



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:12 PM UTC

PDB ID : 3QBV / pdb_00003qbv
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

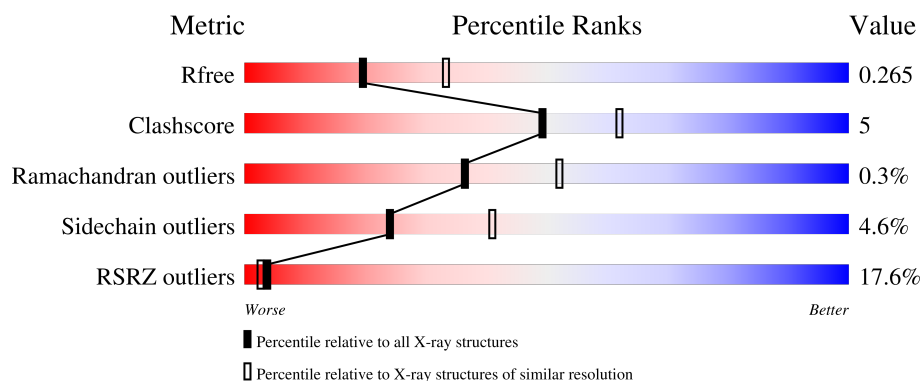
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 $\leq 5\%$. 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	8% 85% 11% ..
1	C	178	6% 87% 11% ..
2	B	351	25% 76% 11% 13%
2	D	351	16% 70% 12% 18%

2 Entry composition

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
1	A	177	Total	C	N	O	S	0	0	0
			1288	818	214	250	6			
1	C	177	Total	C	N	O	S	0	0	0
			1310	835	218	251	6			

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
2	B	307	Total	C	N	O	S	0	0	0
			2164	1367	388	395	14			
2	D	289	Total	C	N	O	S	0	0	0
			2135	1350	379	391	15			

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 (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

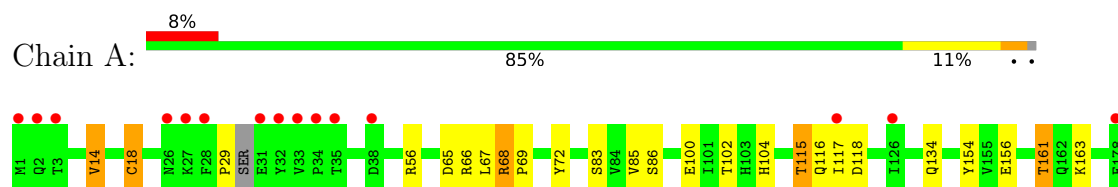
- Molecule 4 is water.

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

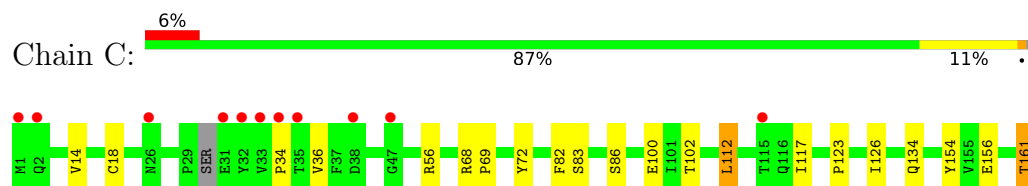
3 Residue-property plots [i](#)

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.

