



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 03:07 pm BST

PDB ID : 3RYT  
Title : The Plexin A1 intracellular region in complex with Rac1  
Authors : Zhang, X.; He, H.  
Deposited on : 2011-05-11  
Resolution : 3.58 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](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

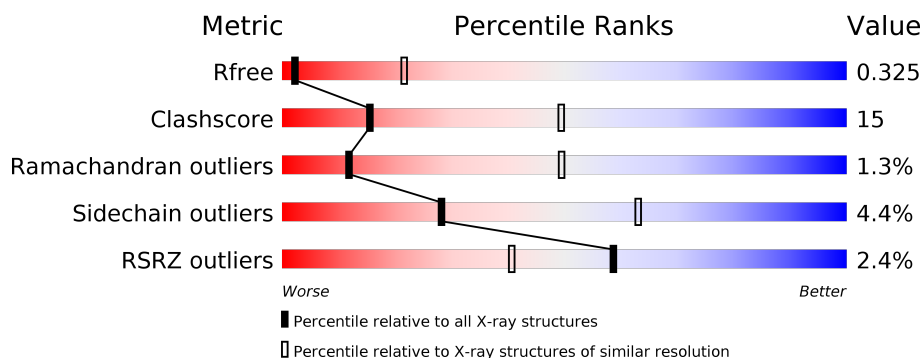
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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	626	<div> <div>2%</div> <div>58%</div> <div>25%</div> <div>•</div> <div>15%</div> </div>
1	B	626	<div> <div>2%</div> <div>64%</div> <div>19%</div> <div>•</div> <div>15%</div> </div>
2	C	180	<div> <div>3%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9112 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 Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			3954	2533	663	737	21			
1	B	531	Total	C	N	O	S	0	0	0
			3852	2447	663	721	21			

- Molecule 2 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1273	820	208	239	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P63000
C	-1	PRO	-	EXPRESSION TAG	UNP P63000
C	0	HIS	-	EXPRESSION TAG	UNP P63000
C	61	LEU	GLN	ENGINEERED MUTATION	UNP P63000

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

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

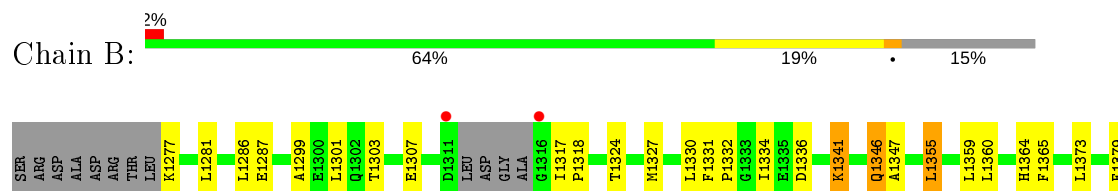
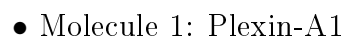
- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

