

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2024 – 12:06 PM EST

PDB ID : 9C76

Title: LRRK2 Roc domain RP (Ras-pocket) complexed to Divarasib

Authors: Zhu, L.Y.; Guiley, K.Z.; Shokat, K.M.

Deposited on : 2024-06-10

Resolution : 2.30 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 2022.3.0, CSD as543be (2022)

Xtriage (Phenix) : 1.21

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.004 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

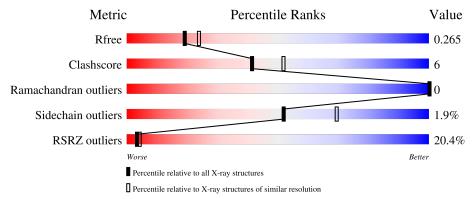
Validation Pipeline (wwPDB-VP) : 2.40

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 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 chair	n
1	A	189	30%	11% 13%
1	В	189	83%	11% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BR	A	204	-	-	X	-
4	MG	A	205	-	-	=	X



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5573 atoms, of which 2684 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 Leucine-rich repeat serine/threonine-protein kinase 2.

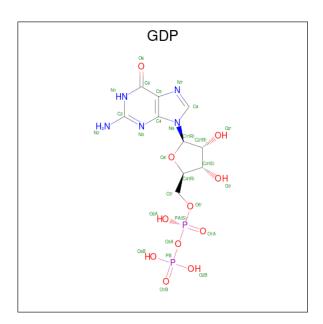
Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	A	165		_	H 1163		O 227	S 6	0	0	0
1	В	178	Total 2836	С		N	О	S 7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q5S007
A	15	ALA	ASN	engineered mutation	UNP Q5S007
A	16	CYS	THR	engineered mutation	UNP Q5S007
A	106	HIS	PRO	engineered mutation	UNP Q5S007
A	107	TYR	TRP	engineered mutation	UNP Q5S007
A	110	GLN	ASN	engineered mutation	UNP Q5S007
A	133	ALA	LYS	engineered mutation	UNP Q5S007
A	136	ALA	LYS	engineered mutation	UNP Q5S007
A	138	ALA	CYS	engineered mutation	UNP Q5S007
В	1	SER	-	expression tag	UNP Q5S007
В	15	ALA	ASN	engineered mutation	UNP Q5S007
В	16	CYS	THR	engineered mutation	UNP Q5S007
В	106	HIS	PRO	engineered mutation	UNP Q5S007
В	107	TYR	TRP	engineered mutation	UNP Q5S007
В	110	GLN	ASN	engineered mutation	UNP Q5S007
В	133	ALA	LYS	engineered mutation	UNP Q5S007
В	136	ALA	LYS	engineered mutation	UNP Q5S007
В	138	ALA	CYS	engineered mutation	UNP Q5S007

• Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
2	Λ	1	Total	С	Н	N	О	Р	0	0	
2	A	1	40	10	12	5	11	2	0	0	
9	D	1	Total	С	Н	N	О	Р	0	0	
	Б	1	40	10	12	5	11	2	U		

• Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Br 3 3	0	0

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

Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0

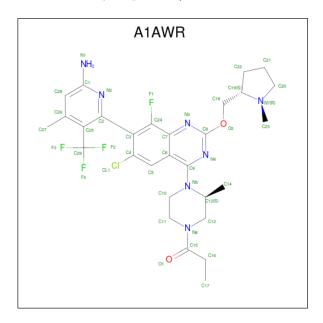
 \bullet Molecule 5 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total F 1 1	0	0

 $\bullet \ \, \text{Molecule 6 is 1-} \{(3S)-4-[(7M)-7-[6-amino-4-methyl-3-(trifluoromethyl)pyridin-2-yl]-6-chloro-8-fluoro-2-\{[(2S)-1-methylpyrrolidin-2-yl]methoxy\} \\ \text{quinazolin-4-yl}-3-methylpiperazin-1-yl} \} \\ \text{Proposition of the proposition of$



propan-1-one (three-letter code: A1AWR) (formula: $C_{29}H_{34}ClF_4N_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atoms						ZeroOcc	AltConf	
6	Λ	1	Total	С	Cl	F	Н	N	О	0	0	
0	A	1	76	29	1	4	33	7	2	U	0	
6	D	1	Total	С	Cl	F	Н	N	О	0	0	
0	Б	1	76	29	1	4	33	7	2	0	U	

• Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total I 1 1	0	0

• Molecule 8 is water.