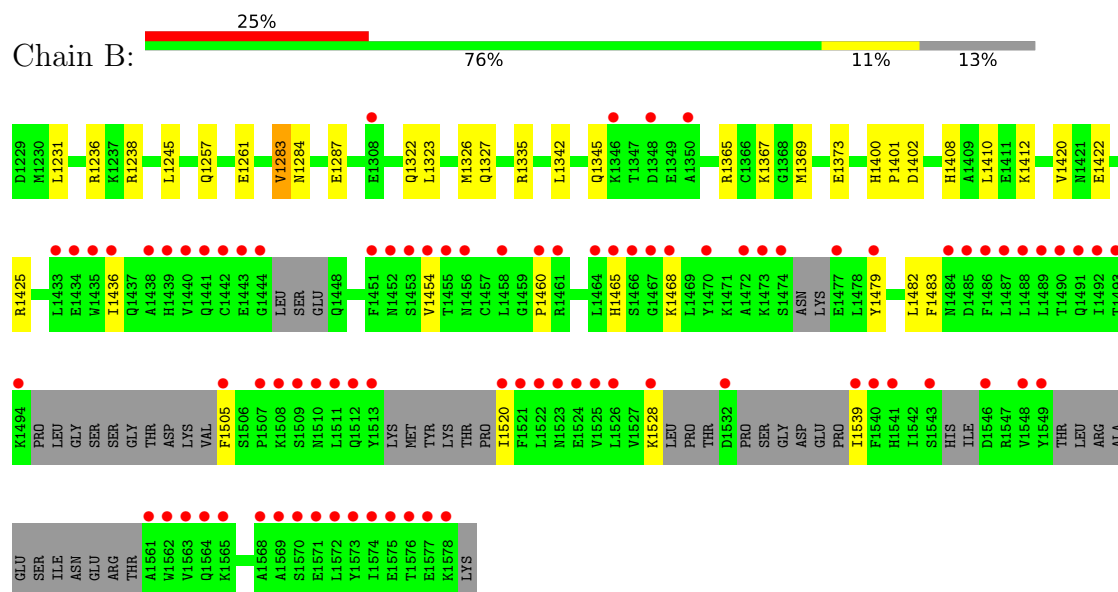
- Molecule 1: Cell division control protein 42 homolog



- Molecule 1: Cell division control protein 42 homolog

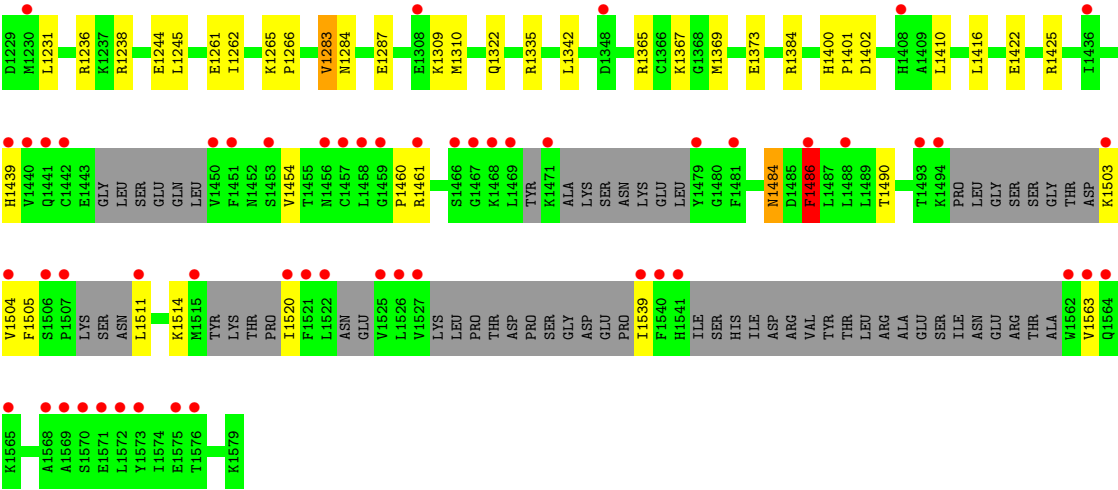


- Molecule 2: Intersectin-1



- Molecule 2: Intersectin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.65Å)	Xtriage
Refinement program	PHENIX dev_847	Depositor
R, R_{free}	0.241 , 0.284 (Not available) , 0.265	Depositor DCC
R_{free} test set	3502 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7068	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.44	0/1314	0.84	2/1799 (0.1%)
1	C	0.41	0/1336	0.83	0/1822
2	B	0.42	0/2194	0.79	2/2977 (0.1%)
2	D	0.41	0/2166	0.78	1/2927 (0.0%)
All	All	0.42	0/7010	0.81	5/9525 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1486	PHE	N-CA-C	6.01	116.50	108.38
2	B	1327	GLN	CA-C-N	-5.80	113.84	119.87
2	B	1327	GLN	C-N-CA	-5.80	113.84	119.87
1	A	68	ARG	CA-C-N	-5.13	114.54	119.87
1	A	68	ARG	C-N-CA	-5.13	114.54	119.87

