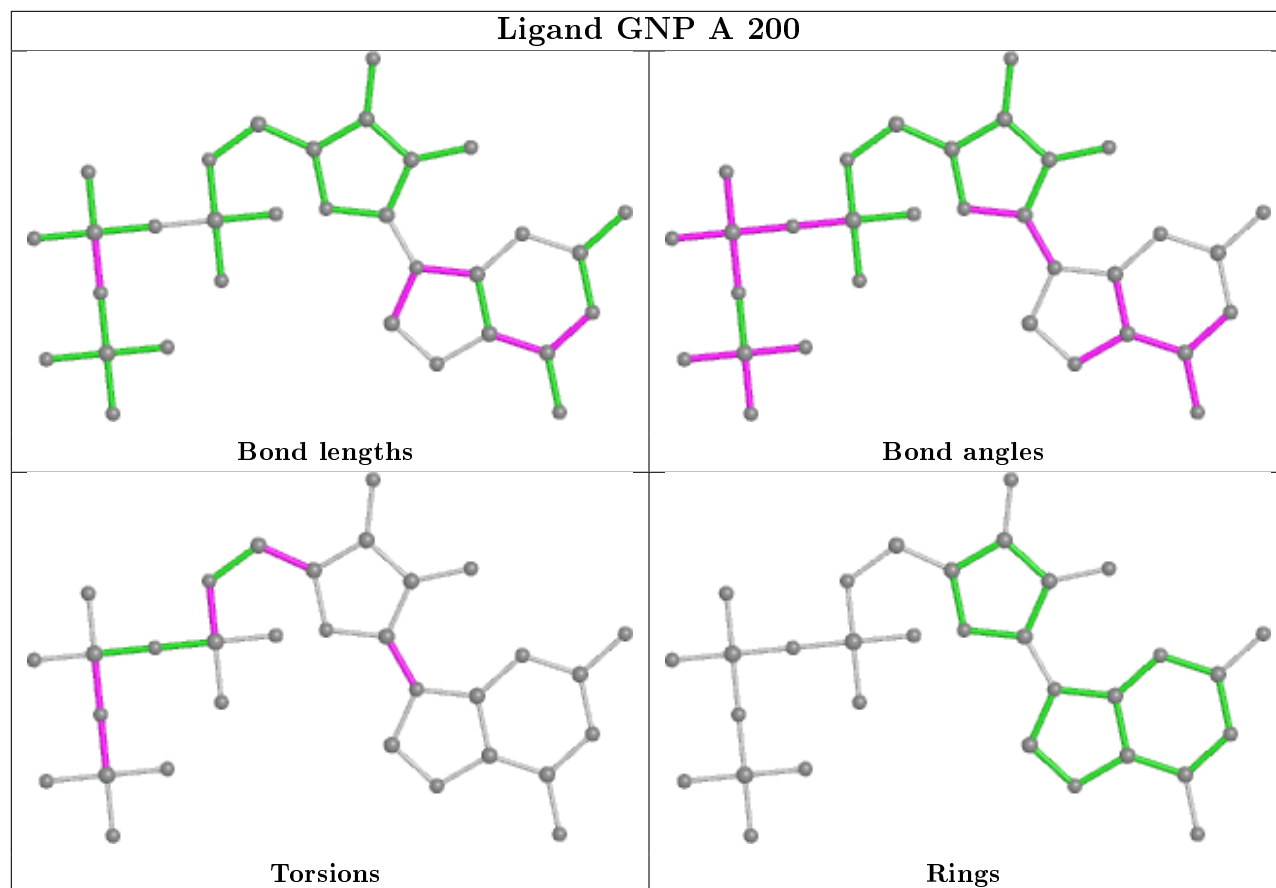
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	200	GNP	3	0
4	C	200	GNP	3	0
4	A	200	GNP	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	178/184 (96%)	0.23	9 (5%) 28 24	41, 112, 244, 271	0
1	B	178/184 (96%)	0.25	4 (2%) 62 52	20, 92, 190, 252	0
1	C	178/184 (96%)	0.59	18 (10%) 7 7	46, 138, 250, 281	0
2	D	503/633 (79%)	0.17	27 (5%) 25 22	21, 90, 253, 287	0
2	E	505/633 (79%)	0.12	12 (2%) 59 49	21, 120, 266, 296	0
2	F	506/633 (79%)	0.18	28 (5%) 25 22	20, 101, 257, 281	0
All	All	2048/2451 (83%)	0.21	98 (4%) 30 26	20, 107, 255, 296	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1722	PRO	5.3
2	E	1591	VAL	4.5
2	F	1961	GLN	4.3
2	F	1882	ARG	4.3
2	D	1733	THR	4.2