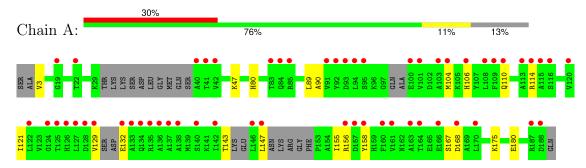
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	43	Total O 43 43	0	0
8	В	53	Total O 53 53	0	0



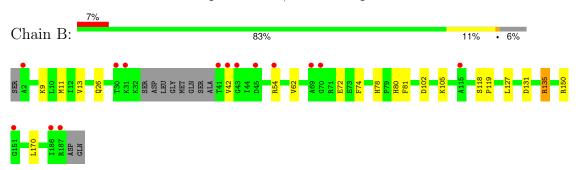
3 Residue-property plots (i)

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: Leucine-rich repeat serine/threonine-protein kinase 2



• Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	40.41Å 98.38Å 105.20Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.22 - 2.30	Depositor
Resolution (A)	35.22 - 2.30	EDS
% Data completeness	99.6 (35.22-2.30)	Depositor
(in resolution range)	99.6 (35.22-2.30)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
D D.	0.227 , 0.267	Depositor
R, R_{free}	0.228 , 0.265	DCC
R_{free} test set	17405 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 41.4	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	0.93	EDS
Total number of atoms	5573	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1AWR, GDP, BR, IOD, F

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		
Wioi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.31	0/1259	0.54	0/1702	
1	В	0.33	0/1430	0.56	0/1925	
All	All	0.32	0/2689	0.55	0/3627	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	135	ARG	Sidechain

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	1239	1163	1172	16	0
1	В	1405	1431	1431	17	0
2	A	28	12	12	0	0
2	В	28	12	12	0	0
3	A	3	0	0	3	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
5	A	1	0	0	0	0
6	A	43	33	0	3	0
6	В	43	33	0	1	0
7	В	1	0	0	0	0
8	A	43	0	0	4	0
8	В	53	0	0	1	0
All	All	2889	2684	2627	34	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 6.

All (34) 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:114:ARG:NH2	3:A:204:BR:BR	2.38	1.10
1:A:143:THR:O	8:A:301:HOH:O	2.01	0.79
1:A:110:GLN:NE2	1:A:114:ARG:HG3	2.06	0.71
6:A:207:A1AWR:N3	6:A:207:A1AWR:N7	2.41	0.69
1:A:110:GLN:HE21	1:A:114:ARG:HG3	1.59	0.68
1:B:150:ARG:O	8:B:301:HOH:O	2.14	0.66
1:A:175:LYS:NZ	8:A:304:HOH:O	2.26	0.66
1:A:3:VAL:N	8:A:305:HOH:O	2.32	0.62
1:B:127:LEU:HD11	1:B:135:ARG:HD3	1.81	0.62
1:B:78:HIS:HB3	1:B:81:PHE:HB3	1.87	0.56
1:A:129:VAL:O	1:A:132:GLU:HG3	2.07	0.53
1:A:110:GLN:O	1:A:114:ARG:HG2	2.13	0.48
1:B:102:ASP:OD2	1:B:105:LYS:CE	2.61	0.48
1:A:167:SER:OG	8:A:302:HOH:O	2.20	0.48
1:B:9:LYS:HE2	1:B:11:MET:SD	2.54	0.47
1:B:42:VAL:HG22	1:B:74:PHE:CD1	2.49	0.47
6:A:207:A1AWR:N3	6:A:207:A1AWR:C20	2.77	0.47
1:A:80:HIS:HA	3:A:202:BR:BR	2.71	0.46
1:B:62:VAL:O	1:B:62:VAL:HG23	2.15	0.46
1:A:110:GLN:NE2	1:A:114:ARG:CG	2.79	0.45
1:A:147:LEU:HA	1:A:155:ILE:HD12	1.99	0.45



