



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 09:40 PM EDT

PDB ID : 3QBV  
Title : Structure of designed orthogonal interaction between CDC42 and nucleotide exchange domains of intersectin  
Authors : Kapp, G.T.; Remenyi, A.; Lim, W.A.; Kortemme, T.  
Deposited on : 2011-01-14  
Resolution : 2.65 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

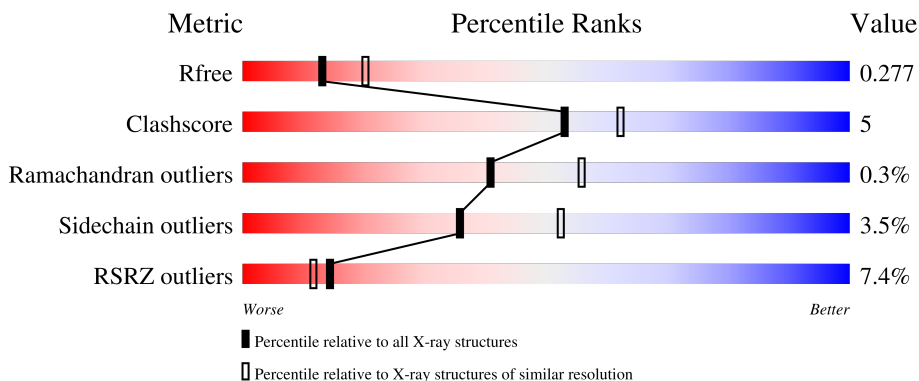
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	178	
1	C	178	
2	B	351	
2	D	351	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7068 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 Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1288	818	214	250	6	0	0	0
1	C	177	1310	835	218	251	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ARG	PHE	engineered mutation	UNP P60953
A	163	LYS	ARG	variant	UNP P60953
C	56	ARG	PHE	engineered mutation	UNP P60953
C	163	LYS	ARG	variant	UNP P60953

- Molecule 2 is a protein called Intersectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	307	2164	1367	388	395	14	0	0	0
2	D	289	2135	1350	379	391	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1373	GLU	SER	engineered mutation	UNP Q15811
D	1373	GLU	SER	engineered mutation	UNP Q15811

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

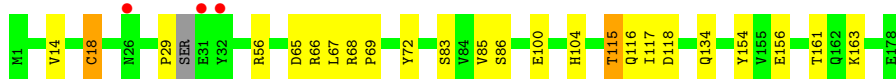
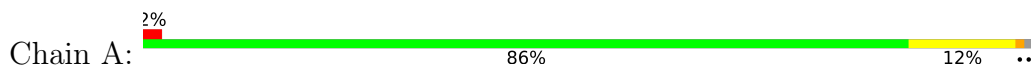
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	34	Total	O	0	0
			34	34		
4	C	18	Total	O	0	0
			18	18		
4	D	42	Total	O	0	0
			42	42		

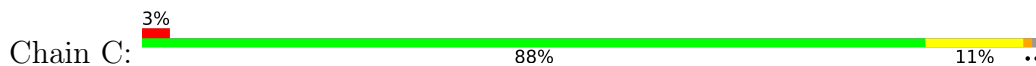
### 3 Residue-property plots

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.

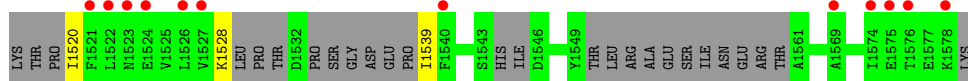
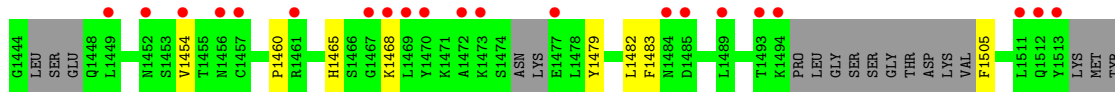
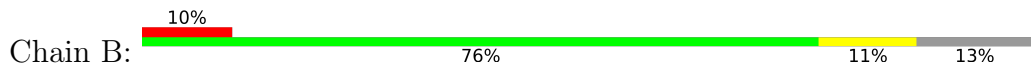
- Molecule 1: Cell division control protein 42 homolog