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	1288	0	1200	17	0
1	C	1310	0	1254	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2164	0	1881	25	0
2	D	2135	0	1944	25	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
4	D	42	0	0	6	0
All	All	7068	0	6303	72	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 (72) 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
2:D:1261:GLU:CD	2:D:1365:ARG:HH22	2.20	0.49
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
2:B:1261:GLU:CD	2:B:1365:ARG:HH22	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1454:VAL:HA	2:D:1460:PRO:HA	2.02	0.41
2:D:1503:LYS:C	2:D:1505:PHE:H	2.29	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%)	36	52
2	D	270/351 (77%)	258 (96%)	10 (4%)	2 (1%)	18	30
All	All	906/1058 (86%)	861 (95%)	42 (5%)	3 (0%)	36	52

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%)	123 (95%)	7 (5%)	20	35
1	C	135/158 (85%)	129 (96%)	6 (4%)	25	43
2	B	185/323 (57%)	179 (97%)	6 (3%)	34	55
2	D	201/323 (62%)	190 (94%)	11 (6%)	19	33
All	All	651/962 (68%)	621 (95%)	30 (5%)	24	41

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	18	CYS
1	A	85	VAL
1	A	102	THR
1	A	115	THR
1	A	134	GLN
1	A	161	THR
2	B	1245	LEU
2	B	1283	VAL
2	B	1322	GLN
2	B	1335	ARG
2	B	1342	LEU
2	B	1410	LEU
1	C	14	VAL
1	C	18	CYS
1	C	102	THR
1	C	112	LEU
1	C	134	GLN
1	C	161	THR
2	D	1245	LEU
2	D	1262	ILE
2	D	1283	VAL
2	D	1322	GLN
2	D	1335	ARG
2	D	1342	LEU
2	D	1410	LEU
2	D	1416	LEU
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
2	B	1400	HIS
2	B	1405	HIS
1	C	39	ASN
2	D	1400	HIS
2	D	1405	HIS

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 oligosaccharides 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	A	200	-	29,30,30	1.21	3 (10%)	45,47,47	1.73	5 (11%)
3	GDP	C	200	-	29,30,30	1.22	3 (10%)	45,47,47	1.79	7 (15%)

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	A	200	-	-	7/16/32/32	0/3/3/3
3	GDP	C	200	-	-	5/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GDP	C5-C4	3.21	1.47	1.38
3	A	200	GDP	C5-C4	3.19	1.47	1.38
3	C	200	GDP	PA-O3A	2.71	1.62	1.59
3	A	200	GDP	C6-N1	-2.50	1.34	1.38
3	C	200	GDP	C6-N1	-2.42	1.34	1.38
3	A	200	GDP	PA-O3A	2.35	1.62	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	200	GDP	C5-C4-N3	-6.03	118.79	128.39
3	A	200	GDP	C5-C4-N3	-5.98	118.87	128.39
3	C	200	GDP	C2-N3-C4	5.03	120.96	112.30
3	A	200	GDP	C2-N3-C4	4.82	120.61	112.30
3	A	200	GDP	N9-C4-N3	4.43	134.81	125.95
3	C	200	GDP	N9-C4-N3	4.42	134.80	125.95
3	C	200	GDP	C6-C5-N7	3.38	136.44	130.29
3	A	200	GDP	C6-C5-N7	3.24	136.19	130.29
3	C	200	GDP	C4-C5-N7	-2.67	106.44	110.67
3	A	200	GDP	C4-C5-N7	-2.63	106.50	110.67
3	C	200	GDP	O2A-PA-O3A	2.22	113.27	107.27
3	C	200	GDP	O6-C6-C5	-2.11	120.97	126.53

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	C	200	GDP	C5'-O5'-PA-O2A
3	A	200	GDP	C3'-C4'-C5'-O5'

