wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 12:24 PM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

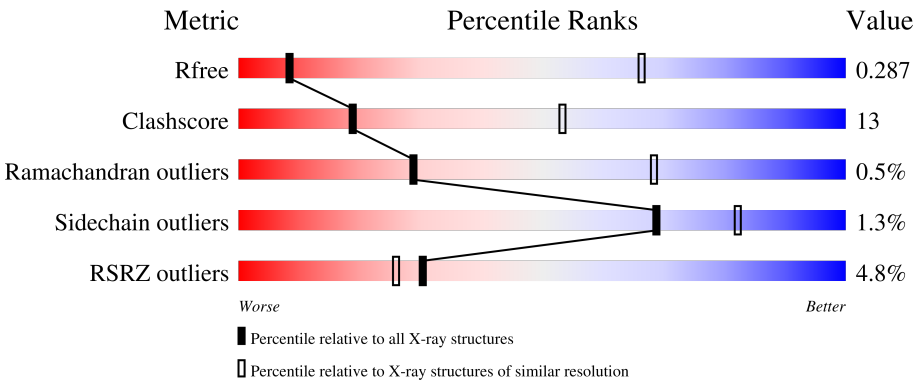
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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 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	184	5%, 70%, 26%, • •
1	B	184	2%, 73%, 23%, • •
1	C	184	10%, 76%, 21%, •
2	D	633	4%, 61%, 17%, •, 21%
2	E	633	2%, 62%, 17%, •, 20%

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Mol	Chain	Length	Quality of chain
2	F	633	4% 59% 19% • 20%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	178	1392	895	230	259	8	0	0	0
1	B	178	1392	895	230	259	8	0	0	0
1	C	178	1392	895	230	259	8	0	0	0

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
			Total	C	N	O	S			
2	D	503	4061	2608	698	741	14	0	0	0
2	E	505	4076	2619	700	743	14	0	0	0
2	F	506	4081	2622	701	744	14	0	0	0

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
			Total	Mg		
3	A	1	1	1	0	0

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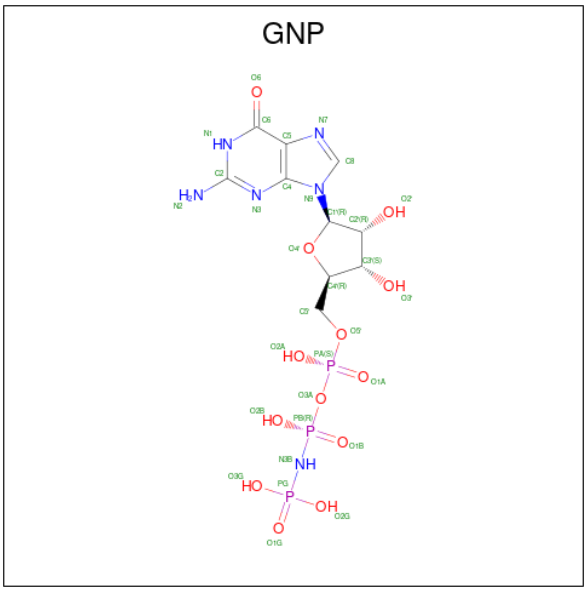
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0
			Total	Mg		
3	C	1	1	1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



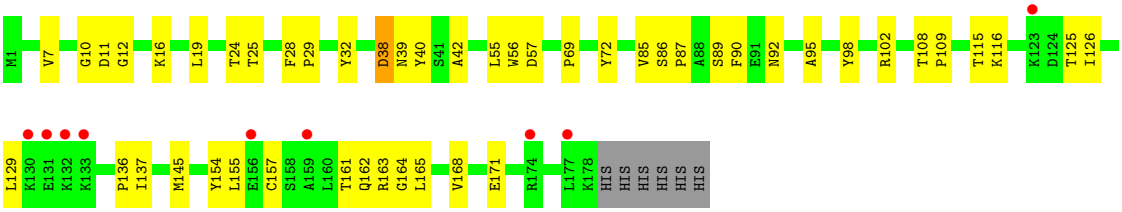
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	32	10	6	13	3	0	0
			Total	C	N	O	P		
4	B	1	32	10	6	13	3	0	0
			Total	C	N	O	P		
4	C	1	32	10	6	13	3	0	0

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.

