



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 01:07 AM EST

PDB ID : 6BCA  
Title : A Complex between PH Domain of LbcRhoGEF (AKAP-Lbc) and Activated RhoA Bound to a GTP Analog  
Authors : Sternweis, P.C.; Chen, Z.  
Deposited on : 2017-10-20  
Resolution : 2.00 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>.

---

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

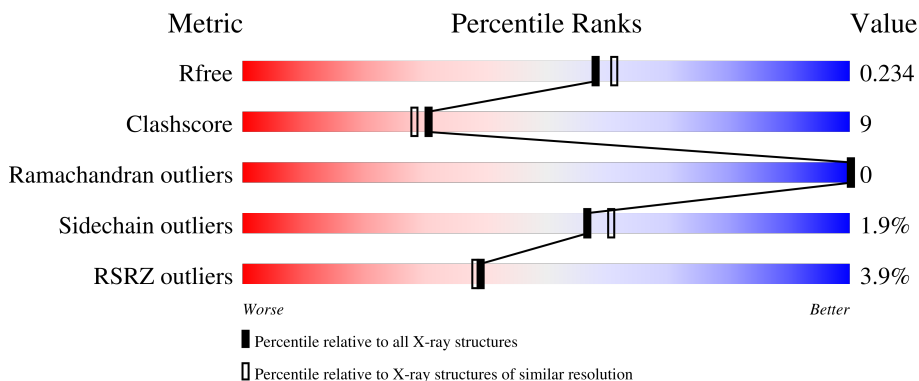
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	C	185	 5% 81% 15% ..
1	F	185	 3% 78% 19% .
2	A	151	 3% 74% 17% . 8%
2	B	151	 3% 72% 17% . 8%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10841 atoms, of which 5197 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 Transforming protein RhoA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	F	179	2829	897	1410	240	272	10	0	0	0
1	C	179	2829	897	1410	240	272	10	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP P61586
F	-2	ILE	-	expression tag	UNP P61586
F	-1	LEU	-	expression tag	UNP P61586
F	0	ASP	-	expression tag	UNP P61586
C	-3	GLY	-	expression tag	UNP P61586
C	-2	ILE	-	expression tag	UNP P61586
C	-1	LEU	-	expression tag	UNP P61586
C	0	ASP	-	expression tag	UNP P61586

- Molecule 2 is a protein called A-kinase anchor protein 13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	A	139	2293	713	1171	194	210	5	0	0	0
2	B	139	2311	719	1180	198	209	5	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2189	GLY	-	expression tag	UNP Q12802
A	2190	ILE	-	expression tag	UNP Q12802
A	2191	LEU	-	expression tag	UNP Q12802
A	2192	ASP	-	expression tag	UNP Q12802

*Continued on next page...*

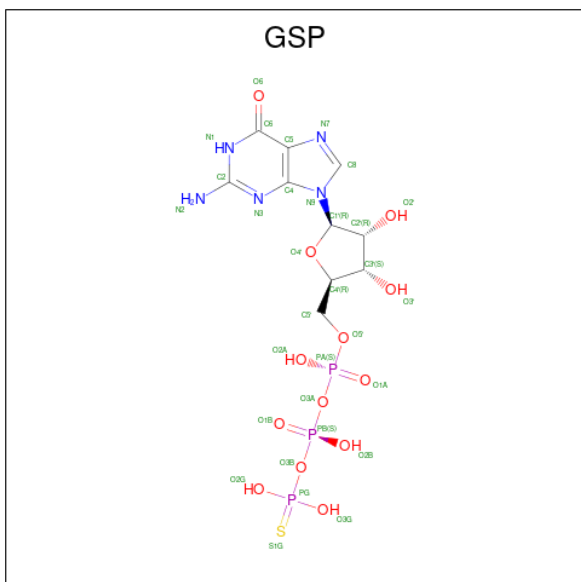
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2334	HIS	-	expression tag	UNP Q12802
A	2335	HIS	-	expression tag	UNP Q12802
A	2336	HIS	-	expression tag	UNP Q12802
A	2337	HIS	-	expression tag	UNP Q12802
A	2338	HIS	-	expression tag	UNP Q12802
A	2339	HIS	-	expression tag	UNP Q12802
B	2189	GLY	-	expression tag	UNP Q12802
B	2190	ILE	-	expression tag	UNP Q12802
B	2191	LEU	-	expression tag	UNP Q12802
B	2192	ASP	-	expression tag	UNP Q12802
B	2334	HIS	-	expression tag	UNP Q12802
B	2335	HIS	-	expression tag	UNP Q12802
B	2336	HIS	-	expression tag	UNP Q12802
B	2337	HIS	-	expression tag	UNP Q12802
B	2338	HIS	-	expression tag	UNP Q12802
B	2339	HIS	-	expression tag	UNP Q12802