- Molecule 1: Cell division control protein 42 homolog



- Molecule 2: Intersectin-1



- Molecule 2: Intersectin-1



GLN	LEU	V1450	V1454	T1455	N1456	C1487	L1488	G1489	P1460	R1461	L1489	TYR	K1471	ALA	LYS	SER	ASN	ASN	LYS	GLU	LEU	Y1479	F1483	N1484	D1485	F1486	L1487	L1488	L1489	T1490	T1493	K1494	PRO	LEU	GLY	SER	SER	GLY	THR	ASP	K1503	V1504	P1507	LYS	SER	ASN	L1511	K1514	M1515	TYR	LYS	THR	PRO	I1520
F1521	L1522	ASN	GLU	V1525	L1526	V1527	LYS	LEU	PRO	THR	ASP	PRO	SER	GLY	ASP	GLU	PRO	I1539	F1540	H1541	ILE	SER	HIS	ILE	ILE	ASP	ARG	VAL	TYR	THR	LEU	ARG	ALA	ALA	V1562	V1563	A1568	A1569	T1576	K1579														

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.46Å 80.06Å 94.59Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	45.85 – 2.65 45.85 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.85-2.65) 99.6 (45.85-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.65Å)	Xtrriage
Refinement program	PHENIX dev_847	Depositor
R, $R_{free}$	0.241 , 0.284 0.232 , 0.277	Depositor DCC
$R_{free}$ test set	3502 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtrriage
Anisotropy	0.399	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: GDP

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	0.32	0/1314	0.53	0/1799
1	C	0.31	0/1336	0.52	0/1822
2	B	0.31	0/2194	0.46	0/2977
2	D	0.31	0/2166	0.47	0/2927
All	All	0.31	0/7010	0.49	0/9525