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Atom-1	Atom-2	Interatomic	Clash
7100111-1	1100111-2	${f distance}({f A})$	overlap (Å)
1:B:13:VAL:HG11	6:B:204:A1AWR:F2	2.06	0.45
1:B:102:ASP:OD2	1:B:105:LYS:HE3	2.17	0.44
1:A:89:LEU:HD12	1:A:121:ILE:HB	1.98	0.44
1:B:42:VAL:HG22	1:B:74:PHE:CG	2.53	0.43
3:A:204:BR:BR	1:B:80:HIS:HA	2.74	0.43
1:B:54:ARG:HG2	1:B:54:ARG:HH11	1.82	0.42
6:A:207:A1AWR:O2	1:B:72:GLU:HG3	2.19	0.42
1:A:90:ALA:HB1	1:A:104:MET:SD	2.61	0.41
1:B:26:GLN:HG3	1:B:170:LEU:CD2	2.50	0.41
1:B:127:LEU:CD1	1:B:135:ARG:HD3	2.48	0.41
1:A:114:ARG:HH12	1:B:80:HIS:CE1	2.38	0.41
1:B:118:SER:HA	1:B:119:PRO:HD3	1.97	0.41
1:A:156:ARG:HE	1:A:180:GLU:CD	2.24	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	Perce	Percentiles	
1	A	153/189 (81%)	152 (99%)	1 (1%)	0	100	100	
1	В	174/189 (92%)	172 (99%)	2 (1%)	0	100	100	
All	All	327/378 (86%)	324 (99%)	3 (1%)	0	100	100	

There are no Ramachandran outliers to report.

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	120/162 (74%)	116 (97%)	4 (3%)	33 48		
1	В	148/162 (91%)	147 (99%)	1 (1%)	81 90		
All	All	268/324 (83%)	263 (98%)	5 (2%)	52 69		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	106	HIS
1	A	158	TYR
1	A	168	ASP
1	В	131	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type	
1	A	110	GLN	

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	Mol Type Chain Res		Link	Bond lengths		Bond angles				
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	A1AWR	В	204	1	46,47,47	0.62	1 (2%)	57,71,71	1.13	4 (7%)
6	A1AWR	A	207	1	46,47,47	0.68	1 (2%)	57,71,71	1.33	4 (7%)
2	GDP	A	201	-	25,30,30	1.01	1 (4%)	30,47,47	0.76	0
2	GDP	В	201	4	25,30,30	1.06	2 (8%)	30,47,47	0.77	0

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
6	A1AWR	В	204	1	-	6/24/48/48	0/5/5/5
6	A1AWR	A	207	1	-	10/24/48/48	0/5/5/5
2	GDP	A	201	-	-	0/12/32/32	0/3/3/3
2	GDP	В	201	4	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
2	A	201	GDP	C5-C6	-2.63	1.42	1.47
2	В	201	GDP	C5-C6	-2.63	1.42	1.47
6	A	207	A1AWR	C13-N5	2.53	1.50	1.47
6	В	204	A1AWR	C9-N4	2.15	1.34	1.32
2	В	201	GDP	C8-N7	-2.07	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
6	A	207	A1AWR	C3-C24-C7	-4.61	120.50	124.07
6	В	204	A1AWR	C3-C24-C7	-4.50	120.58	124.07
6	A	207	A1AWR	C5-C4-C3	-4.43	120.97	122.48
6	A	207	A1AWR	C2-C3-C24	-3.85	117.35	121.56
6	В	204	A1AWR	C5-C4-C3	-2.89	121.50	122.48
6	В	204	A1AWR	C3-C2-N2	-2.38	112.00	115.18
6	A	207	A1AWR	C3-C2-N2	-2.28	112.13	115.18



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
6	В	204	A1AWR	C2-C3-C24	-2.09	119.27	121.56

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	207	A1AWR	N3-C8-O2-C18
6	A	207	A1AWR	N4-C8-O2-C18
6	A	207	A1AWR	C19-C18-O2-C8
6	A	207	A1AWR	O2-C18-C19-C22
6	A	207	A1AWR	O2-C18-C19-N7
6	A	207	A1AWR	N4-C9-N5-C13
6	В	204	A1AWR	C26-C25-C29-F4
6	A	207	A1AWR	C26-C25-C29-F3
6	A	207	A1AWR	C26-C25-C29-F2
6	A	207	A1AWR	C26-C25-C29-F4
6	В	204	A1AWR	C26-C25-C29-F2
6	В	204	A1AWR	C26-C25-C29-F3
6	В	204	A1AWR	N3-C8-O2-C18
6	В	204	A1AWR	C6-C9-N5-C10
6	В	204	A1AWR	N4-C8-O2-C18
6	A	207	A1AWR	O1-C15-N6-C12