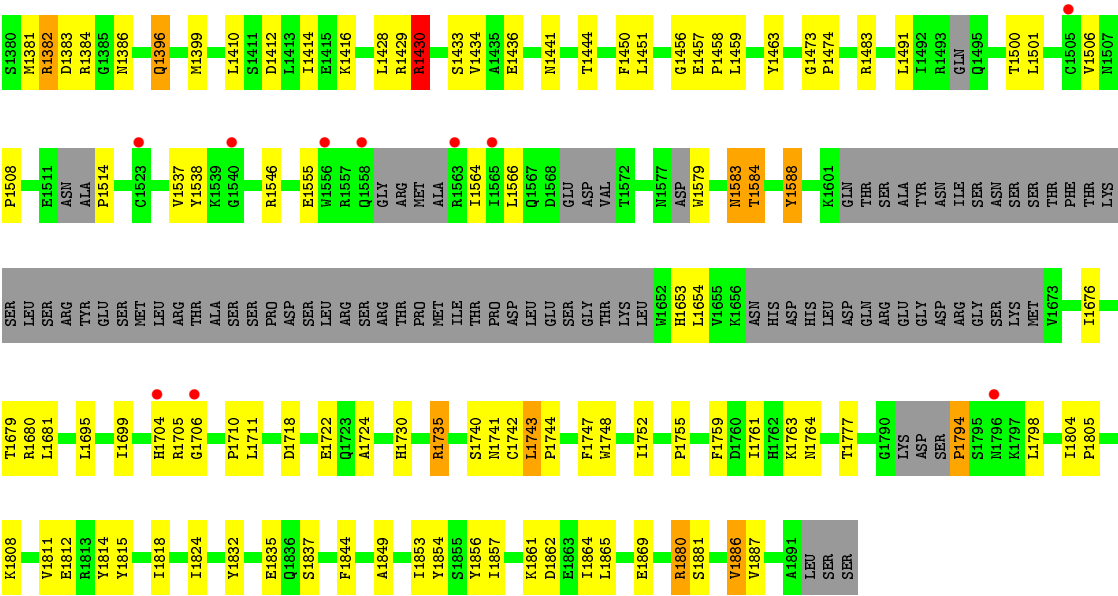


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

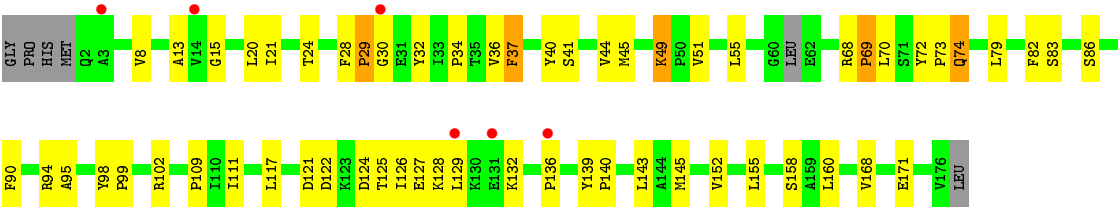


- Molecule 1: Plexin-A1





● Molecule 2: Ras-related C3 botulinum toxin substrate 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.78 Å 110.78 Å 265.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 3.58 49.54 – 3.58	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.54-3.58) 91.4 (49.54-3.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 3.57 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.270 , 0.340 0.248 , 0.325	Depositor DCC
$R_{free}$ test set	970 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 183.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9112	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.26	0/4029	0.37	1/5490 (0.0%)
1	B	0.29	0/3923	0.38	2/5351 (0.0%)
2	C	0.25	0/1302	0.38	0/1787
All	All	0.27	0/9254	0.38	3/12628 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1794	PRO	N-CA-CB	6.01	110.52	103.30
1	B	1514	PRO	N-CA-CB	5.93	110.42	103.30
1	B	1794	PRO	N-CA-CB	5.88	110.35	103.30

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	3954	0	3660	125	0
1	B	3852	0	3398	95	0
2	C	1273	0	1198	45	0
3	C	1	0	0	0	0
4	C	32	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9112	0	8269	258	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 15.