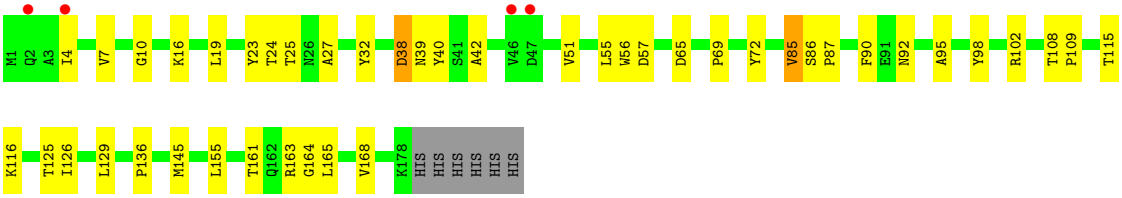
• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain A:



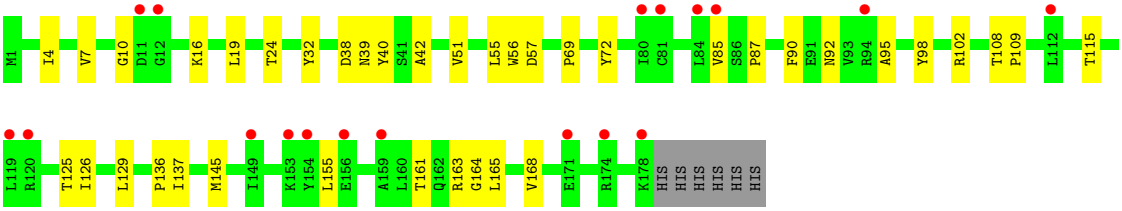
• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain B:



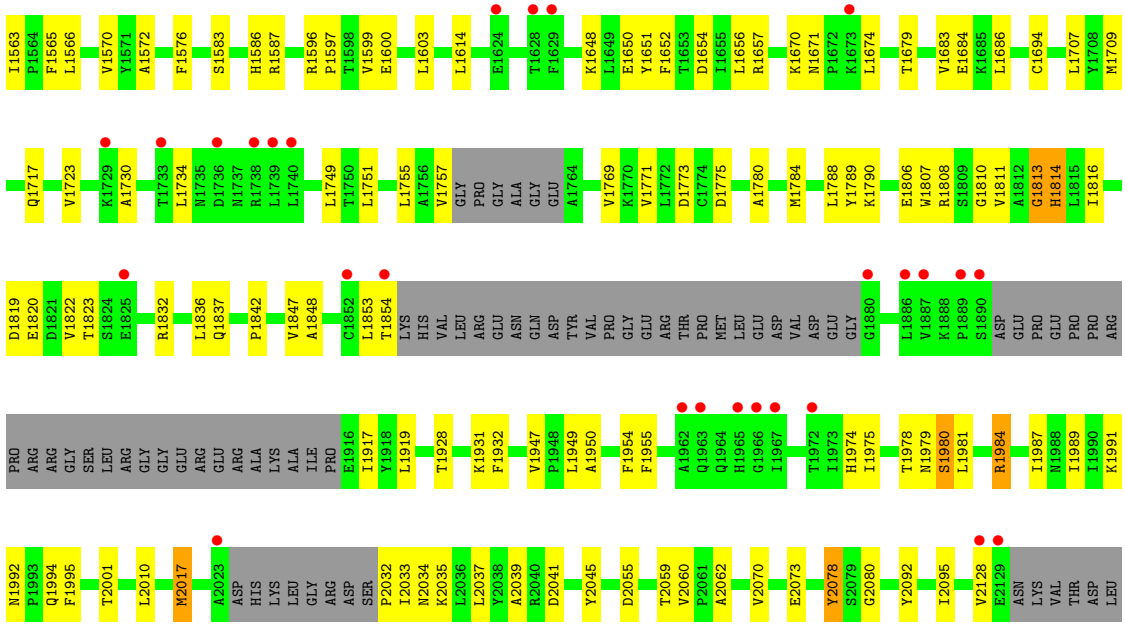
• Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain C:



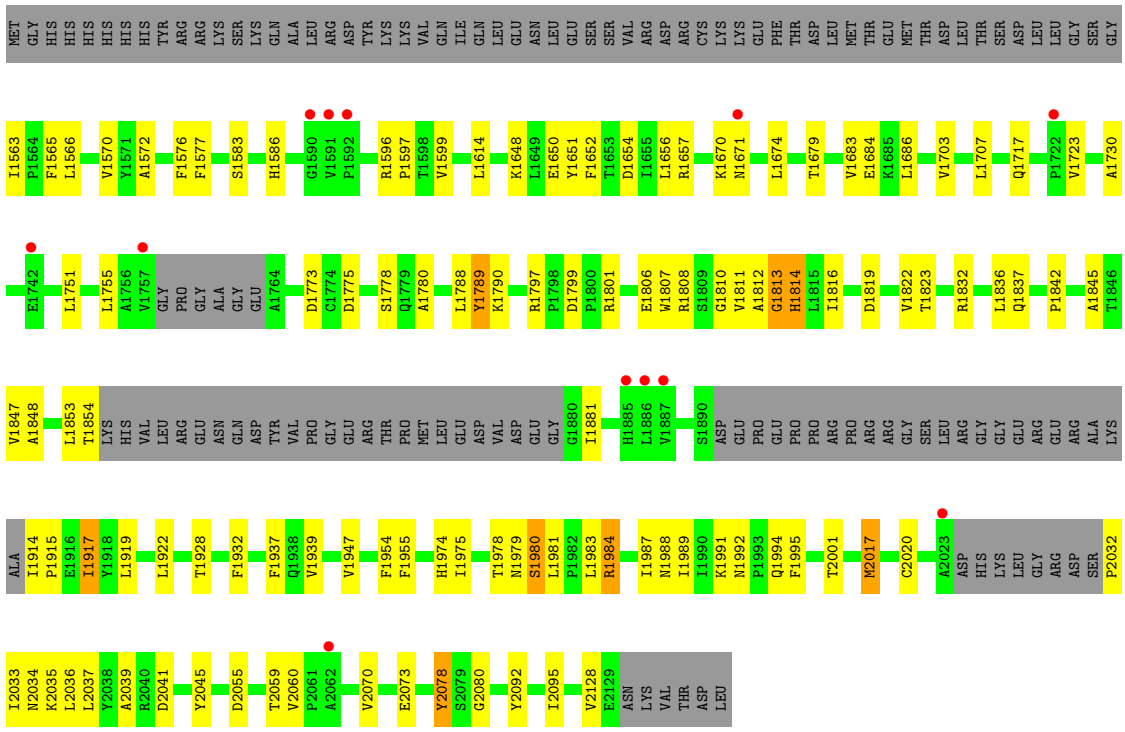
• Molecule 2: Plexin-B1

Chain D:



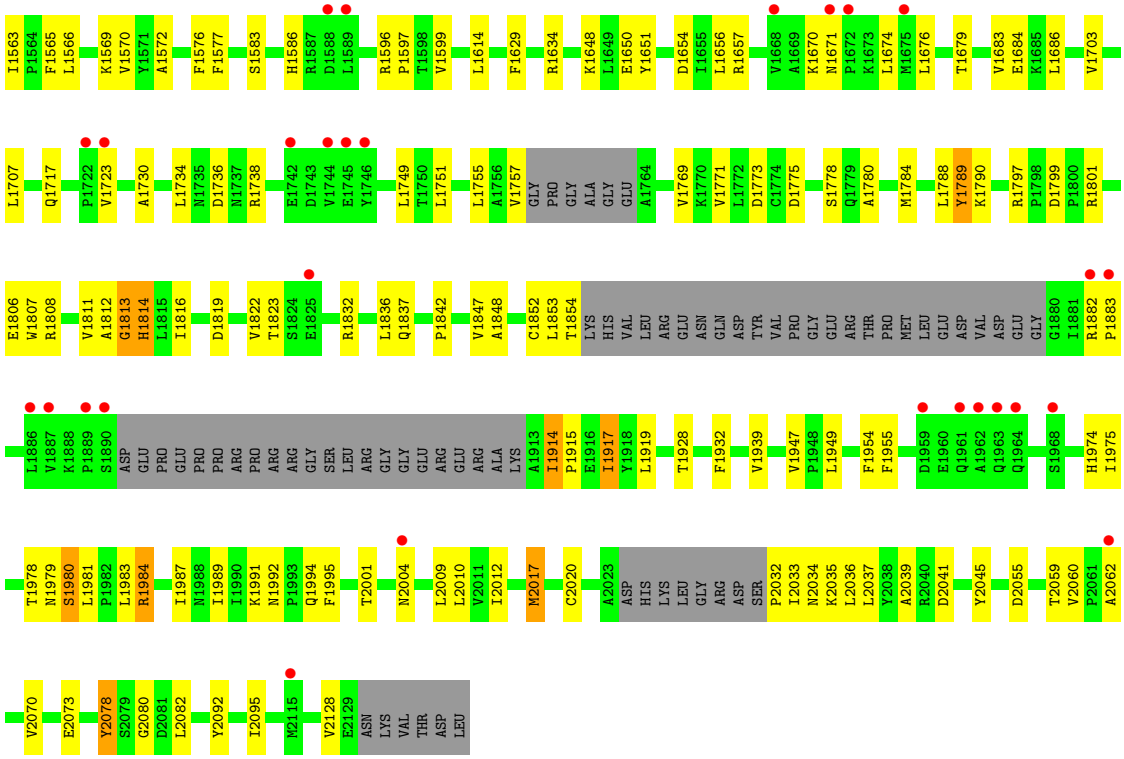
- Molecule 2: Plexin-B1

Chain E: 2% 62% 17% 20%



- Molecule 2: Plexin-B1

Chain F: 4% 59% 19% 20%


I1563 P1564 F1565 L1566 K1569 V1570 Y1571 A1572 F1576 F1577 S1583 H1586 R1587 D1588 L1589 R1596 P1597 T1598 V1599 L1614 F1629 R1634 K1648 L1649 E1650 Y1651 D1654 I1655 L1656 R1657 V1668 A1669 K1670 N1671 P1672 K1673 L1674 M1675 L1676 T1679 V1683 E1684 K1685 L1686 V1703
L1707 Q1717 P1722 V1723 A1730 L1734 N1735 D1736 N1737 R1738 E1742 D1743 V1744 E1745 Y1746 L1749 T1750 L1751 L1755 A1756 V1757 GLY PRO GLY ALA GLY GLU A1764 V1769 K1770 V1771 L1772 D1773 C1774 D1775 S1778 Q1779 A1780 M1784 L1788 Y1789 K1790 R1797 P1798 D1799 P1800 R1801
E1806 W1807 R1808 V1811 A1812 G1813 H1814 L1815 I1816 D1819 V1822 T1823 S1824 E1825 R1832 L1836 Q1837 P1842 V1847 A1848 C1852 L1853 T1854 LYS HIS VAL LEU ARG GLU ASN GLN ASP TYR VAL PRO GLY GLU ARG THR PRO MET LEU GLU ASP VAL ASP GLU GLY G1880 I1881 R1882 P1883
L1886 V1887 K1888 P1889 S1890 ASP GLU PRO GLU PRO PRO ARG PRO ARG ARG ARG GLY SER LEU ARG GLY GLY GLU ARG GLU ARG ALA LYS A1913 I1914 P1915 E1916 I1917 Y1918 L1919 T1928 F1932 V1939 V1947 P1948 L1949 F1954 F1955 D1959 E1960 Q1961 A1962 Q1963 Q1964 S1968 H1974 I1975
T1978 N1979 S1980 L1981 P1982 L1983 R1984 I1987 N1988 I1989 I1990 K1991 N1992 P1993 Q1994 F1995 T2001 N2004 L2009 L2010 V2011 I2012 M2017 C2020 A2023 ASP HIS LYS LEU GLY ARG ASP SER P2032 I2033 N2034 K2035 L2036 L2037 Y2038 A2039 R2040 D2041 Y2045 D2055 T2059 V2060 P2061 A2062
V2070 E2073 Y2078 S2079 G2080 D2081 L2082 Y2092 I2095 M2115 V2128 E2129 ASN LYS VAL THR ASP LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	186.5	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 205.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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^2)	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.*

[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 (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 (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	176/184 (96%)	162 (92%)	14 (8%)	0	100 100

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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 (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	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	F	1736	ASP

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Mol	Chain	Res	Type
2	F	1852	CYS
2	F	1832	ARG
2	F	1914	ILE
2	D	2078	TYR

Sometimes 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	1961	GLN
2	E	2089	HIS
2	F	2000	GLN
2	E	2000	GLN
2	F	1611	ASN

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 monosaccharides 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	A	200	3	29,34,34	1.62	5 (17%)	33,54,54	2.36	13 (39%)
4	GNP	B	200	3	29,34,34	1.72	6 (20%)	33,54,54	2.39	11 (33%)
4	GNP	C	200	3	29,34,34	1.52	6 (20%)	33,54,54	2.42	13 (39%)

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	A	200	3	-	6/14/38/38	0/3/3/3
4	GNP	B	200	3	-	6/14/38/38	0/3/3/3
4	GNP	C	200	3	-	6/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	200	GNP	O4'-C1'	4.03	1.46	1.41
4	A	200	GNP	O4'-C1'	4.02	1.46	1.41
4	C	200	GNP	O4'-C1'	3.53	1.46	1.41
4	B	200	GNP	C2'-C1'	3.34	1.58	1.53
4	A	200	GNP	C2'-C1'	3.02	1.58	1.53

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	200	GNP	C2-N3-C4	6.46	122.74	115.36
4	A	200	GNP	C2-N3-C4	6.14	122.37	115.36
4	B	200	GNP	PB-O3A-PA	-6.00	111.50	132.62
4	C	200	GNP	PB-O3A-PA	-5.95	111.68	132.62
4	B	200	GNP	C2-N3-C4	5.81	121.99	115.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