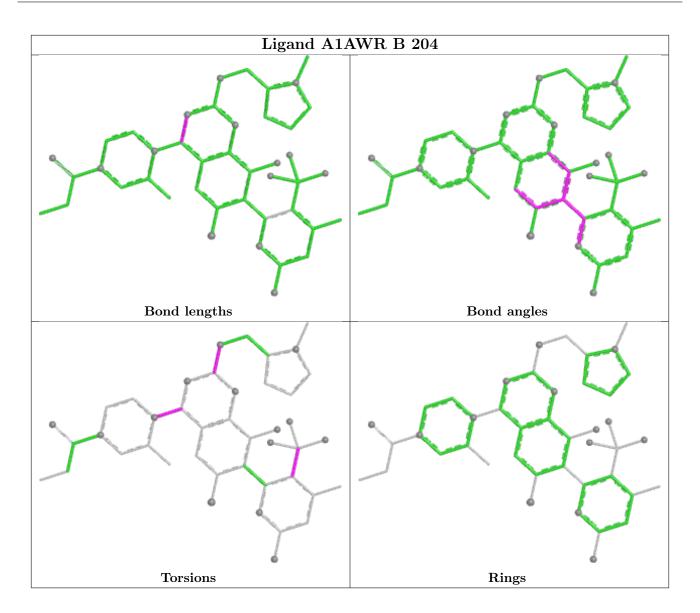
There are no ring outliers.

2 monomers are involved in 4 short contacts:

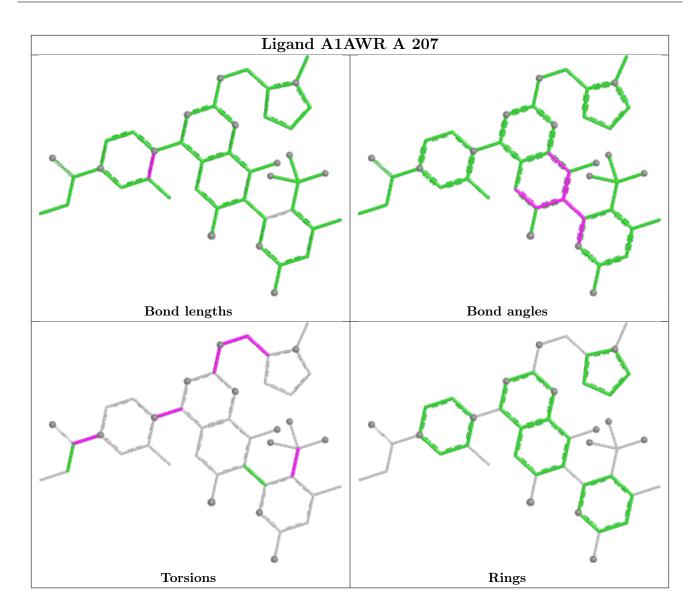
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	204	A1AWR	1	0
6	A	207	A1AWR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