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 [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	1288	0	1200	17	0
1	C	1310	0	1254	12	0
2	B	2164	0	1881	25	0
2	D	2135	0	1944	24	0
3	A	28	0	12	1	0
3	C	28	0	12	0	0
4	A	21	0	0	1	0
4	B	34	0	0	6	0
4	C	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	42	0	0	6	0
All	All	7068	0	6303	71	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 (71) 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:83:SER:HA	1:A:115:THR:HG22	1.59	0.84
1:A:115:THR:HG23	1:A:116:GLN:HG3	1.68	0.75
2:B:1520:ILE:N	4:B:84:HOH:O	2.22	0.72
1:A:14:VAL:O	1:A:115:THR:HG21	1.91	0.69
2:D:1484:ASN:ND2	4:D:64:HOH:O	2.23	0.69
2:D:1490:THR:HA	2:D:1514:LYS:HA	1.78	0.66
2:B:1345:GLN:NE2	4:B:19:HOH:O	2.31	0.62
2:B:1238:ARG:NH2	2:B:1402:ASP:OD2	2.33	0.62
2:D:1238:ARG:NH2	2:D:1402:ASP:OD2	2.35	0.60
2:B:1468:LYS:HA	2:B:1479:TYR:HA	1.83	0.59
2:B:1539:ILE:N	4:B:75:HOH:O	2.38	0.57
2:B:1505:PHE:N	4:B:87:HOH:O	2.38	0.55
1:A:118:ASP:OD2	3:A:200:GDP:N2	2.21	0.55
2:B:1465:HIS:O	2:B:1482:LEU:N	2.40	0.54
2:D:1539:ILE:N	4:D:78:HOH:O	2.42	0.52
2:B:1505:PHE:N	4:B:83:HOH:O	2.42	0.52
2:B:1422:GLU:OE2	2:B:1425:ARG:NH1	2.42	0.51
2:D:1422:GLU:OE2	2:D:1425:ARG:NH1	2.43	0.50
1:C:56:ARG:NH2	2:D:1373:GLU:OE2	2.39	0.49
1:A:117:ILE:HD11	1:A:156:GLU:HB2	1.95	0.49
1:C:154:TYR:CZ	1:C:156:GLU:HG2	2.47	0.49
1:C:161:THR:HG22	1:C:163:LYS:H	1.78	0.48
1:A:67:LEU:HD21	2:B:1420:VAL:HG12	1.94	0.48
1:A:66:ARG:HG3	2:B:1425:ARG:HB2	1.96	0.48
1:A:154:TYR:CZ	1:A:156:GLU:HG2	2.49	0.48
1:C:82:PHE:HE2	1:C:112:LEU:HD23	1.79	0.47
1:A:83:SER:HB3	1:A:86:SER:HB3	1.97	0.46
1:A:161:THR:HG22	1:A:163:LYS:H	1.80	0.46
1:A:104:HIS:HE1	4:A:193:HOH:O	1.99	0.46
1:C:83:SER:HB3	1:C:86:SER:HB3	1.97	0.46
1:C:117:ILE:HD11	1:C:156:GLU:HB2	1.97	0.45
2:D:1461:ARG:HA	4:D:64:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1261:GLU:CD	2:D:1365:ARG:HH22	2.20	0.45
2:D:1284:ASN:HB2	2:D:1287:GLU:HB2	1.99	0.45
1:A:56:ARG:NH2	2:B:1373:GLU:OE2	2.43	0.45
2:D:1400:HIS:CG	2:D:1401:PRO:HD2	2.52	0.45
2:B:1436:ILE:HD13	2:B:1483:PHE:CZ	2.52	0.44
1:C:36:VAL:HG22	2:D:1384:ARG:HD2	1.98	0.44
2:D:1309:LYS:N	4:D:52:HOH:O	2.35	0.44
2:B:1261:GLU:CD	2:B:1365:ARG:HH22	2.20	0.44
2:D:1486:PHE:CB	2:D:1520:ILE:HA	2.48	0.44
2:D:1400:HIS:HD2	2:D:1402:ASP:H	1.65	0.44
2:B:1528:LYS:HA	2:B:1539:ILE:HA	2.00	0.44
2:B:1284:ASN:HB2	2:B:1287:GLU:HB2	2.00	0.44
1:A:69:PRO:HA	1:A:72:TYR:CD1	2.53	0.43
2:D:1520:ILE:N	4:D:85:HOH:O	2.51	0.43
1:C:69:PRO:HA	1:C:72:TYR:CD1	2.53	0.43
2:D:1231:LEU:HB2	2:D:1236:ARG:NH1	2.33	0.43
1:C:117:ILE:HD11	1:C:156:GLU:CB	2.48	0.43
2:D:1486:PHE:HB2	2:D:1520:ILE:HA	2.00	0.43
1:C:68:ARG:HD2	1:C:100:GLU:OE2	2.19	0.43
1:A:117:ILE:HD11	1:A:156:GLU:CB	2.49	0.43
2:D:1310:MET:HG2	4:D:52:HOH:O	2.18	0.43
2:B:1369:MET:HG3	2:B:1373:GLU:HB3	2.02	0.42
2:D:1369:MET:HG3	2:D:1373:GLU:HB3	2.01	0.42
2:D:1439:HIS:O	2:D:1511:LEU:HA	2.20	0.42
2:B:1454:VAL:HA	2:B:1460:PRO:HA	2.02	0.42
2:D:1367:LYS:HE2	2:D:1367:LYS:HB3	1.77	0.42
2:B:1408:HIS:HB3	2:B:1412:LYS:NZ	2.35	0.42
1:A:68:ARG:HD2	1:A:100:GLU:OE2	2.19	0.41
2:B:1400:HIS:CG	2:B:1401:PRO:HD2	2.55	0.41
1:A:65:ASP:OD2	2:B:1425:ARG:NH2	2.47	0.41
1:C:34:PRO:HB3	2:D:1244:GLU:OE2	2.20	0.41
2:D:1265:LYS:HB2	2:D:1266:PRO:HD3	2.03	0.41
2:B:1231:LEU:HD12	2:B:1236:ARG:CZ	2.51	0.41
2:B:1257:GLN:NE2	4:B:101:HOH:O	2.42	0.41
2:D:1454:VAL:HA	2:D:1460:PRO:HA	2.02	0.41
2:B:1323:LEU:HA	2:B:1326:MET:HG3	2.02	0.40
1:C:123:PRO:O	1:C:126:ILE:HG12	2.21	0.40
2:B:1367:LYS:HE2	2:B:1367:LYS:HB3	1.75	0.40
1:A:18:CYS:SG	1:A:29:PRO:HG2	2.62	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	173/178 (97%)	164 (95%)	9 (5%)	0	100	100
1	C	173/178 (97%)	165 (95%)	8 (5%)	0	100	100
2	B	290/351 (83%)	274 (94%)	15 (5%)	1 (0%)	41	56
2	D	270/351 (77%)	258 (96%)	10 (4%)	2 (1%)	22	33
All	All	906/1058 (86%)	861 (95%)	42 (5%)	3 (0%)	41	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1504	VAL
2	B	1283	VAL
2	D	1283	VAL

