Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 11:56 PM EST

PDB ID	:	4LWZ
Title	:	Crystal structure of Myo5b globular tail domain in complex with inactive Rab11a
Authors	:	Pylypenko, O.; Attanda, W.; Gauquelin, C.; Houdusse, A.
Deposited on	:	2013-07-29
Resolution	:	2.55 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:

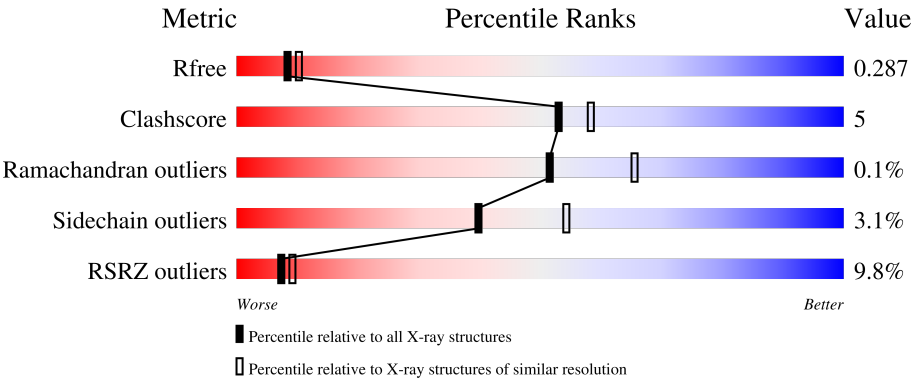
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	177	7% 80% 11% • 8%
1	C	177	12% 71% 15% • 12%
2	B	427	4% 79% 6% 14%
2	D	427	12% 68% 13% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8137 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 protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1265	803	215	246	1			
1	C	155	Total	C	N	O	S	0	0	0
			1174	739	206	228	1			

- Molecule 2 is a protein called Unconventional myosin-Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total	C	N	O	S	0	1	0
			2903	1847	492	539	25			
2	D	346	Total	C	N	O	S	0	0	0
			2612	1651	447	493	21			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1422	MET	-	expression tag	UNP Q9ULV0
B	1423	ARG	-	expression tag	UNP Q9ULV0
B	1424	SER	-	expression tag	UNP Q9ULV0
B	1425	GLU	-	expression tag	UNP Q9ULV0
B	1426	THR	-	expression tag	UNP Q9ULV0
B	1427	MET	-	expression tag	UNP Q9ULV0
B	1428	SER	-	expression tag	UNP Q9ULV0
B	1429	TYR	-	expression tag	UNP Q9ULV0
B	1430	TYR	-	expression tag	UNP Q9ULV0
B	1431	HIS	-	expression tag	UNP Q9ULV0
B	1432	HIS	-	expression tag	UNP Q9ULV0
B	1433	HIS	-	expression tag	UNP Q9ULV0
B	1434	HIS	-	expression tag	UNP Q9ULV0
B	1435	HIS	-	expression tag	UNP Q9ULV0
B	1436	HIS	-	expression tag	UNP Q9ULV0
B	1437	ASP	-	expression tag	UNP Q9ULV0

Continued on next page...

Continued from previous page...