### 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](#)

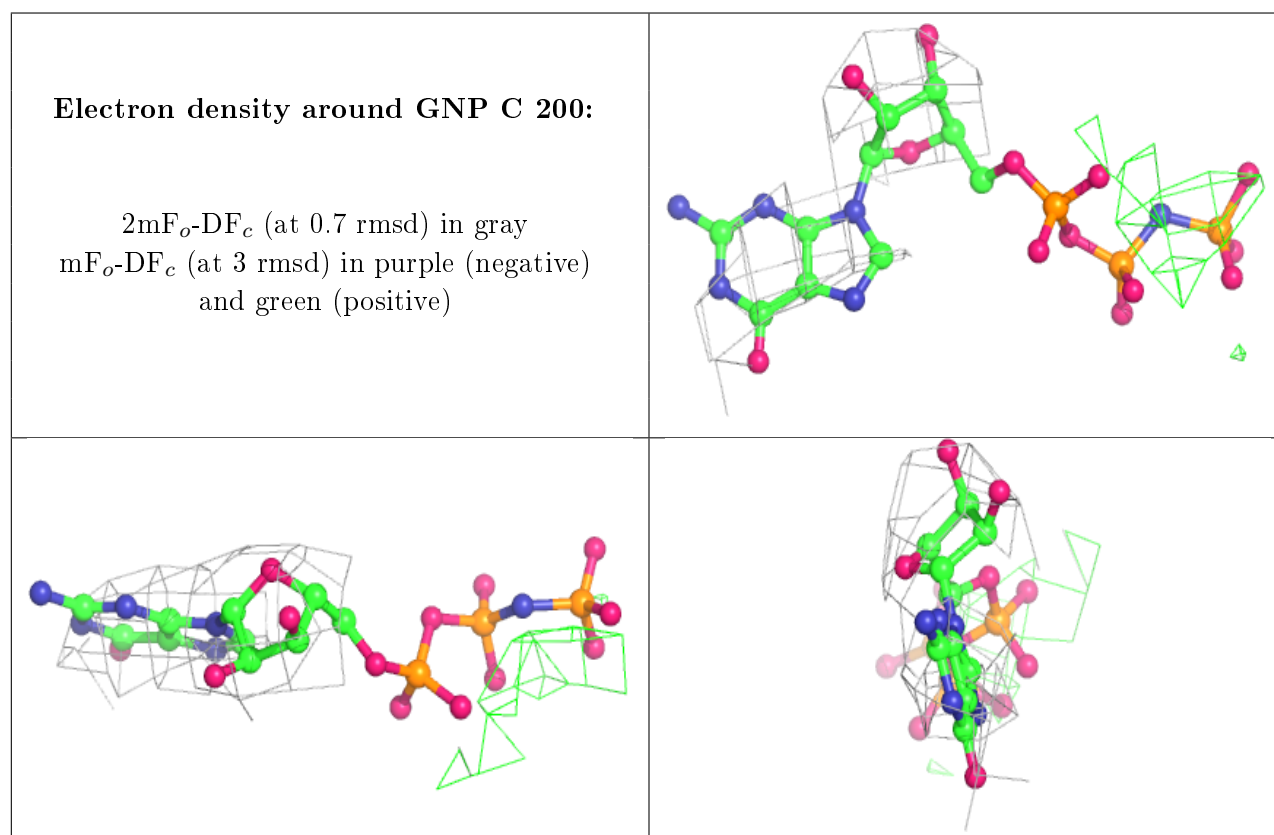
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