### 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	130/158 (82%)	126 (97%)	4 (3%)	40	57
1	C	135/158 (85%)	132 (98%)	3 (2%)	52	70
2	B	185/323 (57%)	180 (97%)	5 (3%)	44	63
2	D	201/323 (62%)	190 (94%)	11 (6%)	21	33
All	All	651/962 (68%)	628 (96%)	23 (4%)	36	52

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	85	VAL
1	A	115	THR
1	A	134	GLN
2	B	1245	LEU
2	B	1322	GLN
2	B	1335	ARG
2	B	1342	LEU
2	B	1410	LEU
1	C	18	CYS
1	C	112	LEU
1	C	134	GLN
2	D	1245	LEU
2	D	1262	ILE
2	D	1322	GLN
2	D	1335	ARG
2	D	1342	LEU
2	D	1410	LEU
2	D	1416	LEU
2	D	1479	TYR
2	D	1484	ASN
2	D	1486	PHE
2	D	1563	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1400	HIS
2	D	1400	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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GDP	C	200	-	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)
3	GDP	A	200	-	24,30,30	0.98	1 (4%)	30,47,47	1.19	3 (10%)

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	200	-	-	5/12/32/32	0/3/3/3
3	GDP	A	200	-	-	7/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	GDP	C6-N1	-2.49	1.34	1.37
3	C	200	GDP	C6-N1	-2.39	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	200	GDP	PA-O3A-PB	-3.02	122.45	132.83
3	C	200	GDP	PA-O3A-PB	-2.83	123.13	132.83
3	C	200	GDP	C3'-C2'-C1'	2.69	105.03	100.98
3	A	200	GDP	C8-N7-C5	2.32	107.42	102.99
3	C	200	GDP	C8-N7-C5	2.32	107.41	102.99
3	C	200	GDP	C5-C6-N1	2.13	117.71	113.95
3	A	200	GDP	C5-C6-N1	2.04	117.55	113.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