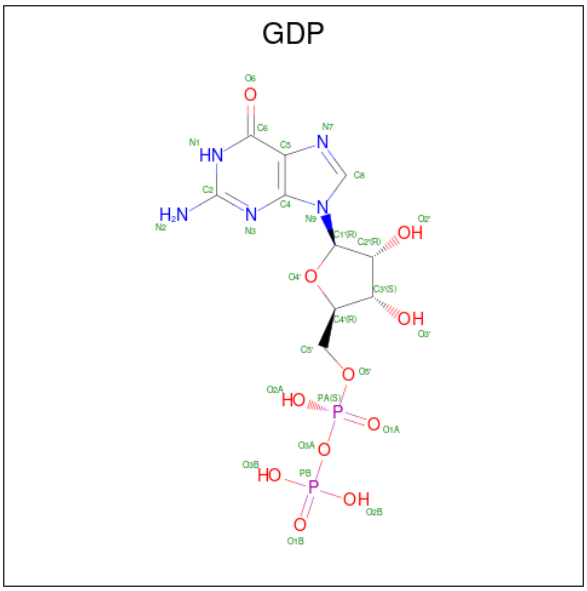
Chain	Residue	Modelled	Actual	Comment	Reference
B	1438	TYR	-	expression tag	UNP Q9ULV0
B	1439	ASP	-	expression tag	UNP Q9ULV0
B	1440	ILE	-	expression tag	UNP Q9ULV0
B	1441	PRO	-	expression tag	UNP Q9ULV0
B	1442	THR	-	expression tag	UNP Q9ULV0
B	1443	THR	-	expression tag	UNP Q9ULV0
B	1444	GLU	-	expression tag	UNP Q9ULV0
B	1445	ASN	-	expression tag	UNP Q9ULV0
B	1446	LEU	-	expression tag	UNP Q9ULV0
B	1447	TYR	-	expression tag	UNP Q9ULV0
B	1448	PHE	-	expression tag	UNP Q9ULV0
B	1449	GLN	-	expression tag	UNP Q9ULV0
B	1450	GLY	-	expression tag	UNP Q9ULV0
B	1451	ALA	-	expression tag	UNP Q9ULV0
B	1452	MET	-	expression tag	UNP Q9ULV0
B	1453	GLY	-	expression tag	UNP Q9ULV0
B	1454	SER	-	expression tag	UNP Q9ULV0
B	1455	MET	-	expression tag	UNP Q9ULV0
D	1422	MET	-	expression tag	UNP Q9ULV0
D	1423	ARG	-	expression tag	UNP Q9ULV0
D	1424	SER	-	expression tag	UNP Q9ULV0
D	1425	GLU	-	expression tag	UNP Q9ULV0
D	1426	THR	-	expression tag	UNP Q9ULV0
D	1427	MET	-	expression tag	UNP Q9ULV0
D	1428	SER	-	expression tag	UNP Q9ULV0
D	1429	TYR	-	expression tag	UNP Q9ULV0
D	1430	TYR	-	expression tag	UNP Q9ULV0
D	1431	HIS	-	expression tag	UNP Q9ULV0
D	1432	HIS	-	expression tag	UNP Q9ULV0
D	1433	HIS	-	expression tag	UNP Q9ULV0
D	1434	HIS	-	expression tag	UNP Q9ULV0
D	1435	HIS	-	expression tag	UNP Q9ULV0
D	1436	HIS	-	expression tag	UNP Q9ULV0
D	1437	ASP	-	expression tag	UNP Q9ULV0
D	1438	TYR	-	expression tag	UNP Q9ULV0
D	1439	ASP	-	expression tag	UNP Q9ULV0
D	1440	ILE	-	expression tag	UNP Q9ULV0
D	1441	PRO	-	expression tag	UNP Q9ULV0
D	1442	THR	-	expression tag	UNP Q9ULV0
D	1443	THR	-	expression tag	UNP Q9ULV0
D	1444	GLU	-	expression tag	UNP Q9ULV0
D	1445	ASN	-	expression tag	UNP Q9ULV0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1446	LEU	-	expression tag	UNP Q9ULV0
D	1447	TYR	-	expression tag	UNP Q9ULV0
D	1448	PHE	-	expression tag	UNP Q9ULV0
D	1449	GLN	-	expression tag	UNP Q9ULV0
D	1450	GLY	-	expression tag	UNP Q9ULV0
D	1451	ALA	-	expression tag	UNP Q9ULV0
D	1452	MET	-	expression tag	UNP Q9ULV0
D	1453	GLY	-	expression tag	UNP Q9ULV0
D	1454	SER	-	expression tag	UNP Q9ULV0
D	1455	MET	-	expression tag	UNP Q9ULV0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

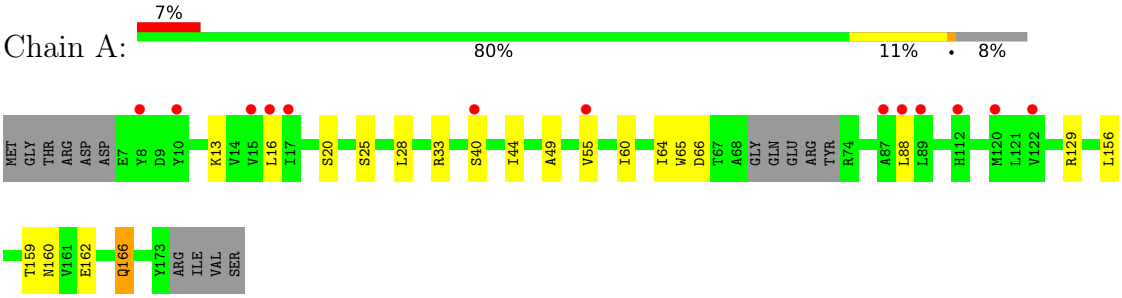
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	33	Total O 33 33	0	0
5	B	49	Total O 49 49	0	0
5	C	17	Total O 17 17	0	0
5	D	26	Total O 26 26	0	0

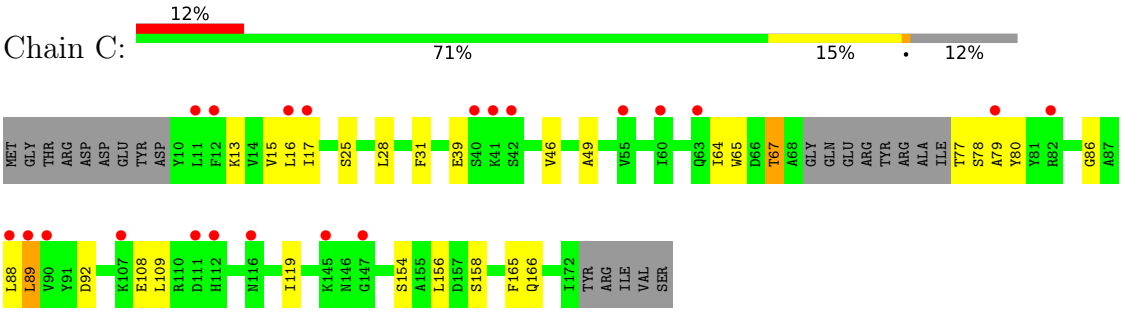
3 Residue-property plots (i)

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.