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

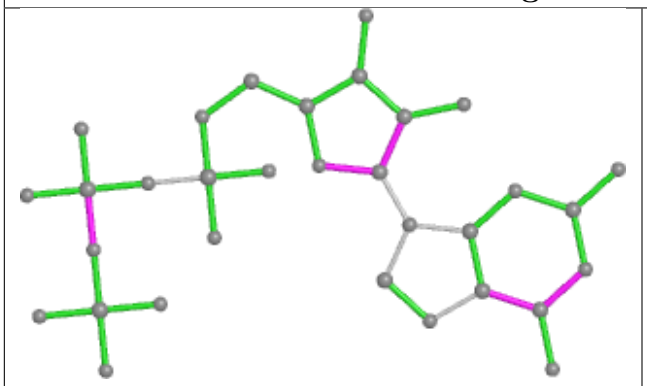
There are no ring outliers.

3 monomers are involved in 9 short contacts:

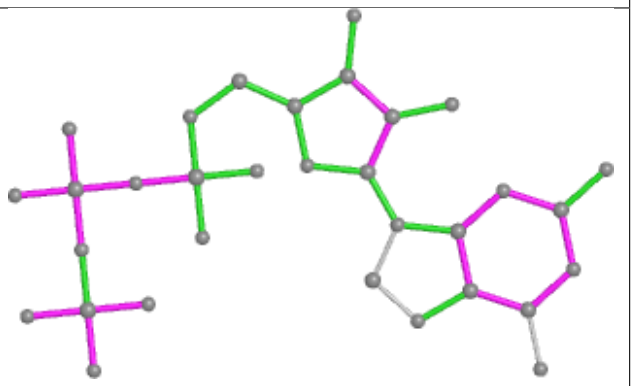
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	GNP	3	0
4	B	200	GNP	3	0
4	C	200	GNP	3	0

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 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.