All (258) 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:A:1337:HIS:HB3	1:A:1338:PRO:HA	1.26	1.09
1:A:1743:LEU:HB3	1:A:1744:PRO:HD3	1.51	0.92
1:B:1373:LEU:HB3	1:B:1379:PHE:HZ	1.35	0.90
1:A:1580:LYS:HB3	1:A:1651:LEU:HG	1.54	0.89
1:A:1381:MET:HA	1:A:1384:ARG:HD3	1.58	0.85
1:A:1365:PHE:HB2	1:A:1879:LEU:HD11	1.59	0.84
1:A:1510:HIS:CD2	1:A:1513:ALA:HB3	2.12	0.84
1:B:1331:PHE:HB3	1:B:1334:ILE:HD12	1.59	0.82
1:A:1508:PRO:HD2	1:A:1537:VAL:HG11	1.63	0.81
1:A:1337:HIS:HB3	1:A:1338:PRO:CA	2.11	0.79
1:B:1373:LEU:HB3	1:B:1379:PHE:CZ	2.20	0.76
1:B:1711:LEU:HD22	1:B:1824:ILE:HD13	1.68	0.76
1:A:1474:PRO:HD2	1:A:1483:ARG:HB2	1.69	0.75
1:A:1477:ALA:HB2	1:A:1528:GLN:HE21	1.52	0.74
1:B:1341:LYS:H	1:B:1341:LYS:HD2	1.51	0.74
1:B:1346:GLN:HA	1:B:1346:GLN:HE21	1.54	0.72
2:C:8:VAL:HG21	2:C:20:LEU:HD21	1.72	0.72
2:C:45:MET:HG2	2:C:49:LYS:H	1.55	0.71
1:B:1743:LEU:HB3	1:B:1744:PRO:HD3	1.71	0.70
1:A:1440:THR:OG1	1:A:1746:ARG:HD3	1.91	0.70
1:A:1695:LEU:O	1:A:1699:ILE:HG13	1.92	0.69
1:B:1459:LEU:HD22	1:B:1759:PHE:HE2	1.57	0.69
1:A:1379:PHE:HB2	1:A:1383:ASP:HB2	1.75	0.69
1:A:1507:ASN:HB3	1:A:1510:HIS:CE1	2.28	0.68
1:A:1561:MET:CE	2:C:41:SER:HB2	2.25	0.67
1:A:1816:ALA:O	1:A:1820:LYS:HG2	1.96	0.66
1:B:1412:ASP:HB3	1:B:1416:LYS:HE3	1.76	0.66
1:B:1396:GLN:HE21	1:B:1396:GLN:HA	1.60	0.66
2:C:36:VAL:O	2:C:37:PHE:HB3	1.96	0.65
1:A:1513:ALA:HB1	1:A:1514:PRO:HD2	1.78	0.64
2:C:83:SER:HB3	2:C:86:SER:HB3	1.78	0.64
1:A:1365:PHE:HD1	1:A:1879:LEU:HD21	1.62	0.64
1:A:1423:HIS:H	1:B:1303:THR:HG21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1382:ARG:HD3	1:B:1382:ARG:C	2.19	0.63
1:B:1755:PRO:HD2	1:B:1763:LYS:HD3	1.80	0.63
1:A:1525:THR:HB	1:A:1528:GLN:HG3	1.81	0.62
1:A:1525:THR:HG22	1:A:1527:THR:H	1.64	0.62
1:A:1800:TYR:O	1:A:1804:ILE:HG12	1.98	0.62
1:B:1832:TYR:O	1:B:1835:GLU:HG2	2.00	0.62
1:A:1808:LYS:O	1:A:1811:VAL:HG12	2.00	0.61
1:B:1491:LEU:HD12	1:B:1681:LEU:HD21	1.83	0.61
1:A:1776:GLN:HB3	1:A:1796:ASN:HD21	1.66	0.61
1:A:1423:HIS:H	1:B:1303:THR:CG2	2.14	0.60
1:A:1564:ILE:HG21	2:C:70:LEU:HB3	1.82	0.60
1:B:1724:ALA:HB1	1:B:1735:ARG:HD2	1.83	0.60
1:B:1428:LEU:O	1:B:1741:ASN:HB3	2.02	0.60
1:A:1355:LEU:HD13	1:A:1886:VAL:HA	1.84	0.59
2:C:13:ALA:H	4:C:179:GNP:HNB3	1.49	0.59
2:C:32:TYR:CE1	2:C:34:PRO:HD3	2.37	0.59
1:A:1337:HIS:CB	1:A:1338:PRO:HA	2.16	0.59
1:B:1346:GLN:HG3	1:B:1347:ALA:H	1.67	0.59
1:B:1330:LEU:HD22	1:B:1441:ASN:ND2	2.19	0.58
1:B:1814:TYR:O	1:B:1818:ILE:HG13	2.04	0.58
1:B:1506:VAL:O	1:B:1508:PRO:HD3	2.03	0.58
1:B:1584:THR:HG22	1:B:1653:HIS:CD2	2.39	0.58
1:A:1555:GLU:HG2	1:A:1565:ILE:HG12	1.85	0.58
1:A:1694:ASP:O	1:A:1698:THR:HG23	2.03	0.58
1:B:1811:VAL:HG22	1:B:1815:TYR:CE2	2.38	0.58
2:C:117:LEU:HB3	2:C:158:SER:HB2	1.85	0.58
1:B:1330:LEU:O	1:B:1332:PRO:HD3	2.03	0.58
1:A:1283:MET:SD	1:A:1798:LEU:HD22	2.45	0.57
1:A:1417:ASN:HB3	1:A:1427:LEU:HD22	1.86	0.57
1:B:1341:LYS:NZ	1:B:1341:LYS:HB3	2.20	0.57
1:A:1574:LYS:O	1:A:1581:ARG:HB3	2.05	0.56
1:B:1854:TYR:O	1:B:1857:ILE:HG22	2.04	0.56
1:B:1864:ILE:HG13	1:B:1865:LEU:N	2.20	0.56
1:A:1392:MET:HB3	1:A:1445:PHE:HE2	1.71	0.56
2:C:21:ILE:HG21	2:C:29:PRO:HG3	1.87	0.56
1:A:1561:MET:HE2	2:C:41:SER:HB2	1.88	0.56
1:A:1431:THR:HG23	1:A:1436:GLU:OE2	2.06	0.55
1:B:1653:HIS:ND1	1:B:1654:LEU:HG	2.21	0.55
1:A:1301:LEU:O	1:A:1305:ILE:HG22	2.06	0.55
1:A:1454:CYS:SG	1:A:1707:SER:HB2	2.46	0.55
2:C:95:ALA:O	2:C:99:PRO:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1777:THR:HG23	1:A:1804:ILE:HD11	1.89	0.55
1:A:1323:ARG:O	1:A:1327:MET:HG2	2.06	0.54
1:A:1328:ARG:NH2	1:A:1335:GLU:HG2	2.22	0.54
1:B:1286:LEU:HD22	1:B:1679:THR:HB	1.89	0.54
1:B:1711:LEU:HD12	1:B:1832:TYR:CB	2.38	0.54
2:C:155:LEU:HD13	2:C:168:VAL:HA	1.88	0.54
1:B:1379:PHE:HB2	1:B:1383:ASP:CB	2.38	0.54
1:A:1388:ALA:O	1:A:1392:MET:HG2	2.08	0.54
2:C:72:TYR:N	2:C:73:PRO:CD	2.71	0.53
1:A:1403:THR:O	1:A:1407:LYS:HG3	2.08	0.53