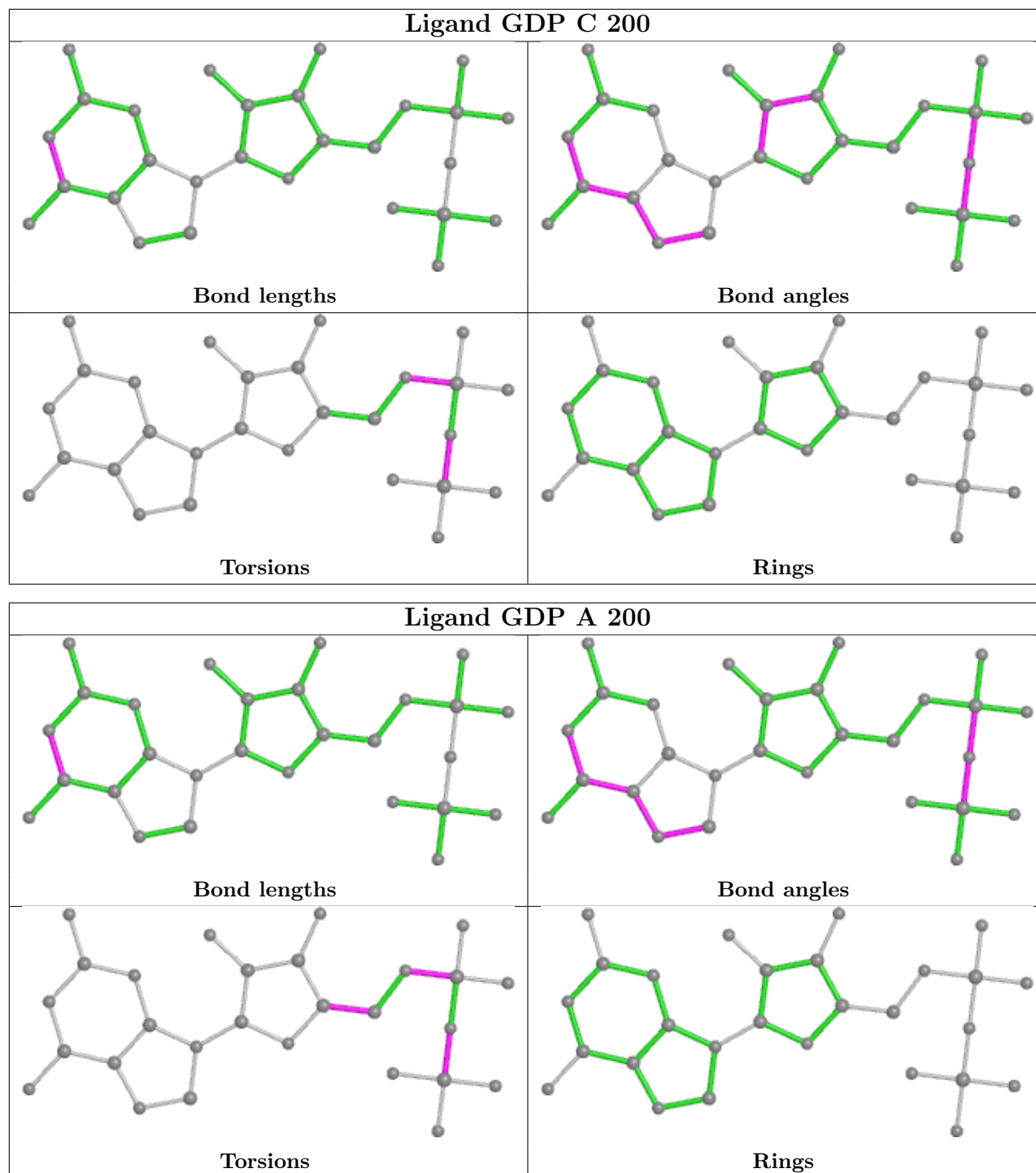
Mol	Chain	Res	Type	Atoms
3	A	200	GDP	PA-O3A-PB-O3B
3	A	200	GDP	C5'-O5'-PA-O3A
3	A	200	GDP	C5'-O5'-PA-O2A
3	C	200	GDP	PA-O3A-PB-O3B
3	C	200	GDP	C5'-O5'-PA-O3A
3	A	200	GDP	C3'-C4'-C5'-O5'
3	A	200	GDP	O4'-C4'-C5'-O5'
3	C	200	GDP	PA-O3A-PB-O2B
3	C	200	GDP	C5'-O5'-PA-O2A
3	A	200	GDP	PA-O3A-PB-O1B
3	C	200	GDP	PA-O3A-PB-O1B
3	A	200	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	200	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 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	177/178 (99%)	0.11	3 (1%) 70 67	28, 45, 81, 117	0
1	C	177/178 (99%)	0.09	5 (2%) 53 49	28, 45, 81, 117	0
2	B	307/351 (87%)	0.47	35 (11%) 5 3	23, 49, 124, 151	0
2	D	289/351 (82%)	0.38	27 (9%) 8 7	23, 48, 122, 142	0
All	All	950/1058 (89%)	0.31	70 (7%) 14 12	23, 47, 117, 151	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1527	VAL	6.9
2	B	1576	THR	5.1
1	C	32	TYR	4.9
2	B	1469	LEU	4.6
2	B	1513	TYR	4.3
1	A	32	TYR	4.3
2	B	1442	CYS	4.1
2	B	1493	THR	4.1
2	B	1485	ASP	3.9
2	B	1468	LYS	3.9
2	B	1522	LEU	3.9
2	B	1521	PHE	3.8
2	B	1523	ASN	3.7
2	B	1574	ILE	3.7
2	D	1489	LEU	3.7
2	B	1477	GLU	3.6
2	B	1489	LEU	3.5
2	D	1483	PHE	3.2
1	A	31	GLU	3.2
1	C	31	GLU	3.2
2	D	1569	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	1229	ASP	3.2
2	D	1486	PHE	3.2
2	B	1467	GLY	3.2
2	D	1494	LYS	3.1
2	D	1490	THR	3.0
1	A	26	ASN	3.0
2	B	1449	LEU	2.9
2	B	1494	LYS	2.9
2	D	1485	ASP	2.8
2	B	1470	TYR	2.8
2	D	1526	LEU	2.8
1	C	48	GLY	2.7
2	D	1488	LEU	2.7
2	D	1568	ALA	2.7
1	C	33	VAL	2.6
2	B	1578	LYS	2.6
2	B	1461	ARG	2.6
2	D	1525	VAL	2.6
2	D	1522	LEU	2.6
2	D	1540	PHE	2.5
2	B	1527	VAL	2.5
2	B	1452	ASN	2.5
2	B	1575	GLU	2.5
2	D	1576	THR	2.5
2	D	1539	ILE	2.5
2	B	1484	ASN	2.4
2	D	1457	CYS	2.4
2	B	1511	LEU	2.4
2	B	1524	GLU	2.4
2	B	1472	ALA	2.3
2	D	1439	HIS	2.3
2	B	1473	LYS	2.3
2	B	1457	CYS	2.3
2	B	1454	VAL	2.2
2	D	1461	ARG	2.2
2	D	1456	ASN	2.2
2	D	1521	PHE	2.2
2	D	1479	TYR	2.1
2	D	1458	LEU	2.1
2	D	1493	THR	2.1
2	D	1484	ASN	2.1
1	C	47	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1456	ASN	2.1
2	B	1526	LEU	2.1
2	B	1512	GLN	2.1
2	B	1440	VAL	2.0
2	D	1230	MET	2.0
2	B	1569	ALA	2.0
2	B	1540	PHE	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](#)