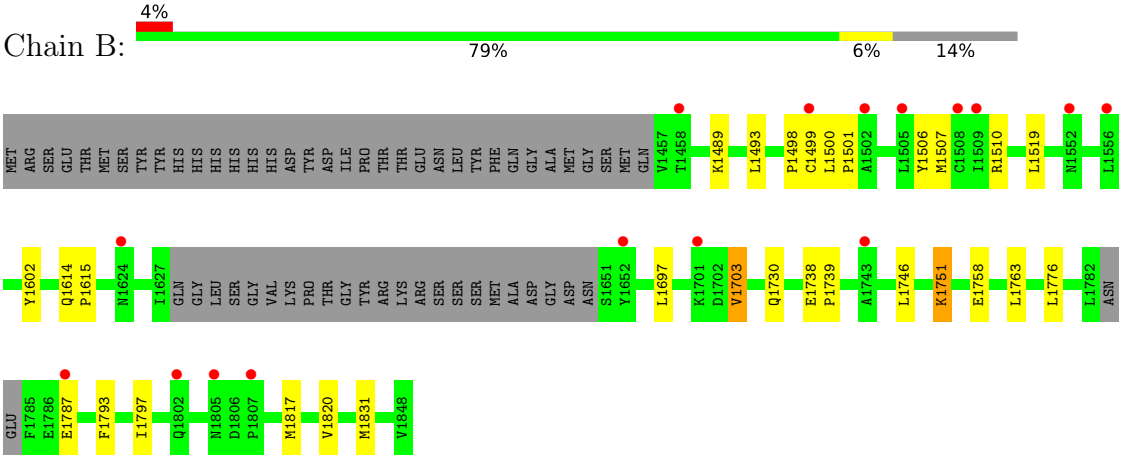
• Molecule 1: Ras-related protein Rab-11A



• Molecule 1: Ras-related protein Rab-11A

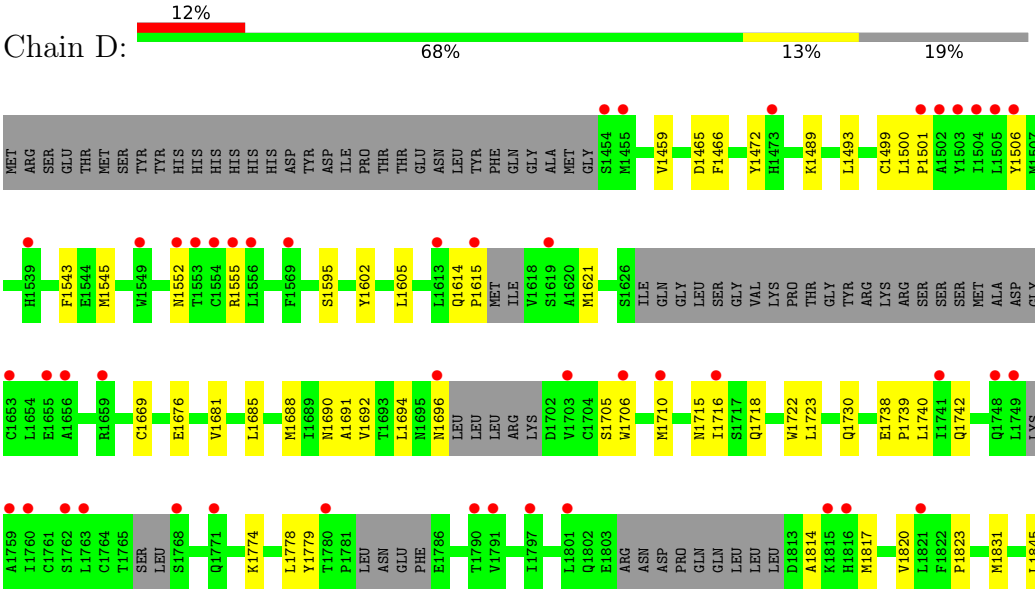


• Molecule 2: Unconventional myosin-Vb



• Molecule 2: Unconventional myosin-Vb

Chain D:


12%
68%
13%
19%
MET ARG SER GLU THR MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET GLY S1454 M1455 V1459 D1465 F1466 Y1472 H1473 K1489 L1493 C1499 L1500 P1501 A1502 Y1503 I1504 L1505 Y1506 M1507 C1508 I1509 L1519
H1539 F1543 E1544 M1545 W1549 N1552 T1553 C1554 R1555 L1556 F1569 S1595 Y1602 L1605 L1613 Q1614 P1615 MET ILE V1618 S1619 A1620 M1621 S1626 ILE GLN GLY GLY LEU SER GLY VAL LYS PRO THR GLY TYR ARG LYS ARG SER SER SER MET ALA ASP GLY ASP ASN SER Y1652
C1653 L1654 E1655 A1656 R1659 C1669 E1676 V1681 L1685 M1688 I1689 N1690 A1691 V1692 T1693 L1694 N1695 N1696 LEU LEU LEU ARG LYS D1702 V1703 C1704 S1705 W1706 M1710 N1715 I1716 S1717 Q1718 W1722 L1723 Q1730 E1738 P1739 L1740 I1741 Q1742 Q1748 L1749 LYS LYS K1752 T1753
A1759 I1760 C1761 S1762 L1763 C1764 T1765 SER LEU S1768 Q1771 K1774 L1778 Y1779 T1780 P1781 LEU ASN GLU PHE E1786 T1790 V1791 I1797 L1801 Q1802 E1803 ARG ASN ASP PRO GLN GLN LEU LEU LEU D1813 A1814 K1815 H1816 M1817 V1820 L1821 F1822 P1823 M1831 L1845 N1846 E1847 V1848