1:A:1460:PHE:HB2	1:A:1759:PHE:CZ	2.44	0.52
1:A:1583:ASN:HB3	1:A:1588:TYR:CE2	2.45	0.52
1:A:1814:TYR:O	1:A:1818:ILE:HG13	2.10	0.52
1:A:1543:TYR:C	1:A:1545:GLN:H	2.13	0.52
2:C:125:THR:O	2:C:129:LEU:HG	2.09	0.51
1:A:1322:TYR:CE2	1:A:1844:PHE:HZ	2.29	0.51
1:A:1561:MET:HE1	2:C:41:SER:HB2	1.92	0.51
1:A:1542:PRO:O	1:A:1546:ARG:HG3	2.11	0.51
1:B:1384:ARG:HH21	1:B:1433:SER:HB2	1.74	0.51
2:C:139:TYR:HB3	2:C:140:PRO:HD3	1.93	0.51
1:B:1444:THR:HA	1:B:1747:PHE:CE1	2.45	0.51
1:A:1504:ASN:HB3	1:A:1515:GLU:HG3	1.92	0.51
1:B:1555:GLU:HA	1:B:1564:ILE:O	2.11	0.51
2:C:109:PRO:HB3	2:C:152:VAL:HG21	1.93	0.51
2:C:20:LEU:HD22	2:C:55:LEU:HD13	1.93	0.51
1:B:1410:LEU:O	1:B:1414:ILE:HG13	2.11	0.51
1:B:1748:TRP:O	1:B:1752:ILE:HG13	2.12	0.50
1:B:1508:PRO:HD2	1:B:1537:VAL:HG11	1.93	0.50
1:B:1869:GLU:OE1	1:B:1880:ARG:HG2	2.11	0.50
1:A:1474:PRO:HD2	1:A:1483:ARG:CB	2.41	0.50
1:A:1320:LEU:HD22	1:A:1324:THR:HG21	1.92	0.50
1:B:1459:LEU:HD22	1:B:1759:PHE:CE2	2.43	0.50
1:B:1744:PRO:HA	1:B:1748:TRP:HB2	1.94	0.50
1:A:1510:HIS:CG	1:A:1511:GLU:N	2.80	0.50
1:A:1376:GLN:HE22	1:A:1860:TYR:HB3	1.77	0.49
1:B:1861:LYS:HG3	1:B:1862:ASP:N	2.28	0.49
1:A:1379:PHE:HB2	1:A:1383:ASP:CB	2.42	0.49
1:A:1305:ILE:O	1:A:1309:THR:HG22	2.13	0.49
1:A:1352:SER:HB3	1:A:1889:THR:HG22	1.94	0.49
1:A:1711:LEU:HD12	1:A:1832:TYR:CG	2.48	0.49
1:B:1336:ASP:HA	1:B:1341:LYS:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1450:PHE:CD2	1:B:1710:PRO:HG3	2.48	0.49
2:C:28:PHE:CD2	2:C:160:LEU:HD13	2.48	0.49
1:A:1330:LEU:HD11	1:A:1445:PHE:CZ	2.48	0.49
1:A:1536:ALA:O	1:A:1539:LYS:HG3	2.12	0.49
1:A:1360:LEU:HD23	1:A:1360:LEU:O	2.12	0.49
2:C:72:TYR:N	2:C:73:PRO:HD2	2.27	0.49
2:C:20:LEU:HD22	2:C:55:LEU:HB3	1.94	0.48
1:B:1740:SER:O	1:B:1744:PRO:HD2	2.13	0.48
2:C:32:TYR:CD2	4:C:179:GNP:H5'1	2.47	0.48
1:A:1331:PHE:HB3	1:A:1334:ILE:HG13	1.94	0.48
1:A:1459:LEU:HD22	1:A:1759:PHE:HE2	1.78	0.48
1:A:1776:GLN:HB3	1:A:1796:ASN:ND2	2.27	0.48
1:B:1444:THR:HA	1:B:1747:PHE:HE1	1.78	0.48
1:A:1437:LYS:O	1:A:1437:LYS:HE2	2.14	0.48
1:B:1360:LEU:HD23	1:B:1360:LEU:O	2.13	0.48
1:A:1322:TYR:HE2	1:A:1844:PHE:HZ	1.59	0.48
2:C:15:GLY:HA2	4:C:179:GNP:H8	1.96	0.48
1:B:1473:GLY:HA3	1:B:1483:ARG:HB3	1.95	0.48
1:B:1695:LEU:O	1:B:1699:ILE:HG13	2.13	0.48
1:B:1864:ILE:HG13	1:B:1865:LEU:H	1.79	0.47
2:C:44:VAL:O	2:C:51:VAL:HG22	2.13	0.47
1:B:1676:ILE:O	1:B:1680:ARG:HG2	2.13	0.47
1:B:1277:LYS:O	1:B:1281:LEU:HG	2.13	0.47
1:A:1764:ASN:ND2	1:A:1767:THR:H	2.12	0.47
1:A:1505:CYS:HA	1:A:1596:VAL:O	2.15	0.47
1:A:1365:PHE:CD1	1:A:1879:LEU:HD21	2.47	0.47
1:A:1743:LEU:HB3	1:A:1744:PRO:CD	2.34	0.47
1:B:1704:HIS:CG	1:B:1705:ARG:H	2.33	0.47
1:A:1503:LEU:O	1:A:1517:PRO:HA	2.15	0.47
1:A:1507:ASN:HB3	1:A:1510:HIS:ND1	2.30	0.46
1:A:1385:GLY:HA2	1:A:1437:LYS:HD3	1.97	0.46
1:B:1396:GLN:CA	1:B:1396:GLN:HE21	2.26	0.46
1:A:1373:LEU:HB3	1:A:1379:PHE:CE2	2.51	0.46
1:B:1711:LEU:HD12	1:B:1832:TYR:CG	2.50	0.46
2:C:139:TYR:HE1	2:C:143:LEU:HD22	1.80	0.46
1:A:1302:GLN:HA	1:A:1305:ILE:HG22	1.96	0.46
1:A:1490:LYS:HD2	1:A:1769:ALA:CB	2.45	0.46
1:B:1463:TYR:CZ	1:B:1761:ILE:HD12	2.51	0.46
1:A:1510:HIS:NE2	1:A:1513:ALA:HB3	2.31	0.46
1:B:1355:LEU:CB	1:B:1886:VAL:HG13	2.46	0.46
1:A:1717:PHE:HE2	1:A:1815:TYR:CD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:ALA:O	1:B:1303:THR:HG23	2.15	0.46
1:B:1324:THR:HG22	1:B:1324:THR:O	2.16	0.46
1:B:1566:LEU:HD22	1:B:1588:TYR:CZ	2.51	0.46
1:B:1500:THR:C	1:B:1501:LEU:HD12	2.36	0.46
1:A:1463:TYR:CZ	1:A:1761:ILE:HD12	2.50	0.46
1:B:1849:ALA:O	1:B:1853:ILE:HG13	2.16	0.46
2:C:24:THR:HG21	2:C:40:TYR:HB3	1.98	0.46
2:C:44:VAL:HG12	2:C:45:MET:N	2.31	0.46
1:A:1528:GLN:HE22	1:A:1653:HIS:CE1	2.33	0.46
1:A:1653:HIS:ND1	1:A:1654:LEU:HD22	2.32	0.45
2:C:124:ASP:O	2:C:127:GLU:HB3	2.15	0.45
1:A:1369:PHE:O	1:A:1373:LEU:HG	2.16	0.45
1:A:1392:MET:HB3	1:A:1445:PHE:CE2	2.52	0.45
1:A:1485:SER:HB3	1:A:1491:LEU:HA	1.98	0.45
1:A:1320:LEU:HD12	1:A:1757:PHE:O	2.17	0.45