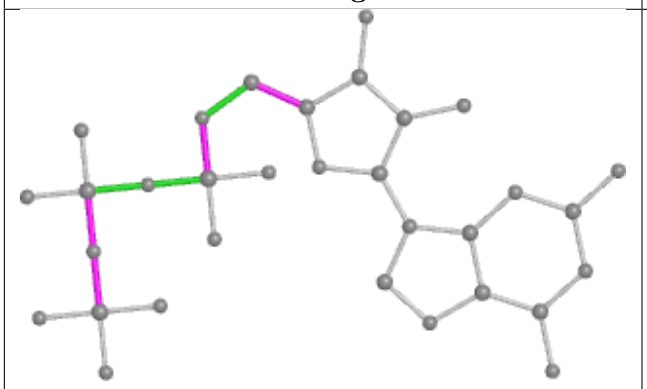
Ligand GNP A 200



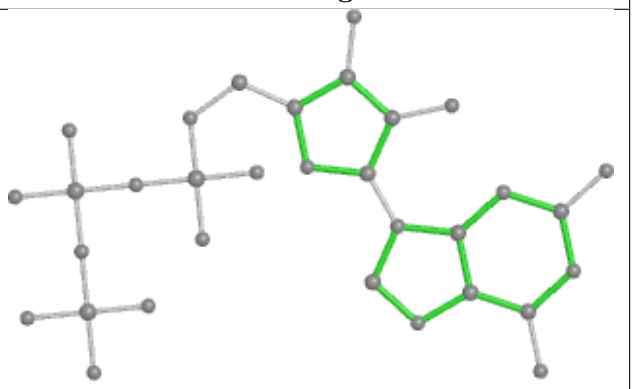
Bond lengths



Bond angles

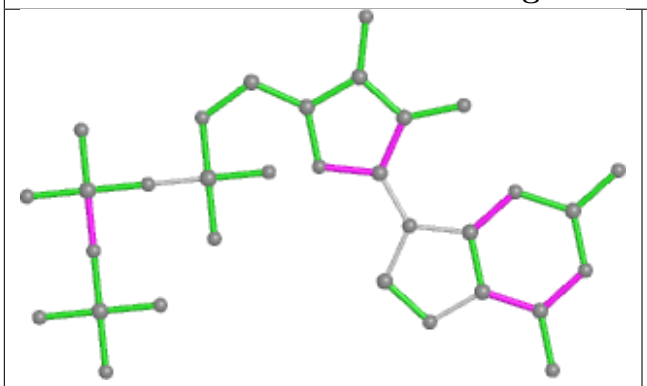


Torsions

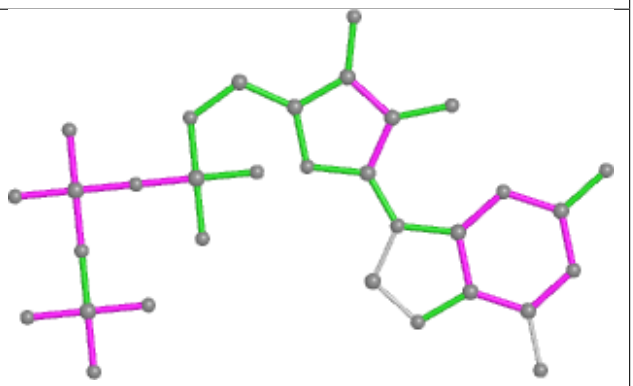


Rings

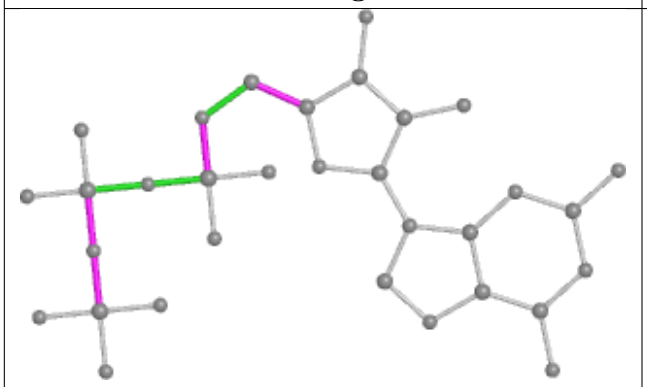
Ligand GNP B 200



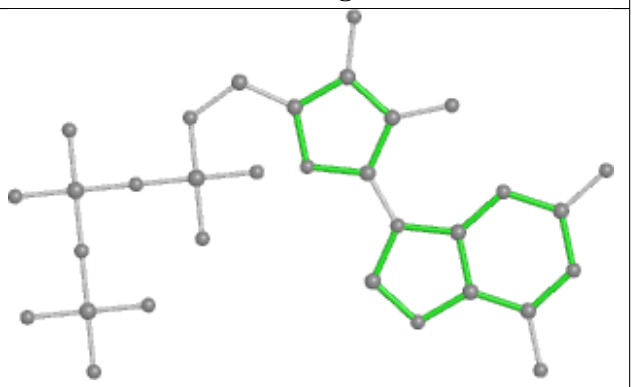
Bond lengths



Bond angles