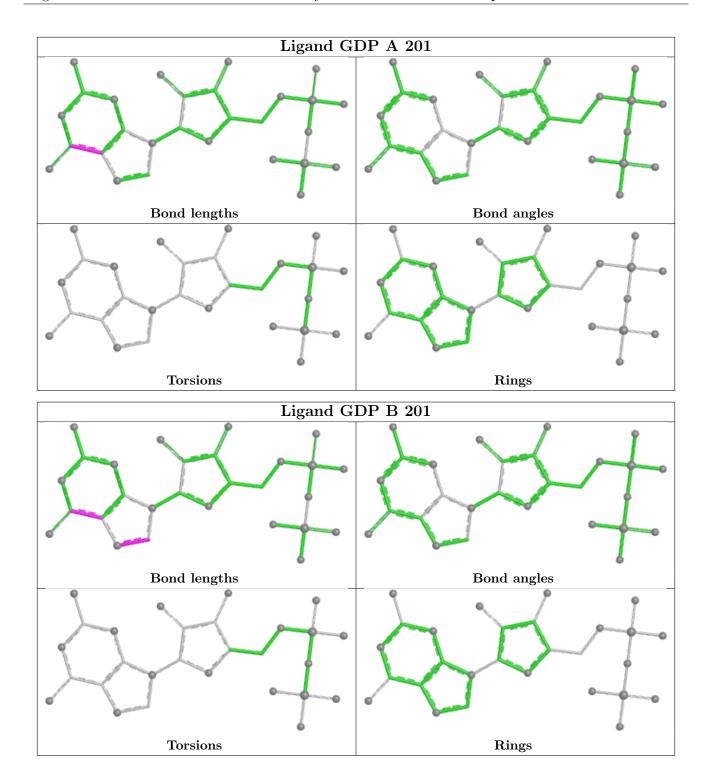












5.7 Other polymers (i)

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^{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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	165/189~(87%)	1.62	56 (33%) 1 1	33, 66, 107, 142	0
1	В	178/189~(94%)	0.61	14 (7%) 20 22	29, 46, 80, 125	0
All	All	343/378~(90%)	1.10	70 (20%) 3 4	29, 55, 104, 142	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ARG	5.4
1	A	92	TYR	5.3
1	A	147	LEU	4.8
1	A	42	VAL	4.6
1	A	94	LEU	4.5
1	A	84	GLN	4.1
1	A	22	THR	4.0
1	A	101	VAL	3.9
1	В	41	THR	3.9
1	A	127	LEU	3.9
1	A	146	LEU	3.8
1	В	42	VAL	3.8
1	A	133	ALA	3.7
1	A	135	ARG	3.6
1	A	140	SER	3.6
1	A	85	ARG	3.6
1	В	2	ALA	3.5
1	A	129	VAL	3.5
1	A	142	ILE	3.5
1	A	100	GLU	3.4
1	A	106	HIS	3.3
1	A	170	LEU	3.3
1	A	41	THR	3.1
1	В	30	THR	3.0



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Mol	Chain	Res	Type	RSRZ				
1	A	116	SER	3.0				
1	A	110	GLN	3.0				
1	В	43	GLY	3.0				
1	A	109	PHE	3.0				
1	A	108	LEU	2.9				
1	A	95	SER	2.9				
1	В	54	ARG	2.8				
1	A	157	ASP	2.8				
1	A	188	ASP	2.8				
1	В	151	GLY	2.8				
1	A	136	ALA	2.7				
1	A	83	THR	2.7				
1	В	70	GLY	2.6				
1	В	187	ARG	2.6				
1	A	163	ALA	2.6				
1	A	134	GLN	2.6				
1	A	91	VAL	2.5				
1	A	125	THR	2.5				
1	A	156	ARG	2.5				
1	A	120	VAL	2.5				
1	A	138	ALA	2.5				
1	A	168	ASP	2.5				
1	В	31	LYS	2.4				
1	A	93	ASP	2.4				
1	A	124	GLY	2.4				
1	A	115	ALA	2.4				
1	A	137	ALA	2.4				
1	A	126	HIS	2.4				
1	A	158	TYR	2.3				
1	A	132	GLU	2.3				
1	В	45	ASP	2.3				
1	A	113	ALA	2.3				
1	A	161	VAL	2.3				
1	A	19	GLY	2.3				
1	В	69	ALA	2.2				
1	A	104	MET	2.2				
1	A	122	LEU	2.2				
1	A	103	ALA	2.2				
1	В	115	ALA	2.2				
1	A	166	GLU	2.2				
1	A	114	ARG	2.1				
1	A	128	ASP	2.1				



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Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	2.1
1	A	164	THR	2.1
1	A	160	PHE	2.1
1	В	186	ILE	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.

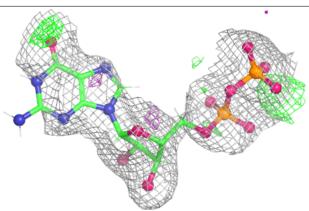
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$ m B ext{-}factors(\AA^2)$	Q < 0.9
4	MG	A	205	1/1	0.21	0.48	137,137,137,137	0
2	GDP	A	201	28/28	0.84	0.17	56,85,142,171	0
6	A1AWR	A	207	43/43	0.85	0.18	52,75,104,107	0
5	F	A	206	1/1	0.91	0.28	43,43,43,43	0
6	A1AWR	В	204	43/43	0.91	0.10	30,43,56,58	0
2	GDP	В	201	28/28	0.96	0.07	27,37,49,50	0
3	BR	A	203	1/1	0.96	0.08	63,63,63,63	0
3	BR	A	204	1/1	0.97	0.13	75,75,75,75	0
3	BR	A	202	1/1	0.98	0.08	67,67,67	0
4	MG	В	203	1/1	0.99	0.02	36,36,36,36	0
7	IOD	В	202	1/1	0.99	0.03	47,47,47,47	0