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.68Å 143.14Å 162.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 2.55 24.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.97-2.55) 99.7 (24.97-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.231 , 0.295 0.226 , 0.287	Depositor DCC
R_{free} test set	2606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.7	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	0.95	EDS
Total number of atoms	8137	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: GDP, 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	0.39	0/1285	0.54	0/1742
1	C	0.40	0/1191	0.55	0/1614
2	B	0.38	0/2955	0.49	0/4000
2	D	0.38	0/2653	0.51	0/3598
All	All	0.39	0/8084	0.51	0/10954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1265	0	1236	15	0
1	C	1174	0	1123	24	0
2	B	2903	0	2882	17	0
2	D	2612	0	2435	31	0
3	A	28	0	12	1	0
3	C	28	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	49	0	0	0	0
5	C	17	0	0	0	0
5	D	26	0	0	0	0
All	All	8137	0	7700	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (85) 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)
2:D:1602:TYR:CZ	2:D:1820:VAL:HG11	2.19	0.78
2:B:1602:TYR:CZ	2:B:1820:VAL:HG11	2.26	0.71
2:B:1507:MET:HG3	2:B:1831:MET:CE	2.25	0.67
1:C:13:LYS:HE3	1:C:65:TRP:CE2	2.32	0.64
2:D:1602:TYR:CE2	2:D:1820:VAL:HG11	2.33	0.63
1:A:55:VAL:HB	1:A:60:ILE:CD1	2.30	0.61
2:B:1507:MET:CG	2:B:1831:MET:CE	2.79	0.60
1:C:13:LYS:HE3	1:C:65:TRP:CD2	2.37	0.59
2:D:1705:SER:HA	2:D:1779:TYR:CE1	2.39	0.56
1:C:109:LEU:HD23	1:C:119:ILE:HD13	1.88	0.56
2:D:1706:TRP:O	2:D:1710:MET:HG2	2.07	0.55
2:D:1614:GLN:HB3	2:D:1615:PRO:HD3	1.89	0.55
2:D:1614:GLN:HB3	2:D:1615:PRO:CD	2.38	0.54
1:C:16:LEU:HD23	1:C:88:LEU:HB2	1.90	0.54
1:C:13:LYS:HG3	1:C:65:TRP:CD1	2.43	0.54
2:B:1738:GLU:HA	2:B:1738:GLU:OE2	2.08	0.53
1:C:156:LEU:C	1:C:156:LEU:HD23	2.29	0.53
2:D:1555:ARG:O	2:D:1555:ARG:HD3	2.10	0.51
1:C:15:VAL:HB	1:C:80:TYR:CE2	2.46	0.51
2:D:1738:GLU:O	2:D:1742:GLN:HG3	2.12	0.50
1:C:77:THR:C	1:C:79:ALA:N	2.63	0.50
2:B:1493:LEU:HD21	2:B:1501:PRO:HD3	1.94	0.50
2:D:1688:MET:C	2:D:1690:ASN:N	2.65	0.50
2:B:1614:GLN:N	2:B:1615:PRO:HD2	2.27	0.50
2:D:1543:PHE:CE1	2:D:1605:LEU:HD11	2.47	0.50
1:A:28:LEU:HD11	1:A:49:ALA:HB3	1.94	0.49
1:C:13:LYS:HG3	1:C:65:TRP:NE1	2.27	0.49
2:D:1506:TYR:HD1	2:D:1831:MET:CE	2.25	0.49
2:D:1774:LYS:O	2:D:1778:LEU:HG	2.11	0.49
2:B:1697:LEU:HD12	2:B:1703:VAL:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LEU:HD12	1:C:89:LEU:C	2.34	0.48
1:C:109:LEU:CD2	1:C:119:ILE:HD13	2.44	0.48
2:B:1500:LEU:HB3	2:B:1501:PRO:HD3	1.95	0.48
1:A:159:THR:O	1:A:160:ASN:HB2	2.14	0.47
2:D:1506:TYR:CD1	2:D:1831:MET:CE	2.97	0.47
1:C:77:THR:O	1:C:78:SER:C	2.51	0.47
2:D:1681:VAL:O	2:D:1685:LEU:HG	2.14	0.47
1:A:28:LEU:HD13	1:A:64:ILE:HG21	1.96	0.47
2:D:1738:GLU:N	2:D:1739:PRO:CD	2.78	0.47
2:D:1692:VAL:O	2:D:1696:ASN:ND2	2.49	0.46
1:A:40:SER:HB3	3:A:201:GDP:H3'	1.98	0.46
1:A:55:VAL:HB	1:A:60:ILE:HD13	1.97	0.46
2:B:1500:LEU:N	2:B:1501:PRO:CD	2.79	0.46
2:D:1506:TYR:HD1	2:D:1831:MET:HE3	1.81	0.46
2:D:1715:ASN:O	2:D:1718:GLN:HB2	2.16	0.46
1:C:77:THR:O	1:C:80:TYR:N	2.49	0.45
2:B:1498:PRO:O	2:B:1499:CYS:HB2	2.17	0.45
2:D:1716:ILE:HD11	2:D:1740:LEU:HG	1.98	0.45
1:C:31:PHE:CE1	1:C:165:PHE:HB2	2.52	0.45
1:C:92:ASP:OD1	1:C:92:ASP:C	2.56	0.44
1:C:46:VAL:HG22	1:C:67:THR:CG2	2.47	0.43
2:D:1500:LEU:N	2:D:1501:PRO:CD	2.81	0.43
2:B:1602:TYR:CE2	2:B:1820:VAL:HG11	2.52	0.43
2:D:1506:TYR:CD1	2:D:1506:TYR:C	2.91	0.43
1:A:13:LYS:HE3	1:A:65:TRP:CE2	2.53	0.43
1:C:15:VAL:HG22	1:C:86:GLY:O	2.19	0.43
1:A:25:SER:OG	1:A:66:ASP:OD2	2.33	0.43
1:C:28:LEU:HD11	1:C:49:ALA:HB3	2.01	0.43
2:D:1621:MET:O	2:D:1715:ASN:ND2	2.51	0.43
1:C:31:PHE:CE1	1:C:165:PHE:CB	3.01	0.43
1:C:46:VAL:HG22	1:C:67:THR:HG23	2.00	0.43
2:D:1738:GLU:HB3	2:D:1739:PRO:HD3	2.00	0.43
1:A:16:LEU:HD23	1:A:88:LEU:HB2	2.01	0.42
1:A:162:GLU:O	1:A:166:GLN:HB2	2.20	0.42
2:D:1472:TYR:HB3	2:D:1845:LEU:CD2	2.49	0.42
1:A:156:LEU:C	1:A:156:LEU:HD23	2.40	0.42
1:A:55:VAL:HB	1:A:60:ILE:HD12	2.02	0.42
2:D:1499:CYS:HA	2:D:1552:ASN:OD1	2.20	0.42
1:A:129:ARG:HD2	2:D:1669:CYS:HB3	2.00	0.42
2:D:1466:PHE:CD1	2:D:1847:GLU:HB3	2.54	0.42
2:B:1738:GLU:HB3	2:B:1739:PRO:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1506:TYR:CE2	2:B:1510:ARG:HG3	2.55	0.41
2:B:1751:LYS:HD2	2:B:1776:LEU:CD2	2.51	0.41
1:C:154:SER:O	1:C:158:SER:N	2.50	0.41
1:C:108:GLU:O	1:C:108:GLU:HG2	2.19	0.41
1:C:28:LEU:HD13	1:C:64:ILE:CG2	2.51	0.41
2:D:1722:TRP:CZ3	2:D:1723:LEU:HD23	2.56	0.41
2:B:1507:MET:CG	2:B:1831:MET:HE2	2.48	0.41
2:D:1676:GLU:HB2	2:D:1823:PRO:HG3	2.03	0.41
1:A:13:LYS:HE3	1:A:65:TRP:CD2	2.55	0.41
2:B:1793:PHE:CE2	2:B:1797:ILE:HD11	2.56	0.41
1:A:44:ILE:HD13	2:B:1763:LEU:HD13	2.02	0.41
1:C:13:LYS:CE	1:C:65:TRP:CE2	3.01	0.41
2:D:1691:ALA:CB	2:D:1814:ALA:HB2	2.51	0.40
2:D:1459:VAL:O	2:D:1459:VAL:HG13	2.22	0.40