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

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

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	F	1	Total	C	H	N	O	P	S	0	0
			45	10	13	5	13	3	1		
4	C	1	Total	C	H	N	O	P	S	0	0
			45	10	13	5	13	3	1		

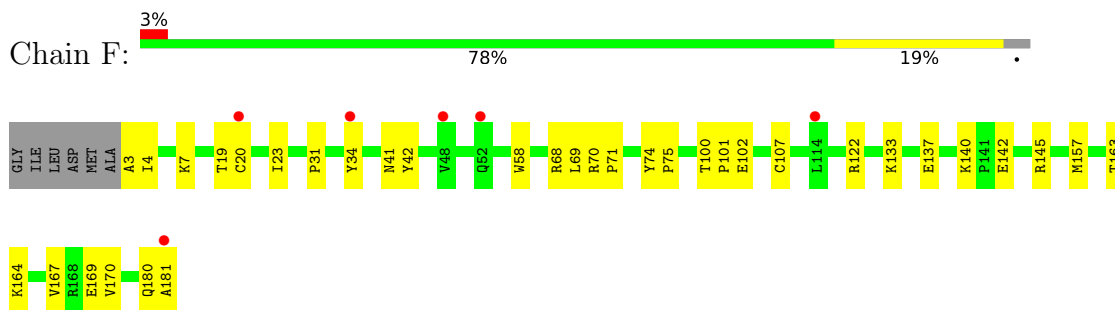
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	156	Total	O	0	0
			156	156		
5	A	87	Total	O	0	0
			87	87		
5	B	89	Total	O	0	0
			89	89		
5	C	155	Total	O	0	0
			155	155		

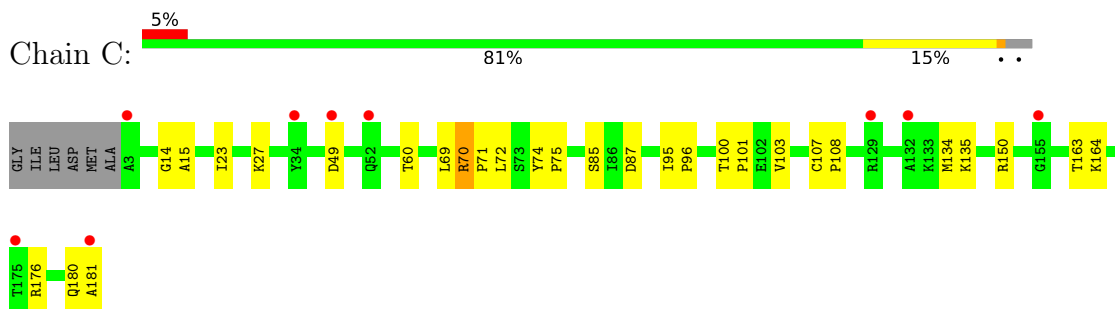
### 3 Residue-property plots [i](#)

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.