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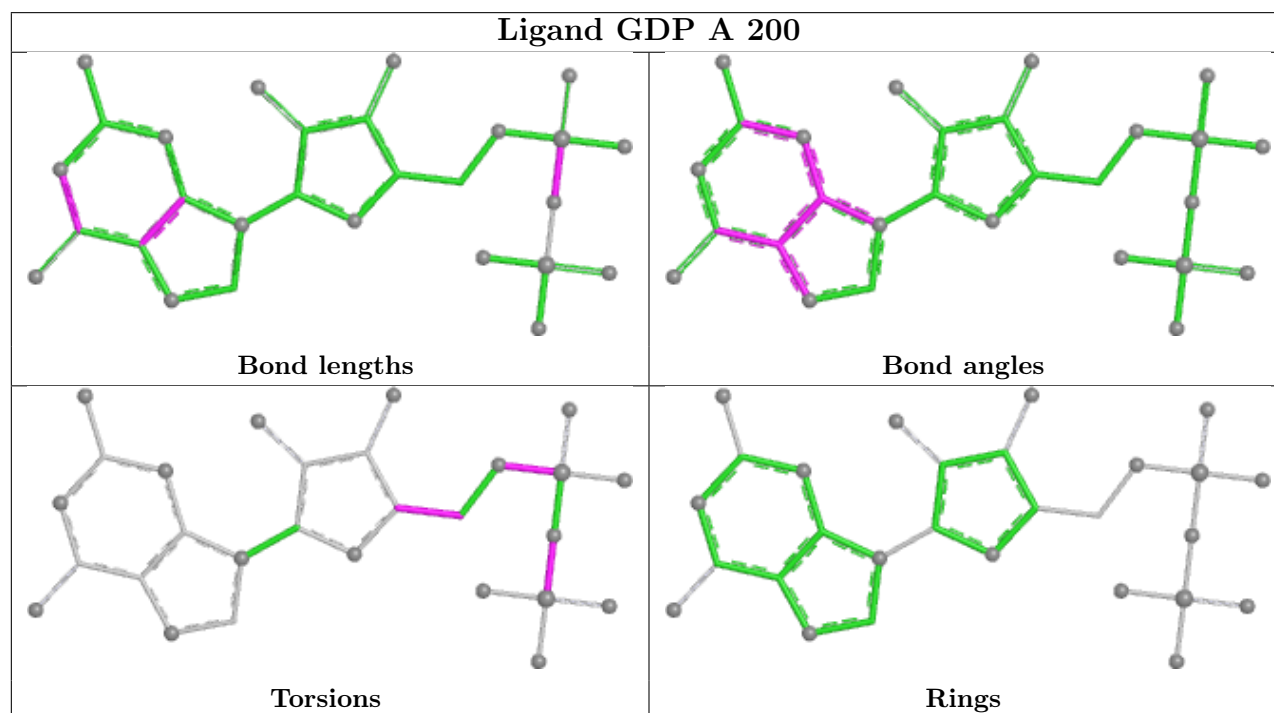
Mol	Chain	Res	Type	Atoms
3	A	200	GDP	O4'-C4'-C5'-O5'
3	C	200	GDP	PA-O3A-PB-O2B
3	A	200	GDP	PA-O3A-PB-O1B
3	C	200	GDP	PA-O3A-PB-O1B
3	A	200	GDP	PA-O3A-PB-O2B