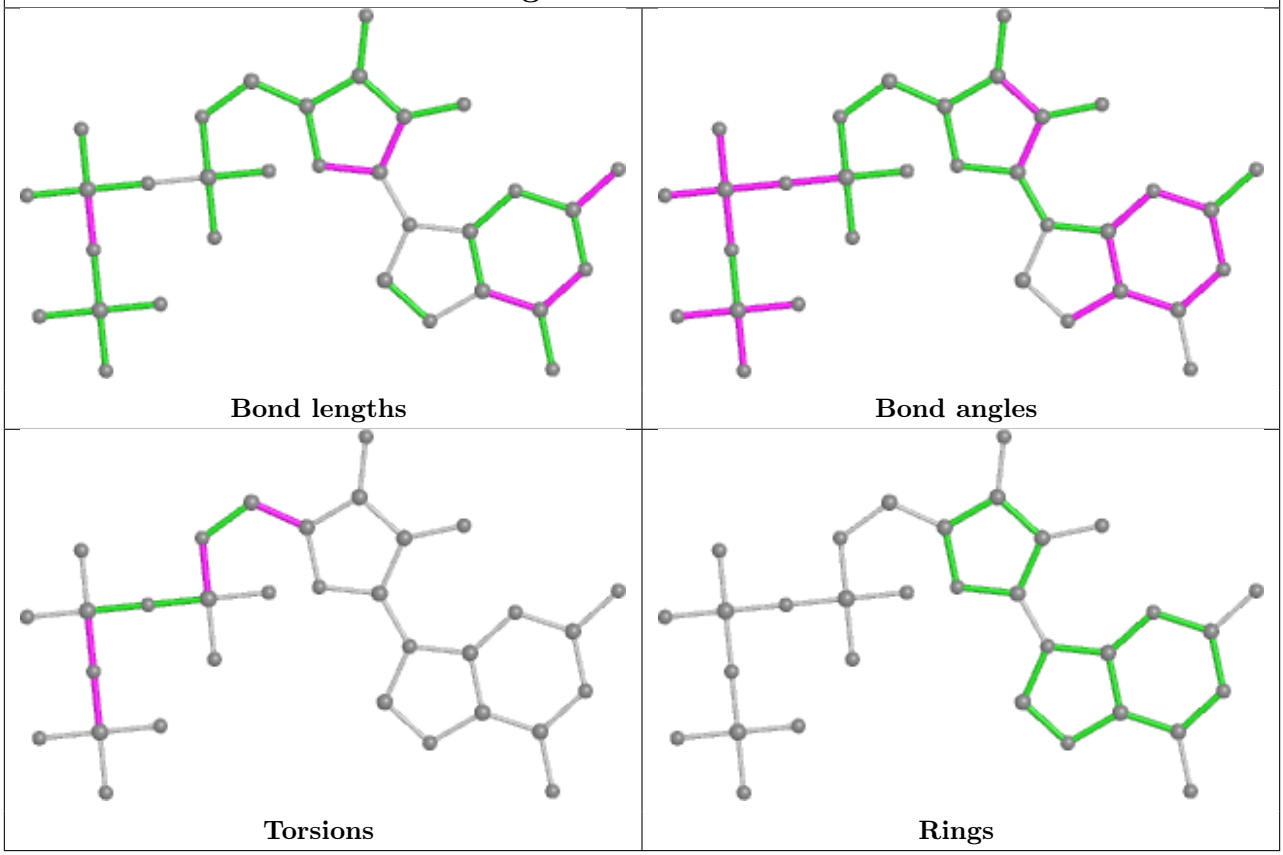


Torsions



Rings

Ligand GNP C 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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 monosaccharides in this entry.

6.4 Ligands (i)

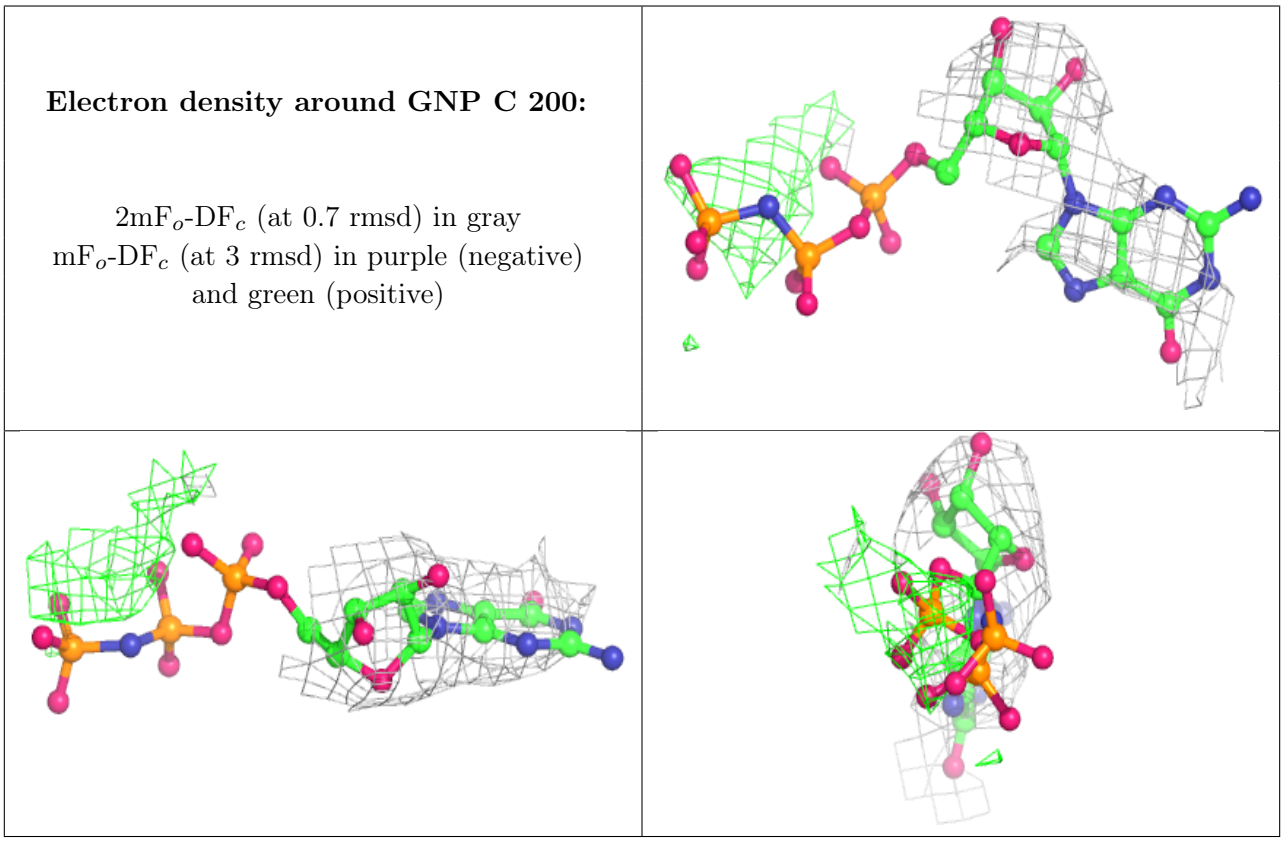
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	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.