1:A:1363:LYS:O	1:A:1367:LEU:HG	2.16	0.45
1:B:1428:LEU:HD13	1:B:1742:CYS:SG	2.57	0.45
2:C:20:LEU:CD2	2:C:55:LEU:HD13	2.47	0.45
1:A:1441:ASN:N	1:A:1441:ASN:HD22	2.14	0.45
1:B:1451:LEU:O	1:B:1456:GLY:HA3	2.17	0.45
1:B:1886:VAL:HG12	1:B:1887:VAL:N	2.32	0.45
1:B:1808:LYS:O	1:B:1811:VAL:HG12	2.17	0.45
1:B:1880:ARG:HG3	1:B:1881:SER:N	2.32	0.45
1:A:1360:LEU:HA	1:A:1365:PHE:CD2	2.52	0.45
1:A:1554:LEU:HD11	1:A:1596:VAL:HG11	1.98	0.45
1:A:1709:LEU:HD12	1:A:1710:PRO:HD2	1.99	0.44
1:B:1704:HIS:CG	1:B:1705:ARG:N	2.85	0.44
2:C:68:ARG:HB3	2:C:69:PRO:HD3	1.99	0.44
1:A:1462:LEU:O	1:A:1466:ILE:HG12	2.17	0.44
2:C:155:LEU:HD11	2:C:171:GLU:HB2	1.99	0.44
1:A:1320:LEU:HD13	1:A:1324:THR:HG22	1.99	0.44
1:B:1705:ARG:HA	1:B:1706:GLY:HA2	1.53	0.44
2:C:82:PHE:CE2	2:C:90:PHE:HD1	2.36	0.44
1:A:1386:ASN:O	1:A:1390:LEU:HG	2.17	0.44
1:A:1432:GLU:OE2	1:A:1432:GLU:HA	2.17	0.44
2:C:37:PHE:CG	2:C:37:PHE:O	2.71	0.44
1:B:1359:LEU:O	1:B:1365:PHE:CD1	2.71	0.44
1:A:1423:HIS:HB2	1:B:1303:THR:HB	1.99	0.44
1:A:1868:LEU:HD22	1:A:1879:LEU:HD22	2.00	0.43
1:B:1301:LEU:O	1:B:1301:LEU:HD23	2.17	0.43
1:B:1538:TYR:HB2	1:B:1546:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44:VAL:HG12	2:C:45:MET:H	1.84	0.43
1:A:1817:ASP:O	1:A:1821:MET:HG3	2.19	0.43
1:B:1869:GLU:HG3	1:B:1869:GLU:O	2.18	0.43
1:B:1584:THR:HG22	1:B:1653:HIS:NE2	2.34	0.43
1:A:1455:ALA:O	1:A:1458:PRO:HD2	2.19	0.43
1:B:1396:GLN:O	1:B:1837:SER:HB2	2.18	0.43
1:A:1651:LEU:HD12	1:A:1651:LEU:N	2.33	0.43
1:A:1411:SER:O	1:A:1415:GLU:HG2	2.19	0.42
1:A:1580:LYS:O	1:A:1651:LEU:HA	2.19	0.42
1:A:1678:LEU:HD12	1:A:1682:LEU:CD1	2.49	0.42
1:A:1740:SER:O	1:A:1744:PRO:HD2	2.19	0.42
1:B:1399:MET:HB2	1:B:1837:SER:HB3	2.00	0.42
1:B:1869:GLU:HA	1:B:1869:GLU:OE1	2.19	0.42
2:C:129:LEU:HD13	2:C:136:PRO:HG3	2.01	0.42
1:B:1428:LEU:HD23	1:B:1436:GLU:OE2	2.19	0.42
1:A:1330:LEU:HD22	1:A:1441:ASN:CG	2.40	0.42
1:A:1305:ILE:HG23	1:A:1306:HIS:N	2.34	0.42
1:A:1306:HIS:O	1:A:1310:SER:N	2.45	0.42
1:B:1566:LEU:HD22	1:B:1588:TYR:CE1	2.53	0.42
2:C:68:ARG:N	2:C:69:PRO:CD	2.82	0.42
1:A:1373:LEU:HD22	1:A:1860:TYR:HD2	1.85	0.42
1:A:1745:LEU:HD21	1:A:1779:MET:HA	2.01	0.42
2:C:98:TYR:HE1	2:C:102:ARG:HH11	1.68	0.42
1:A:1528:GLN:O	1:A:1531:GLU:HB2	2.19	0.42
1:A:1804:ILE:N	1:A:1805:PRO:CD	2.82	0.42
1:A:1290:VAL:O	1:A:1290:VAL:HG12	2.19	0.42
1:A:1877:GLN:O	1:A:1878:ARG:C	2.58	0.42
1:A:1487:SER:C	1:A:1489:ASP:H	2.24	0.42
1:A:1490:LYS:HD2	1:A:1769:ALA:HB2	2.01	0.42
1:B:1777:THR:HG23	1:B:1804:ILE:HD11	2.01	0.42
1:A:1367:LEU:CD2	1:A:1405:VAL:HG13	2.50	0.41
1:A:1653:HIS:C	1:A:1654:LEU:HD13	2.41	0.41
1:B:1384:ARG:HB3	1:B:1434:VAL:HG22	2.01	0.41
2:C:94:ARG:HE	2:C:145:MET:HE1	1.85	0.41
2:C:74:GLN:HE21	2:C:74:GLN:HB2	1.72	0.41
1:A:1463:TYR:CE1	1:A:1761:ILE:HD12	2.54	0.41
1:B:1794:PRO:O	1:B:1798:LEU:HB2	2.20	0.41
2:C:79:LEU:CD2	2:C:111:ILE:HB	2.50	0.41
1:A:1711:LEU:HD22	1:A:1824:ILE:HD11	2.03	0.41
1:B:1724:ALA:HB3	1:B:1735:ARG:HH11	1.85	0.41
1:A:1424:PRO:O	1:A:1427:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1317:ILE:HA	1:B:1318:PRO:HD3	1.84	0.41
2:C:128:LYS:O	2:C:132:LYS:HG3	2.21	0.41
2:C:139:TYR:N	2:C:140:PRO:CD	2.84	0.41
2:C:68:ARG:O	2:C:70:LEU:N	2.54	0.41
1:A:1417:ASN:O	1:A:1422:ASN:HB2	2.20	0.41
1:A:1482:ALA:N	1:A:1492:ILE:HG13	2.35	0.41
1:B:1457:GLU:N	1:B:1458:PRO:HD2	2.35	0.41
2:C:122:ASP:O	2:C:126:ILE:HG12	2.20	0.41
1:A:1376:GLN:NE2	1:A:1863:GLU:HB2	2.36	0.41
1:A:1469:GLN:NE2	1:A:1469:GLN:HA	2.36	0.41
1:B:1441:ASN:N	1:B:1441:ASN:HD22	2.19	0.41
1:B:1808:LYS:O	1:B:1812:GLU:HG3	2.21	0.40
1:B:1474:PRO:HD2	1:B:1483:ARG:HB2	2.01	0.40
1:B:1583:ASN:HB3	1:B:1588:TYR:HE2	1.85	0.40
1:B:1382:ARG:HD3	1:B:1383:ASP:N	2.36	0.40
1:A:1447:LEU:HD11	1:A:1743:LEU:HD11	2.04	0.40
1:B:1718:ASP:O	1:B:1722:GLU:HG3	2.22	0.40
1:B:1384:ARG:HH21	1:B:1433:SER:CB	2.33	0.40
1:B:1429:ARG:O	1:B:1430:ARG:C	2.60	0.40
1:B:1804:ILE:N	1:B:1805:PRO:CD	2.85	0.40