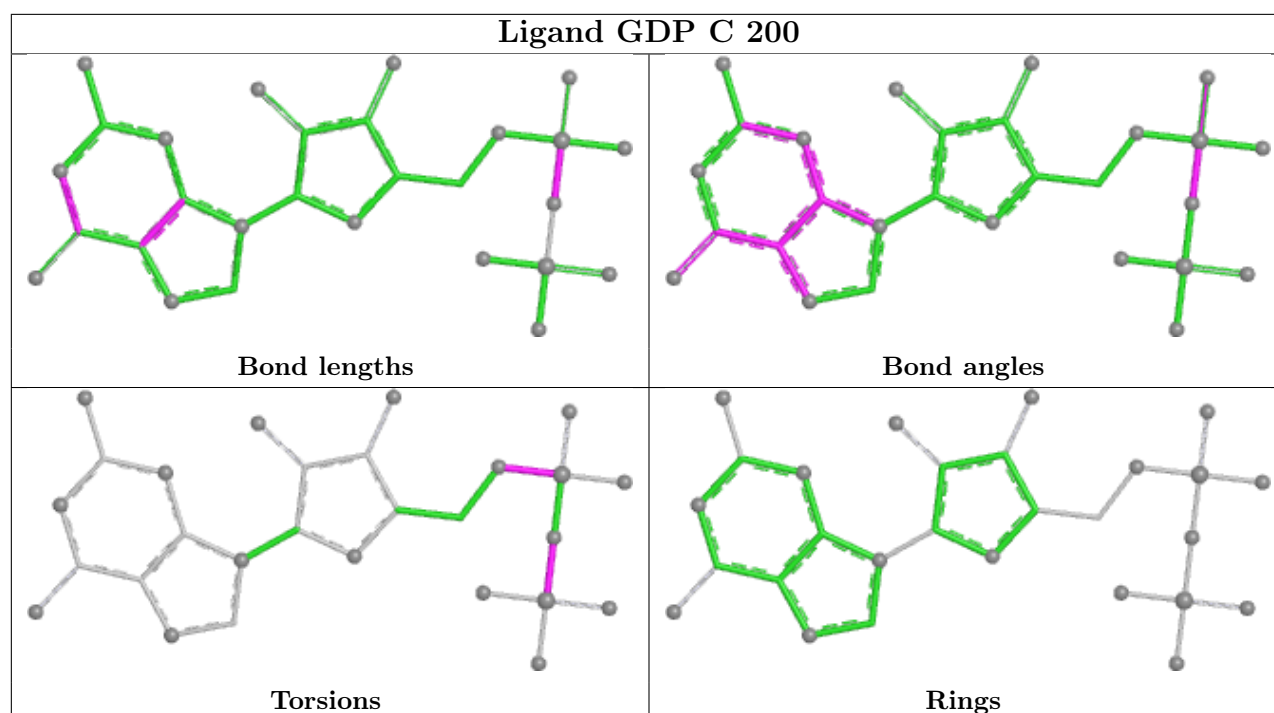
There are no ring outliers.