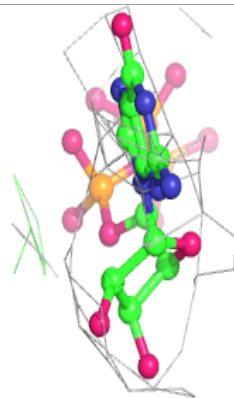
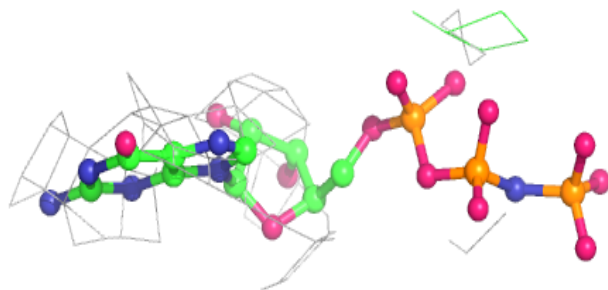
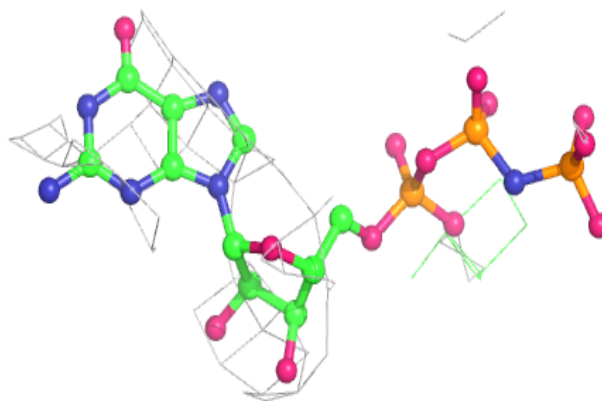
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GNP	C	200	32/32	0.87	0.29	99,127,142,151	0
4	GNP	A	200	32/32	0.88	0.26	69,89,107,121	0
4	GNP	B	200	32/32	0.90	0.27	47,62,77,79	0
3	MG	B	201	1/1	0.94	0.16	19,19,19,19	0
3	MG	A	201	1/1	0.97	0.09	38,38,38,38	0
3	MG	C	201	1/1	0.98	0.16	57,57,57,57	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.

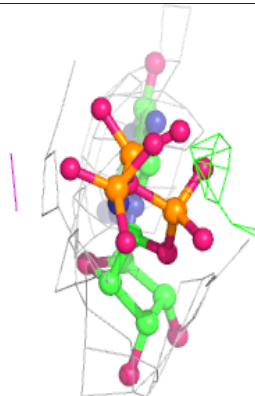
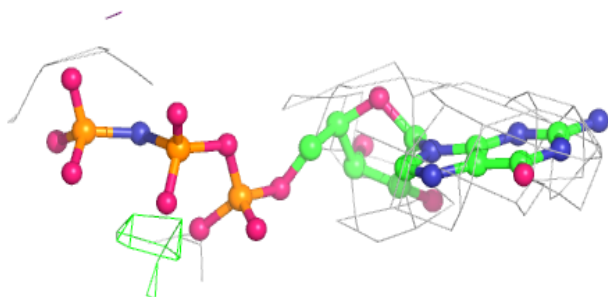
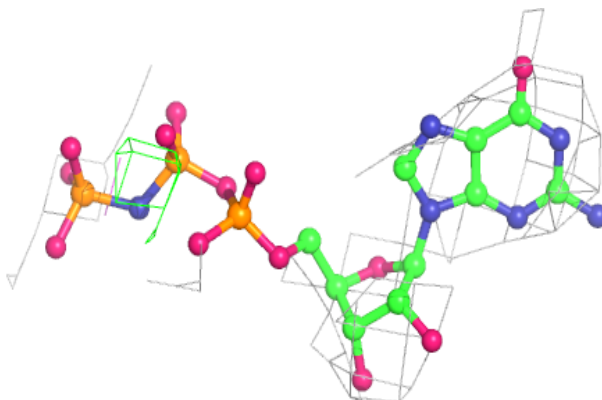


**Electron density around GNP A 200:**

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

**Electron density around GNP B 200:**

$2mF_o-DF_c$  (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.