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	158/177 (89%)	153 (97%)	5 (3%)	0	100	100
1	C	151/177 (85%)	141 (93%)	10 (7%)	0	100	100
2	B	362/427 (85%)	345 (95%)	17 (5%)	0	100	100
2	D	330/427 (77%)	312 (94%)	17 (5%)	1 (0%)	41	51
All	All	1001/1208 (83%)	951 (95%)	49 (5%)	1 (0%)	51	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1694	LEU

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	132/150 (88%)	129 (98%)	3 (2%)	50	65
1	C	118/150 (79%)	112 (95%)	6 (5%)	24	32
2	B	321/391 (82%)	312 (97%)	9 (3%)	43	58
2	D	266/391 (68%)	258 (97%)	8 (3%)	41	55
All	All	837/1082 (77%)	811 (97%)	26 (3%)	40	54

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	33	ARG
1	A	166	GLN
2	B	1489	LYS
2	B	1519	LEU
2	B	1703	VAL
2	B	1730	GLN
2	B	1746	LEU
2	B	1751	LYS
2	B	1758	GLU
2	B	1787	GLU
2	B	1817	MET
1	C	17	ILE
1	C	25	SER
1	C	39	GLU
1	C	67	THR
1	C	89	LEU
1	C	166	GLN
2	D	1465	ASP
2	D	1489	LYS
2	D	1493	LEU
2	D	1519	LEU
2	D	1545	MET
2	D	1595	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1730	GLN
2	D	1817	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1511	HIS
2	B	1539	HIS
2	D	1539	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GDP	C	201	4	24,30,30	1.05	2 (8%)	30,47,47	1.15	3 (10%)
3	GDP	A	201	4	24,30,30	1.03	1 (4%)	30,47,47	1.31	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	C	201	4	-	0/12/32/32	0/3/3/3
3	GDP	A	201	4	-	1/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	GDP	C6-N1	-2.61	1.34	1.37
3	C	201	GDP	O4'-C1'	2.40	1.44	1.41
3	A	201	GDP	C6-N1	-2.32	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	GDP	PA-O3A-PB	-3.08	122.25	132.83
3	C	201	GDP	PA-O3A-PB	-3.06	122.32	132.83
3	A	201	GDP	C8-N7-C5	2.58	107.90	102.99
3	C	201	GDP	C5-C6-N1	2.43	118.25	113.95
3	A	201	GDP	C2'-C3'-C4'	2.37	107.24	102.64
3	C	201	GDP	C8-N7-C5	2.03	106.85	102.99
3	A	201	GDP	C5-C6-N1	2.01	117.50	113.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GDP	PA-O3A-PB-O2B

There are no ring outliers.