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 ⓘ

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, 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	177/178 (99%)	0.39	15 (8%)	16 12	28, 45, 81, 117	0
1	C	177/178 (99%)	0.31	11 (6%)	26 20	28, 45, 81, 117	0
2	B	307/351 (87%)	0.99	86 (28%)	1 1	23, 49, 124, 151	0
2	D	289/351 (82%)	0.76	55 (19%)	3 2	23, 48, 122, 142	0
All	All	950/1058 (89%)	0.68	167 (17%)	4 3	23, 47, 117, 151	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1522	LEU	5.9
1	C	32	TYR	5.3
2	D	1522	LEU	5.2
2	D	1515	MET	5.1
2	B	1513	TYR	5.1
1	A	32	TYR	5.0
2	B	1474	SER	4.9
2	B	1561	ALA	4.9
2	B	1484	ASN	4.6
2	B	1521	PHE	4.4
2	B	1466	SER	4.3
1	A	26	ASN	4.2
1	C	1	MET	4.2
2	D	1563	VAL	4.2
2	B	1452	ASN	4.1
2	D	1572	LEU	4.1
2	B	1470	TYR	4.1
1	A	31	GLU	4.0
2	B	1467	GLY	4.0
2	B	1442	CYS	3.9
2	B	1532	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	1562	TRP	3.9
2	B	1468	LYS	3.9
2	D	1442	CYS	3.9
1	A	35	THR	3.8
2	D	1562	TRP	3.7
2	D	1570	SER	3.7
2	B	1507	PRO	3.7
2	B	1479	TYR	3.7
1	C	31	GLU	3.7
2	B	1546	ASP	3.7
1	A	28	PHE	3.7
2	D	1568	ALA	3.6
2	D	1471	LYS	3.6
1	A	33	VAL	3.6
2	B	1441	GLN	3.5
2	B	1569	ALA	3.5
2	B	1485	ASP	3.5
2	D	1461	ARG	3.5
2	D	1576	THR	3.4
2	B	1461	ARG	3.4
2	D	1541	HIS	3.4
2	D	1486	PHE	3.4
2	D	1507	PRO	3.4
1	C	33	VAL	3.4
2	B	1549	TYR	3.3
2	B	1563	VAL	3.3
2	D	1573	TYR	3.3
2	B	1439	HIS	3.3
1	C	34	PRO	3.3
2	D	1469	LEU	3.3
1	A	34	PRO	3.2
2	B	1573	TYR	3.2
2	B	1565	LYS	3.2
2	B	1510	ASN	3.2
2	D	1511	LEU	3.2
2	B	1490	THR	3.2
2	D	1540	PHE	3.2
2	B	1526	LEU	3.1
2	D	1527	VAL	3.1
2	D	1575	GLU	3.1
2	B	1458	LEU	3.1
2	B	1477	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	1434	GLU	3.1
2	B	1440	VAL	3.1
2	D	1525	VAL	3.1
2	B	1512	GLN	3.0
2	B	1455	THR	3.0
2	B	1571	GLU	3.0
2	B	1472	ALA	3.0
2	B	1489	LEU	2.9
2	B	1572	LEU	2.9
1	C	38	ASP	2.9
1	A	1	MET	2.9
2	B	1539	ILE	2.9
2	B	1435	TRP	2.9
2	B	1509	SER	2.9
1	C	35	THR	2.8
2	B	1465	HIS	2.8
2	D	1441	GLN	2.8
2	B	1456	ASN	2.8
2	D	1456	ASN	2.8
2	D	1493	THR	2.8
2	B	1443	GLU	2.8
2	B	1574	ILE	2.7
1	C	26	ASN	2.7
2	D	1457	CYS	2.7
2	B	1491	GLN	2.7
2	B	1570	SER	2.7
2	B	1473	LYS	2.7
2	D	1569	ALA	2.7
2	B	1436	ILE	2.6
2	B	1433	LEU	2.6
2	D	1468	LYS	2.6
2	D	1564	GLN	2.6
2	B	1543	SER	2.6
2	D	1571	GLU	2.6
1	C	2	GLN	2.6
2	B	1487	LEU	2.5
2	B	1454	VAL	2.5
2	B	1486	PHE	2.5
2	D	1466	SER	2.5
2	D	1565	LYS	2.5
2	B	1524	GLU	2.5
2	B	1346	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1348	ASP	2.5
2	D	1436	ILE	2.5
2	D	1459	GLY	2.5
2	B	1576	THR	2.5
2	B	1528	LYS	2.5
1	A	27	LYS	2.4
2	B	1564	GLN	2.4
2	B	1505	PHE	2.4
1	A	126	ILE	2.4
2	B	1464	LEU	2.4
2	B	1525	VAL	2.4
2	D	1504	VAL	2.4
2	B	1578	LYS	2.4
2	D	1494	LYS	2.4
2	B	1444	GLY	2.4
2	B	1438	ALA	2.4
2	B	1511	LEU	2.3
2	D	1458	LEU	2.3
2	B	1493	THR	2.3
2	B	1494	LYS	2.3
2	B	1350	ALA	2.3
1	A	117	ILE	2.3
2	D	1506	SER	2.3
2	B	1548	VAL	2.3
2	B	1540	PHE	2.3
2	B	1577	GLU	2.3
2	B	1453	SER	2.3
2	B	1508	LYS	2.2
1	A	3	THR	2.2
2	B	1308	GLU	2.2
2	B	1451	PHE	2.2
2	D	1230	MET	2.2
2	D	1308	GLU	2.2
2	B	1523	ASN	2.2
1	A	38	ASP	2.2
2	D	1453	SER	2.2
2	B	1520	ILE	2.2
2	D	1439	HIS	2.2
2	B	1460	PRO	2.1
1	A	2	GLN	2.1
2	B	1488	LEU	2.1
2	B	1492	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	1521	PHE	2.1
2	B	1568	ALA	2.1
1	A	178	GLU	2.1
1	C	115	THR	2.1
2	D	1467	GLY	2.1
2	D	1520	ILE	2.1
2	D	1451	PHE	2.1
2	D	1539	ILE	2.1
2	B	1541	HIS	2.1
2	D	1503	LYS	2.0
2	D	1450	VAL	2.0
2	B	1575	GLU	2.0
2	D	1481	PHE	2.0
2	D	1348	ASP	2.0
2	D	1488	LEU	2.0
2	D	1526	LEU	2.0
2	D	1408	HIS	2.0
1	C	47	GLY	2.0
2	D	1440	VAL	2.0
2	D	1479	TYR	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](#)