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	518/626 (83%)	455 (88%)	56 (11%)	7 (1%)	11	48
1	B	511/626 (82%)	460 (90%)	46 (9%)	5 (1%)	15	55
2	C	170/180 (94%)	149 (88%)	17 (10%)	4 (2%)	6	37
All	All	1199/1432 (84%)	1064 (89%)	119 (10%)	16 (1%)	12	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	29	PRO
1	A	1575	ILE
1	B	1430	ARG
1	B	1583	ASN
2	C	37	PHE
1	A	1578	ASP
1	B	1584	THR
1	A	1433	SER
1	A	1845	ASN
1	B	1355	LEU
1	B	1743	LEU
1	A	1337	HIS
1	A	1542	PRO
2	C	30	GLY
1	A	1743	LEU
2	C	69	PRO

### 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	383/563 (68%)	368 (96%)	15 (4%)	32	65
1	B	350/563 (62%)	330 (94%)	20 (6%)	20	55
2	C	127/155 (82%)	124 (98%)	3 (2%)	49	76
All	All	860/1281 (67%)	822 (96%)	38 (4%)	28	63

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1325	TYR
1	A	1396	GLN
1	A	1431	THR
1	A	1437	LYS
1	A	1510	HIS

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Mol	Chain	Res	Type
1	A	1561	MET
1	A	1579	TRP
1	A	1654	LEU
1	A	1678	LEU
1	A	1764	ASN
1	A	1776	GLN
1	A	1798	LEU
1	A	1813	ARG
1	A	1844	PHE
1	A	1878	ARG
1	B	1287	GLU
1	B	1307	GLU
1	B	1327	MET
1	B	1341	LYS
1	B	1346	GLN
1	B	1364	HIS
1	B	1381	MET
1	B	1382	ARG
1	B	1386	ASN
1	B	1396	GLN
1	B	1430	ARG
1	B	1579	TRP
1	B	1588	TYR
1	B	1730	HIS
1	B	1735	ARG
1	B	1764	ASN
1	B	1844	PHE
1	B	1856	TYR
1	B	1880	ARG
1	B	1886	VAL
2	C	49	LYS
2	C	74	GLN
2	C	121	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1358	GLN
1	A	1376	GLN
1	A	1441	ASN
1	A	1468	GLN
1	A	1469	GLN

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Mol	Chain	Res	Type
1	A	1528	GLN
1	A	1545	GLN
1	A	1583	ASN
1	A	1589	GLN
1	A	1602	GLN
1	A	1723	GLN
1	A	1727	HIS
1	A	1764	ASN
1	A	1776	GLN
1	A	1836	GLN
1	A	1845	ASN
1	B	1346	GLN
1	B	1376	GLN
1	B	1386	ASN
1	B	1396	GLN
1	B	1441	ASN
1	B	1468	GLN
1	B	1469	GLN
1	B	1545	GLN
1	B	1689	GLN
1	B	1723	GLN
1	B	1762	HIS
1	B	1764	ASN
1	B	1836	GLN
1	B	1845	ASN
2	C	74	GLN
2	C	104	HIS
2	C	107	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	C	179	3	28,34,34	2.61	9 (32%)	30,54,54	2.28	7 (23%)