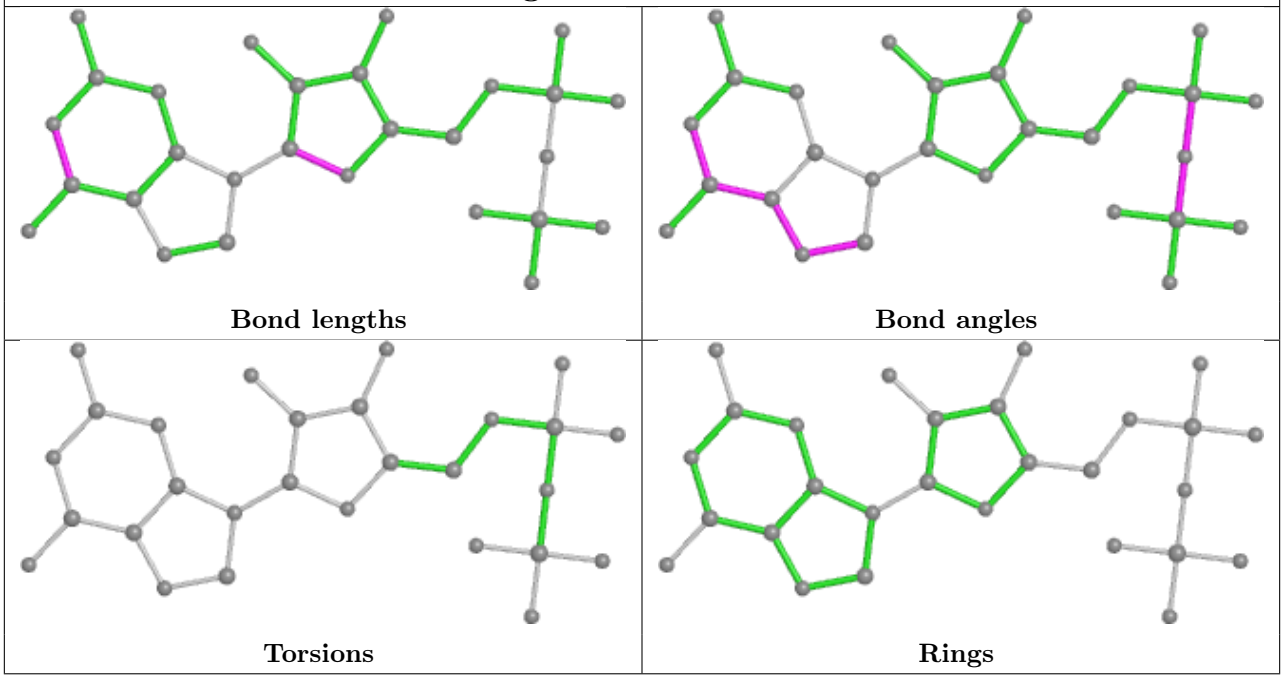
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	GDP	1	0

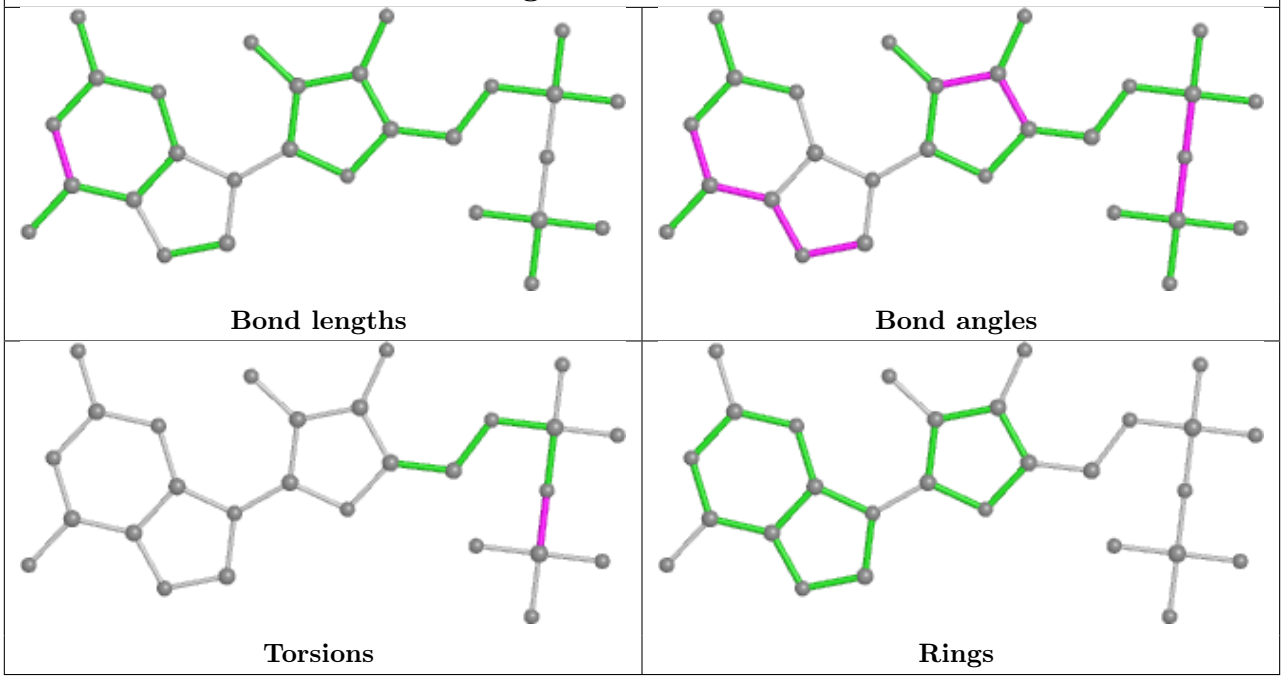
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GDP C 201