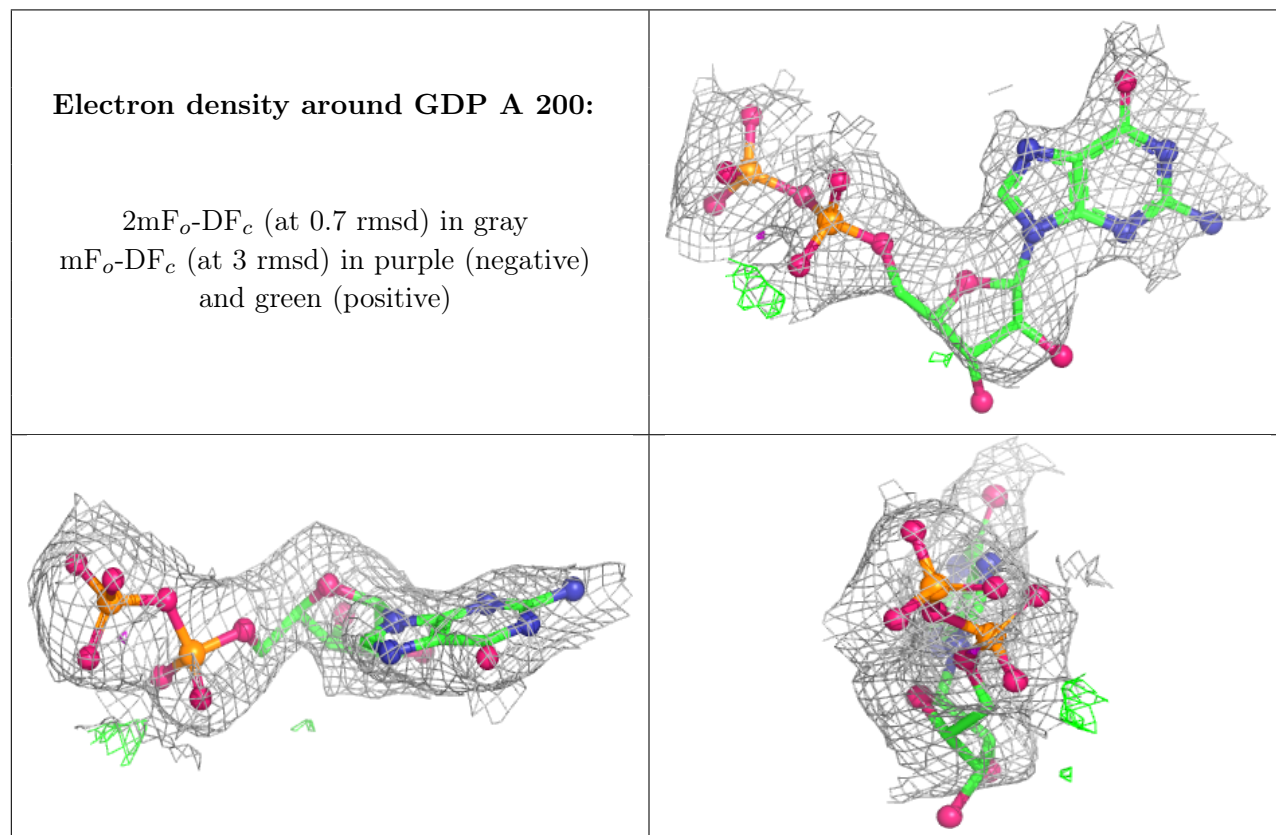
There are no oligosaccharides in this entry.