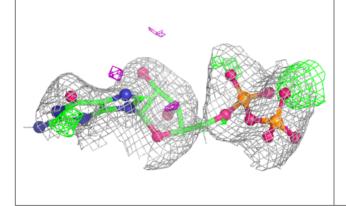
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

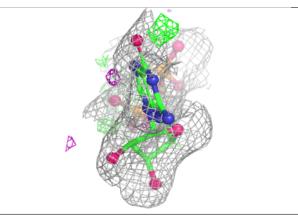


Electron density around GDP A 201:

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

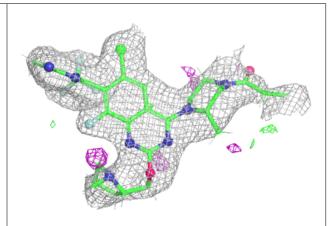


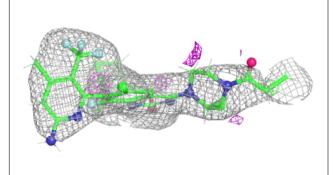


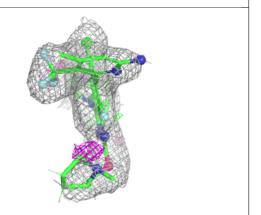


Electron density around A1AWR A 207:

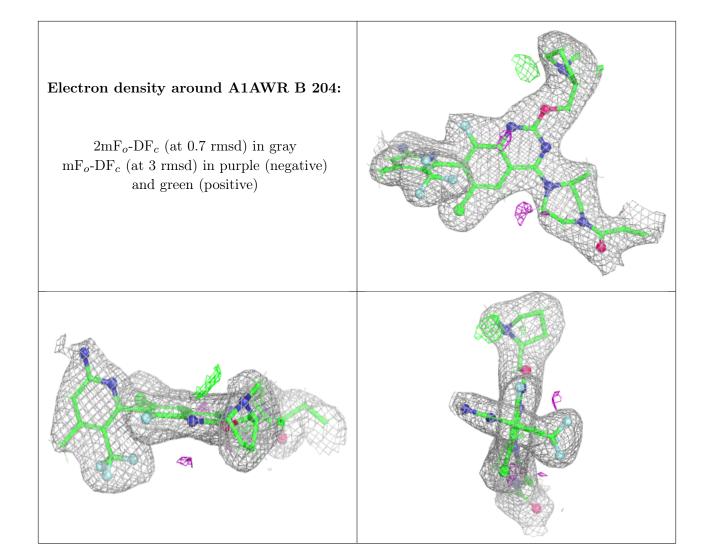
 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



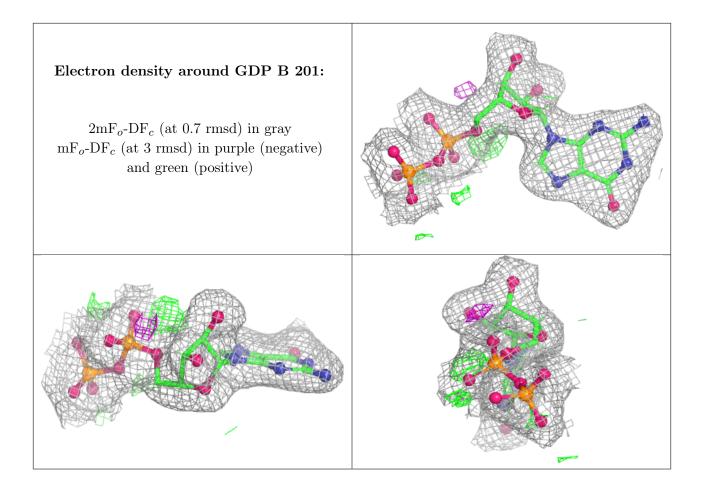












6.5 Other polymers (i)

There are no such residues in this entry.