Ligand GDP A 201



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^{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	162/177 (91%)	0.17	13 (8%) 12 15	52, 76, 128, 162	0
1	C	155/177 (87%)	0.75	21 (13%) 3 4	60, 97, 141, 181	0
2	B	367/427 (85%)	0.05	16 (4%) 34 41	54, 81, 140, 188	0
2	D	346/427 (81%)	0.49	51 (14%) 2 3	59, 98, 146, 178	0
All	All	1030/1208 (85%)	0.32	101 (9%) 7 9	52, 90, 142, 188	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1652	TYR	6.4
2	B	1624	ASN	5.7
2	D	1710	MET	5.6
2	D	1763	LEU	5.5
1	C	55	VAL	5.5
2	D	1760	ILE	5.3
2	D	1801	LEU	4.5
2	B	1701	LYS	4.4
2	D	1505	LEU	4.2
2	D	1780	THR	4.1
1	A	88	LEU	4.0
2	B	1458	THR	4.0
1	C	16	LEU	3.7
2	D	1615	PRO	3.6
1	A	10	TYR	3.5
2	D	1748	GLN	3.5
2	D	1502	ALA	3.4
1	C	79	ALA	3.4
1	C	82	ARG	3.4
1	C	116	ASN	3.3
2	D	1703	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1749	LEU	3.2
1	A	16	LEU	3.2
1	A	17	ILE	3.1
1	C	40	SER	3.1
1	C	145	LYS	3.1
2	D	1741	ILE	3.1
2	D	1455	MET	3.1
2	B	1502	ALA	3.1
1	C	90	VAL	3.0
1	C	147	GLY	3.0
2	D	1556	LEU	3.0
2	D	1554	CYS	3.0
2	D	1569	PHE	3.0
2	D	1508	CYS	2.9
1	A	8	TYR	2.9
2	D	1506	TYR	2.9
2	D	1552	ASN	2.9
2	B	1743	ALA	2.9
2	B	1508	CYS	2.9
2	D	1706	TRP	2.8
1	C	12	PHE	2.8
2	B	1805	ASN	2.7
2	D	1815	LYS	2.7
1	C	89	LEU	2.7
2	B	1509	ILE	2.7
2	D	1509	ILE	2.6
2	D	1553	THR	2.6
2	D	1716	ILE	2.6
2	D	1659	ARG	2.6
2	D	1816	HIS	2.6
2	D	1759	ALA	2.6
2	D	1503	TYR	2.6
2	B	1552	ASN	2.5
1	C	11	LEU	2.5
2	D	1797	ILE	2.5
1	C	42	SER	2.5
2	B	1807	PRO	2.5
1	C	60	ILE	2.5
1	A	55	VAL	2.5
2	B	1802	GLN	2.5
2	D	1696	ASN	2.5
1	A	87	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1771	GLN	2.4
2	D	1656	ALA	2.4
1	C	17	ILE	2.4
1	A	40	SER	2.4
1	A	89	LEU	2.4
1	C	107	LYS	2.4
2	D	1791	VAL	2.4
2	D	1655	GLU	2.4
2	D	1768	SER	2.4
2	D	1504	ILE	2.4
1	C	88	LEU	2.4
2	B	1556	LEU	2.3
2	D	1613	LEU	2.3
1	A	120	MET	2.3
2	D	1555	ARG	2.3
2	B	1652	TYR	2.3
1	A	15	VAL	2.3
2	D	1790	THR	2.3
1	C	112	HIS	2.3
2	D	1821	LEU	2.2
2	B	1499	CYS	2.2
2	D	1752	LYS	2.2
1	A	122	VAL	2.2
1	C	41	LYS	2.2
2	B	1787	GLU	2.2
2	D	1473	HIS	2.1
2	D	1619	SER	2.1
2	B	1505	LEU	2.1
1	A	112	HIS	2.1
2	D	1454	SER	2.1
2	D	1501	PRO	2.1
2	D	1653	CYS	2.1
2	D	1539	HIS	2.1
2	D	1762	SER	2.1
2	D	1549	TRP	2.1
1	C	111	ASP	2.0
2	D	1753	THR	2.0
1	C	63	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