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	C	179	3	-	7/17/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	179	GNP	C4-N9	-7.32	1.38	1.47
4	C	179	GNP	C5-C6	-6.43	1.41	1.52
4	C	179	GNP	PB-O3A	-5.15	1.52	1.59
4	C	179	GNP	C6-N1	3.88	1.39	1.33
4	C	179	GNP	PG-O1G	3.27	1.51	1.46
4	C	179	GNP	PB-O2B	-3.11	1.48	1.56
4	C	179	GNP	C5-C4	-2.42	1.38	1.53
4	C	179	GNP	C8-N9	-2.30	1.37	1.45
4	C	179	GNP	PG-O3G	-2.01	1.51	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	179	GNP	C4-C5-N7	6.38	110.92	102.46
4	C	179	GNP	C5-C6-N1	-5.29	111.66	118.19
4	C	179	GNP	O2B-PB-O1B	4.01	118.33	109.92
4	C	179	GNP	O6-C6-C5	4.00	128.03	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	179	GNP	O3G-PG-O1G	-3.61	104.38	113.45
4	C	179	GNP	PA-O3A-PB	-3.52	120.23	132.62
4	C	179	GNP	O3G-PG-O2G	3.24	116.28	107.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

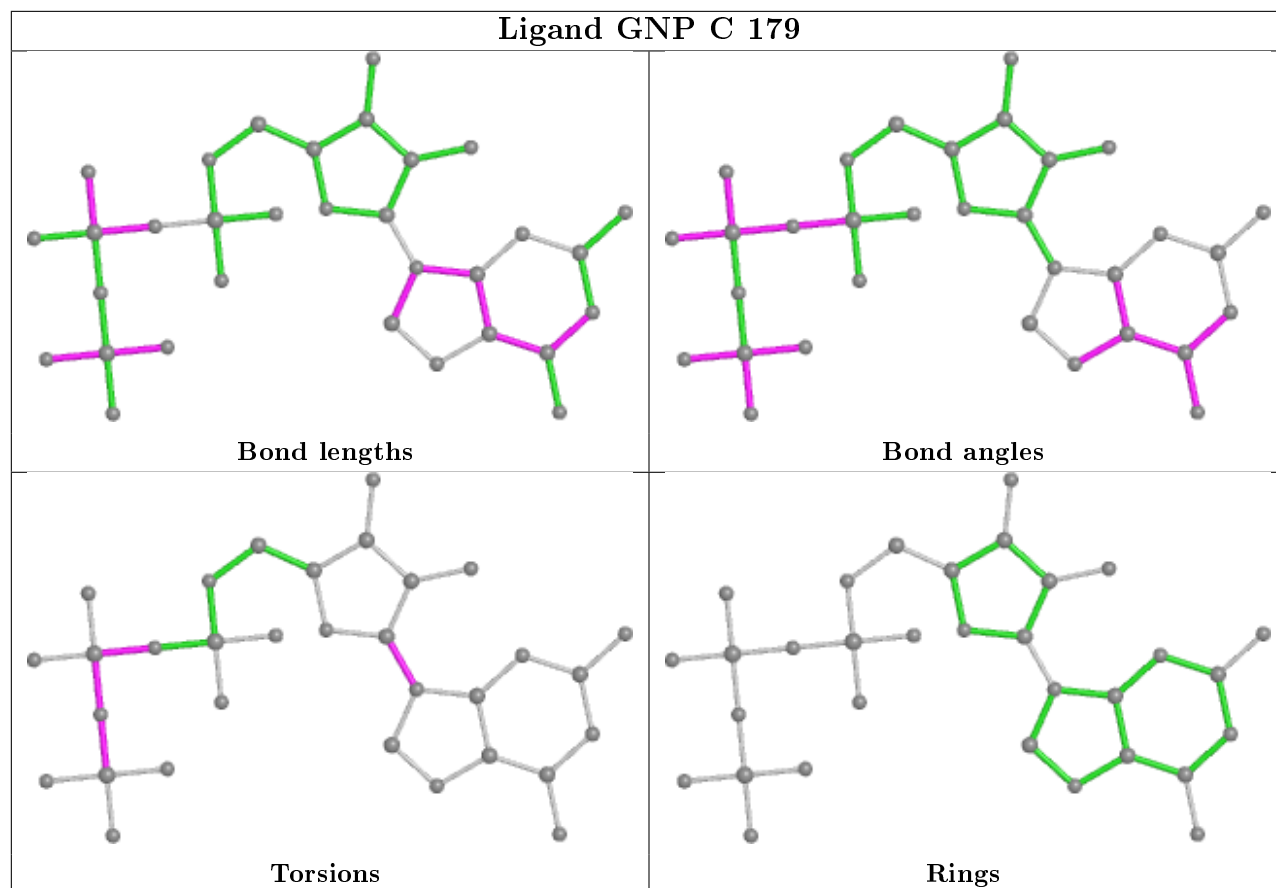
Mol	Chain	Res	Type	Atoms
4	C	179	GNP	PB-N3B-PG-O1G
4	C	179	GNP	PG-N3B-PB-O1B
4	C	179	GNP	PA-O3A-PB-O1B
4	C	179	GNP	PA-O3A-PB-O2B
4	C	179	GNP	O4'-C1'-N9-C4
4	C	179	GNP	C2'-C1'-N9-C8
4	C	179	GNP	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	179	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