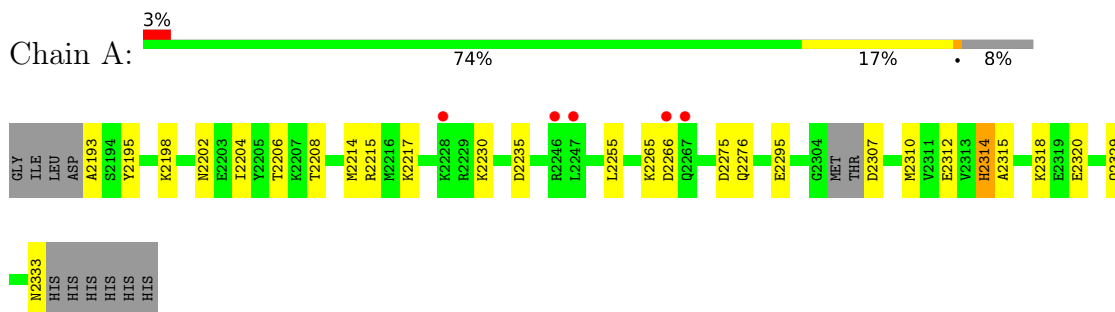
- Molecule 1: Transforming protein RhoA



- Molecule 1: Transforming protein RhoA

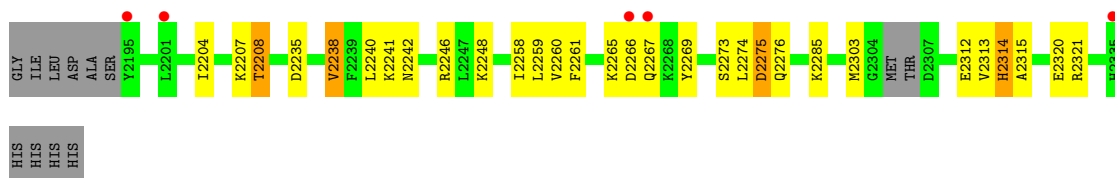


- Molecule 2: A-kinase anchor protein 13



- Molecule 2: A-kinase anchor protein 13





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.35Å 60.52Å 63.62Å 91.83° 92.97° 90.01°	Depositor
Resolution (Å)	34.21 – 2.00 39.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (34.21-2.00) 97.2 (39.15-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.196 , 0.234 0.199 , 0.234	Depositor DCC
$R_{free}$ test set	2500 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.165 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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: GSP, 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	C	0.68	0/1447	0.77	2/1956 (0.1%)
1	F	0.74	2/1447 (0.1%)	0.83	4/1956 (0.2%)
2	A	0.57	0/1133	0.70	1/1511 (0.1%)
2	B	0.60	0/1144	0.72	1/1526 (0.1%)
All	All	0.66	2/5171 (0.0%)	0.76	8/6949 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	107	CYS	CB-SG	-6.32	1.71	1.82
1	F	34	TYR	CD2-CE2	-5.48	1.31	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	F	122	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	C	70	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	70	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	70	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	2235	ASP	CB-CG-OD2	5.20	122.98	118.30
2	A	2235	ASP	CB-CG-OD2	5.18	122.97	118.30
1	F	70	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	C	1419	1410	1408	21	0
1	F	1419	1410	1408	25	0
2	A	1122	1171	1179	19	0
2	B	1131	1180	1183	36	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	C	32	13	12	0	0
4	F	32	13	12	0	0
5	A	87	0	0	2	0
5	B	89	0	0	8	0
5	C	155	0	0	1	0
5	F	156	0	0	3	0
All	All	5644	5197	5202	95	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 9.