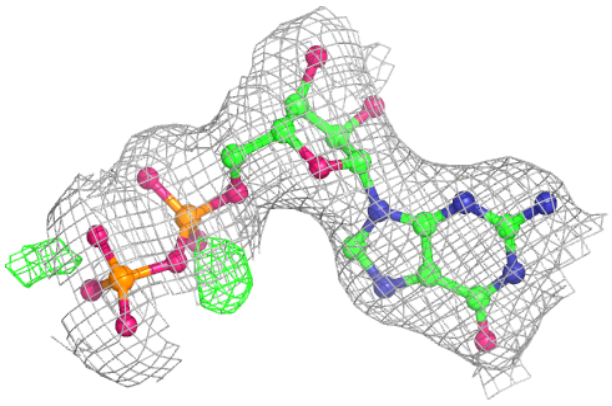
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

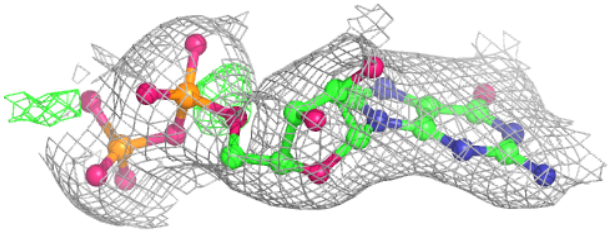
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	202	1/1	0.69	0.16	90,90,90,90	0
3	GDP	C	201	28/28	0.96	0.13	56,70,84,96	0
4	MG	A	202	1/1	0.97	0.11	74,74,74,74	0
3	GDP	A	201	28/28	0.98	0.11	47,61,72,83	0

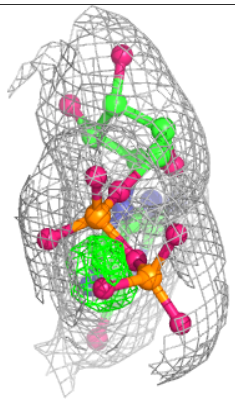
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP 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)

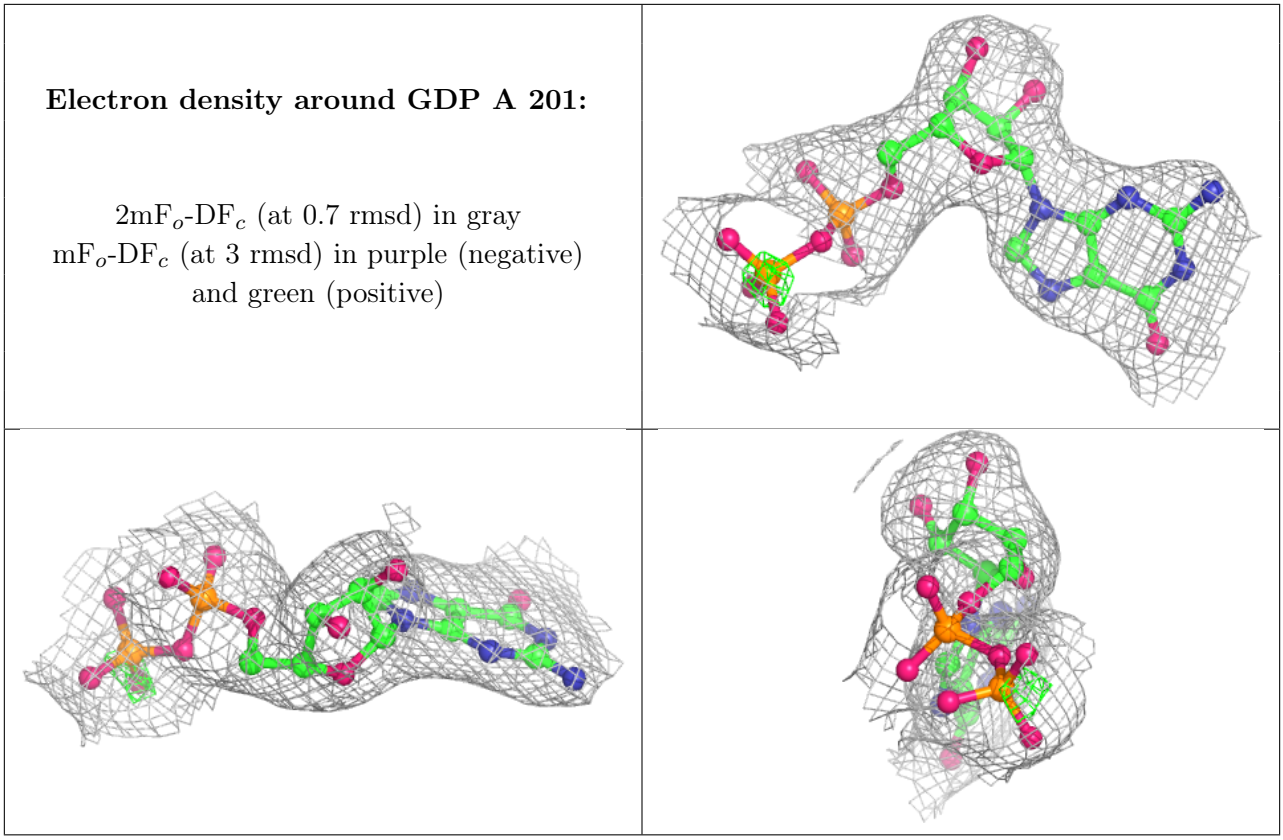






Electron density around GDP A 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.