### 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<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	532/626 (84%)	-0.15	12 (2%) 60 42	88, 179, 275, 337	0
1	B	531/626 (84%)	-0.06	12 (2%) 60 42	126, 216, 304, 371	0
2	C	174/180 (96%)	0.12	6 (3%) 45 29	92, 183, 346, 410	7 (4%)
All	All	1237/1432 (86%)	-0.07	30 (2%) 59 41	88, 196, 302, 410	7 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	30	GLY	5.7
1	A	1555	GLU	4.3
1	B	1316	GLY	4.2
1	A	1564	ILE	4.1
1	B	1706	GLY	3.8
1	A	1844	PHE	3.8
1	A	1849	ALA	3.8
1	B	1796	ASN	3.3
1	A	1706	GLY	3.3
1	A	1565	ILE	3.2
1	B	1565	ILE	3.0
1	A	1356	PHE	2.9
1	B	1558	GLN	2.9
1	A	1598	LEU	2.9
1	A	1559	GLY	2.5
1	A	1681	LEU	2.4
1	B	1311	ASP	2.4
1	B	1563	ARG	2.3
1	B	1704	HIS	2.3
1	A	1430	ARG	2.3
2	C	14	VAL	2.3
1	B	1523	CYS	2.3
1	A	1554	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1505	CYS	2.2
1	B	1556	TRP	2.2
2	C	136	PRO	2.1
2	C	131	GLU	2.1
2	C	3	ALA	2.1
2	C	129	LEU	2.0
1	B	1540	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

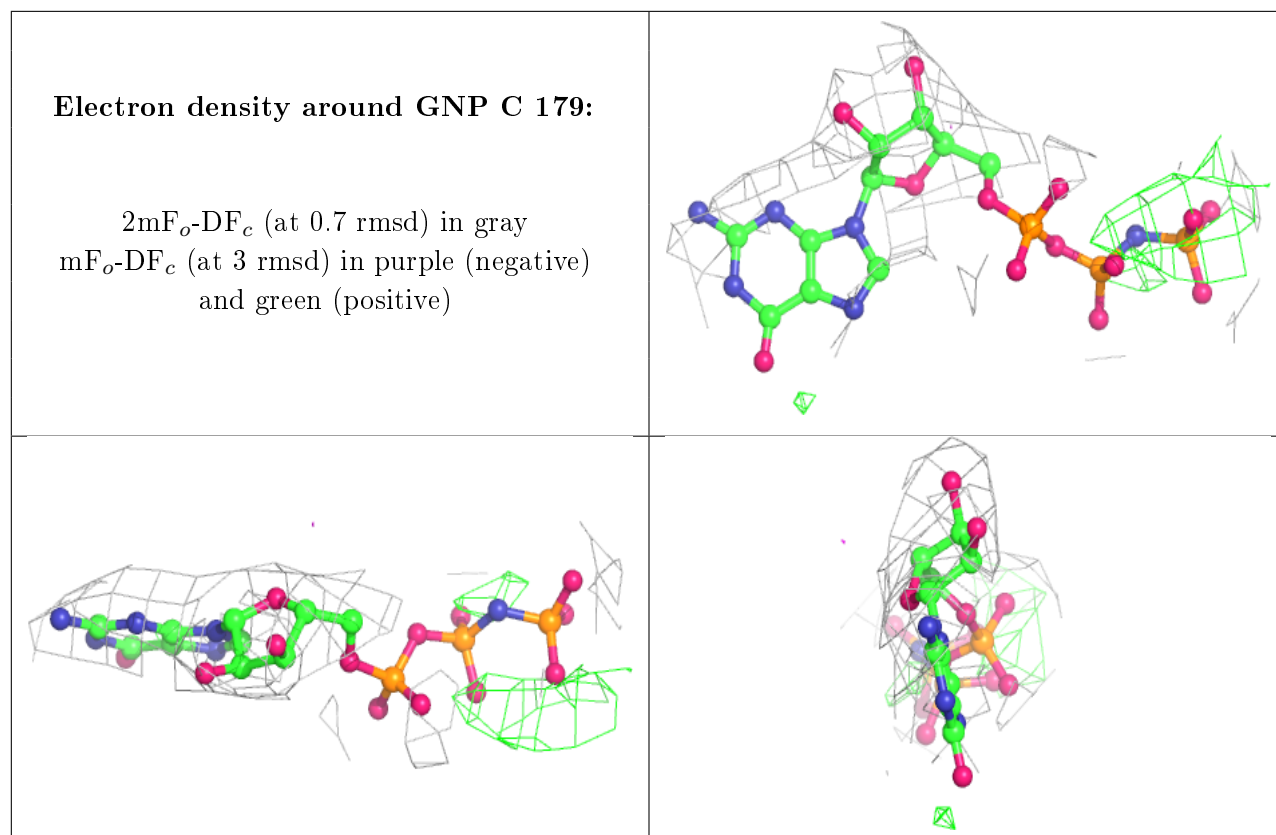
There are no carbohydrates in this entry.

## 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<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	179	32/32	0.94	0.18	126,165,181,392	0
3	MG	C	178	1/1	0.96	0.18	148,148,148,148	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.