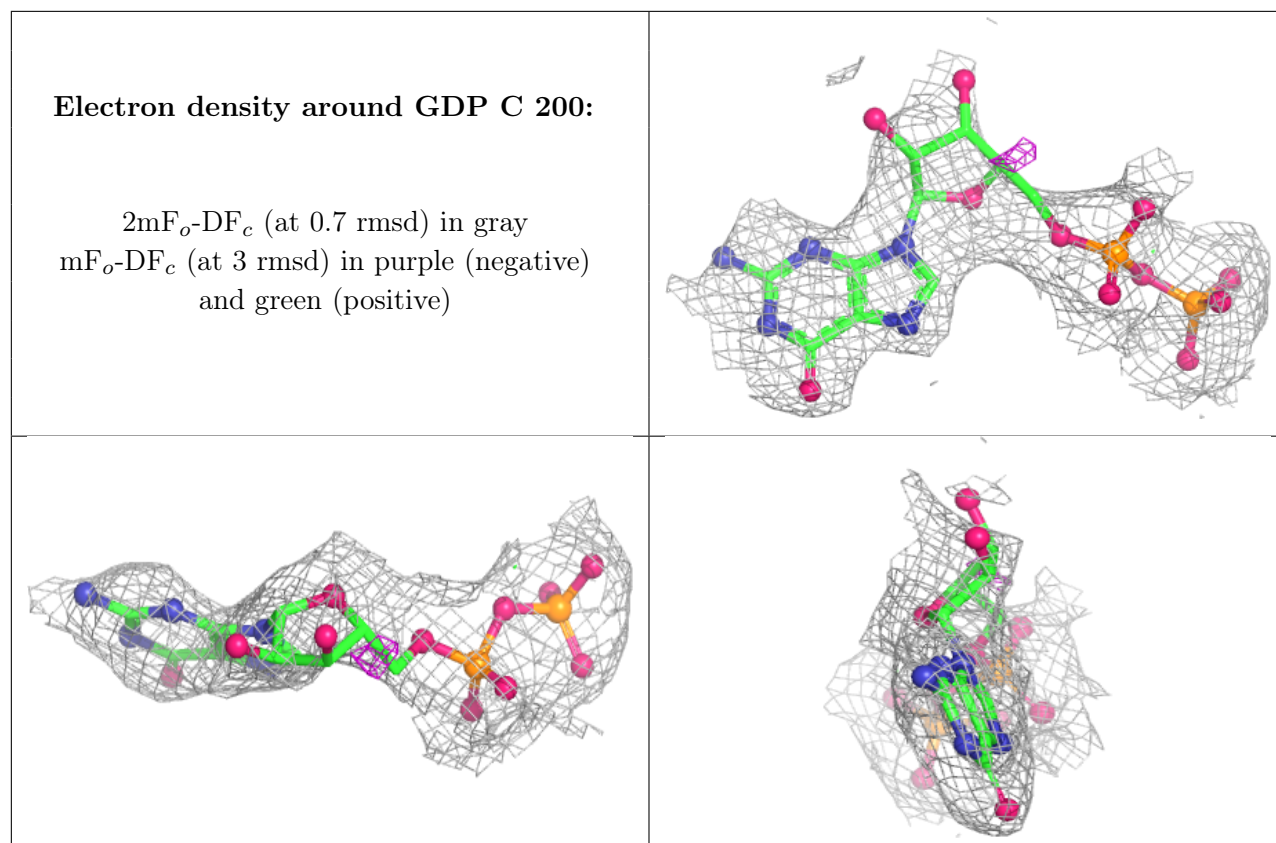
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	GDP	A	200	28/28	0.92	0.12	36,84,97,101	0
3	GDP	C	200	28/28	0.93	0.12	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.