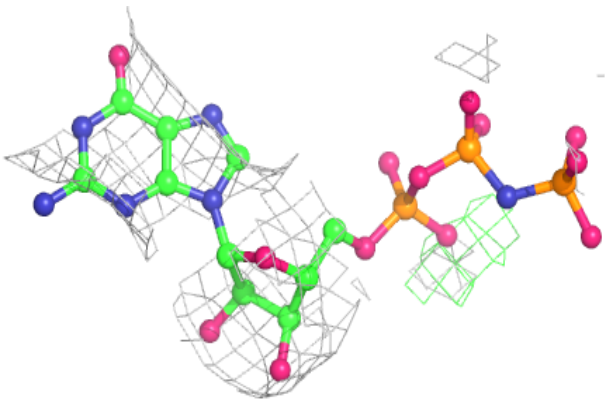
Electron density around GNP C 200:

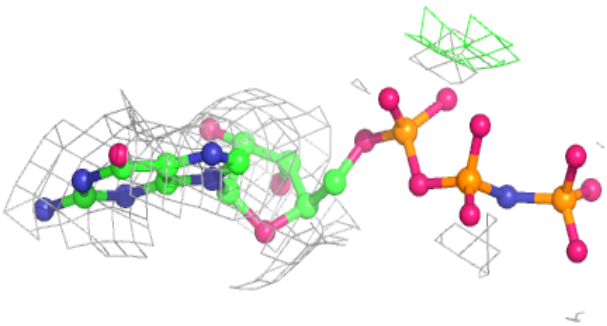
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

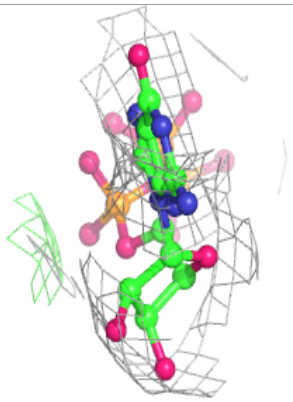


Electron density around GNP A 200:

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

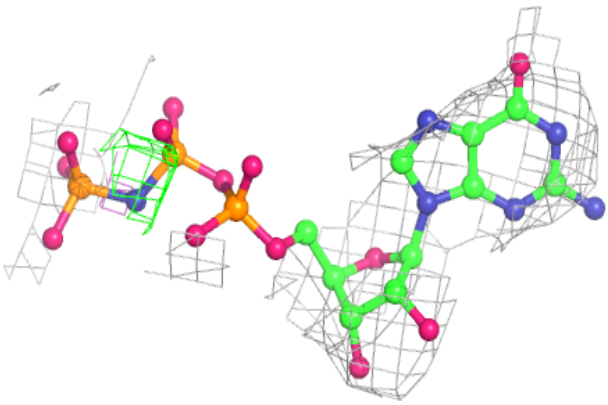


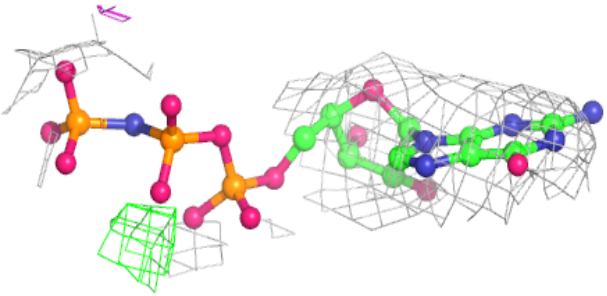


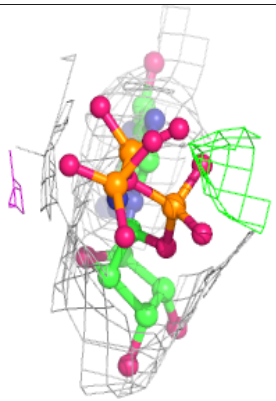


Electron density around GNP B 200:

$2mF_o$-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.