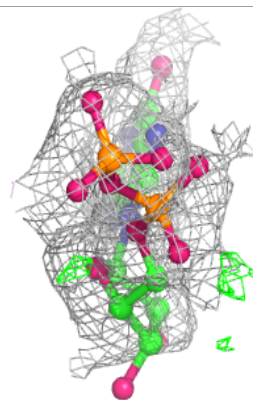
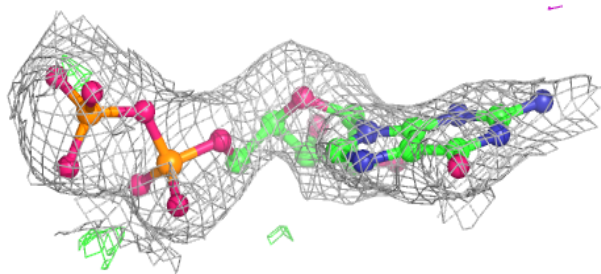
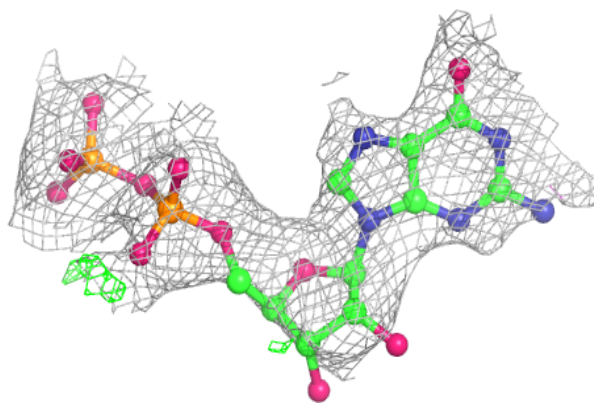
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GDP	A	200	28/28	0.92	0.21	36,84,97,101	0
3	GDP	C	200	28/28	0.93	0.26	27,79,95,111	0

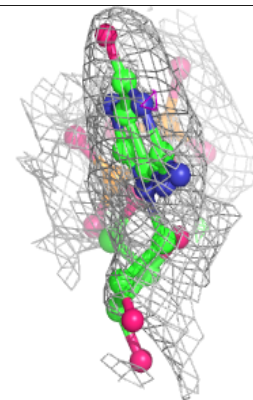
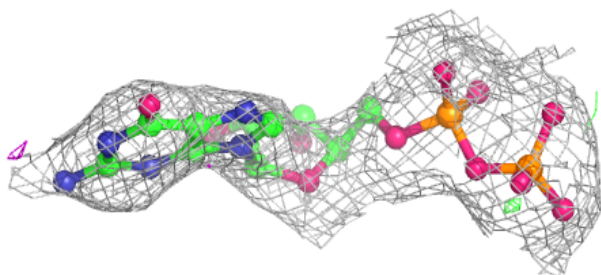
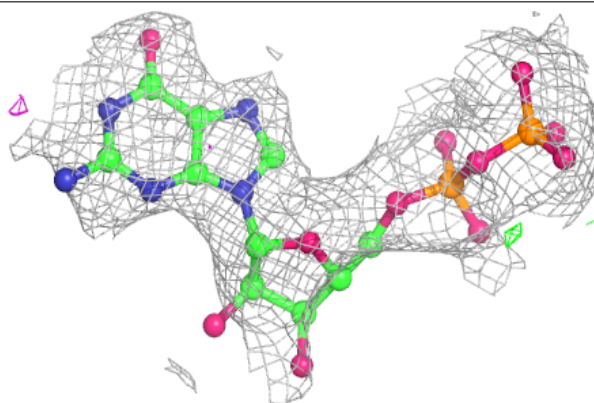
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GDP 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 GDP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.