All (95) 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:B:2312:GLU:OE2	2:B:2314:HIS:HE1	1.67	0.77
2:A:2204:ILE:O	2:A:2208:THR:HG23	1.85	0.77
2:B:2259:LEU:C	2:B:2259:LEU:HD13	2.05	0.77
1:F:167:VAL:O	1:F:170:VAL:HG12	1.85	0.75
2:A:2217:LYS:HD2	2:A:2307:ASP:O	1.86	0.74
1:F:167:VAL:O	1:F:170:VAL:CG1	2.37	0.73
1:F:3:ALA:O	5:F:301:HOH:O	2.08	0.72
2:A:2193:ALA:N	5:A:2401:HOH:O	2.22	0.71
2:B:2275:ASP:OD2	5:B:2401:HOH:O	2.09	0.69
2:B:2259:LEU:HD13	2:B:2260:VAL:N	2.10	0.67
1:C:49:ASP:OD2	1:C:176:ARG:NH1	2.29	0.66
2:A:2312:GLU:OE2	2:A:2314:HIS:HE1	1.80	0.64
2:B:2207:LYS:HE3	2:B:2269:TYR:CE2	2.31	0.64
2:B:2276:GLN:N	5:B:2403:HOH:O	2.17	0.63
2:B:2204:ILE:O	2:B:2208:THR:HG23	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2202:ASN:O	2:A:2206:THR:HG23	1.99	0.62
2:B:2207:LYS:O	2:B:2207:LYS:HG3	2.00	0.62
1:F:163:THR:O	1:F:164:LYS:HB2	2.00	0.61
2:B:2241:LYS:NZ	5:B:2402:HOH:O	2.14	0.61
2:A:2214:MET:HE2	2:A:2215:ARG:O	2.01	0.60
1:C:69:LEU:HD12	1:C:72:LEU:HD12	1.85	0.59
2:B:2285:LYS:O	2:B:2303:MET:HG3	2.03	0.58
2:B:2275:ASP:HB2	5:B:2401:HOH:O	2.03	0.58
2:B:2259:LEU:HD11	2:B:2261:PHE:CZ	2.39	0.57
1:C:85:SER:OG	1:C:87:ASP:OD1	2.19	0.57
2:B:2275:ASP:N	5:B:2403:HOH:O	2.38	0.56
1:C:134:MET:C	1:C:135:LYS:HD2	2.27	0.56
2:B:2204:ILE:O	2:B:2208:THR:CG2	2.56	0.54
2:A:2275:ASP:O	2:A:2276:GLN:HB2	2.09	0.53
2:B:2259:LEU:C	2:B:2259:LEU:CD1	2.77	0.52
1:F:74:TYR:N	1:F:75:PRO:CD	2.73	0.52
2:A:2214:MET:CE	2:A:2215:ARG:O	2.58	0.51
2:B:2315:ALA:HB1	2:B:2320:GLU:HG2	1.93	0.51
1:F:102:GLU:OE1	5:F:302:HOH:O	2.19	0.51
1:F:180:GLN:HG2	1:F:181:ALA:H	1.76	0.51
2:A:2310:MET:CE	1:C:72:LEU:HB3	2.41	0.50
1:C:74:TYR:N	1:C:75:PRO:CD	2.74	0.50
1:C:180:GLN:HG2	1:C:181:ALA:H	1.77	0.50
2:A:2295:GLU:HG2	2:A:2318:LYS:HB2	1.94	0.49
2:A:2214:MET:HE3	2:A:2215:ARG:N	2.27	0.49
1:C:163:THR:O	1:C:164:LYS:HB2	2.13	0.49
2:B:2266:ASP:O	2:B:2267:GLN:HB2	2.12	0.49
2:A:2333:ASN:C	5:A:2432:HOH:O	2.50	0.49
1:F:69:LEU:HD13	2:B:2303:MET:CE	2.43	0.49
1:F:167:VAL:O	1:F:170:VAL:HG13	2.13	0.49
2:B:2275:ASP:CA	5:B:2403:HOH:O	2.61	0.48
2:B:2315:ALA:HB1	2:B:2320:GLU:CG	2.44	0.48
2:B:2207:LYS:O	2:B:2207:LYS:CG	2.61	0.47
2:B:2321:ARG:C	2:B:2321:ARG:HD2	2.35	0.47
1:F:69:LEU:HD13	2:B:2303:MET:HE2	1.97	0.47
1:F:69:LEU:CD1	2:B:2303:MET:CE	2.92	0.47
1:C:107:CYS:N	1:C:108:PRO:CD	2.77	0.47
1:F:157:MET:HE1	1:F:169:GLU:HB3	1.96	0.46
1:F:180:GLN:O	1:F:181:ALA:HB3	2.15	0.46
2:A:2295:GLU:HG2	2:A:2318:LYS:HD2	1.96	0.46
2:A:2310:MET:HE3	1:C:72:LEU:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:THR:O	1:F:23:ILE:HG12	2.14	0.46
2:B:2240:LEU:CD2	2:B:2313:VAL:HG22	2.45	0.46
2:B:2265:LYS:HD2	5:B:2479:HOH:O	2.15	0.46
1:F:137:GLU:OE1	1:F:140:LYS:NZ	2.49	0.46
1:C:71:PRO:HA	1:C:74:TYR:CD2	2.51	0.46
2:A:2265:LYS:O	2:A:2266:ASP:C	2.53	0.45
1:C:180:GLN:O	1:C:181:ALA:HB3	2.16	0.45
1:F:100:THR:HB	1:F:101:PRO:HD3	1.99	0.45
2:B:2274:LEU:O	2:B:2275:ASP:C	2.55	0.45
1:C:181:ALA:HA	5:C:371:HOH:O	2.16	0.45
2:B:2242:ASN:HB2	2:B:2246:ARG:O	2.17	0.44
1:F:7:LYS:HE3	1:F:58:TRP:CD2	2.53	0.44
1:F:142:GLU:HG3	1:F:145:ARG:NH2	2.32	0.44
1:C:14:GLY:O	1:C:15:ALA:HB3	2.17	0.44
1:F:180:GLN:HG2	1:F:181:ALA:N	2.32	0.44
1:C:100:THR:HB	1:C:101:PRO:HD3	2.00	0.44
2:A:2195:TYR:O	2:A:2198:LYS:HB3	2.18	0.43
2:A:2315:ALA:HB1	2:A:2320:GLU:HB3	2.00	0.43
1:C:103:VAL:O	1:C:107:CYS:HB2	2.17	0.43
2:B:2258:ILE:CG2	2:B:2259:LEU:N	2.81	0.43
2:B:2312:GLU:OE2	2:B:2314:HIS:CE1	2.59	0.43
2:B:2259:LEU:HD11	2:B:2261:PHE:CE2	2.53	0.43
2:B:2259:LEU:CD1	2:B:2261:PHE:CE2	3.01	0.43
1:F:23:ILE:HD11	1:F:42:TYR:CZ	2.54	0.42
1:F:4:ILE:HA	5:F:301:HOH:O	2.19	0.42
2:B:2238:VAL:HG13	2:B:2313:VAL:HG13	2.01	0.42
1:C:180:GLN:O	1:C:181:ALA:CB	2.68	0.42
1:C:23:ILE:HG23	1:C:27:LYS:HD2	2.02	0.41
1:F:133:LYS:HE2	1:F:133:LYS:HB3	1.73	0.41
2:A:2230:LYS:HG3	2:A:2255:LEU:HD13	2.03	0.41
2:B:2258:ILE:HG22	2:B:2259:LEU:N	2.35	0.41
1:F:71:PRO:HA	1:F:74:TYR:CD2	2.55	0.41
2:A:2217:LYS:CD	2:A:2307:ASP:O	2.64	0.41
1:C:60:THR:HB	1:C:70:ARG:HG3	2.01	0.41
2:B:2266:ASP:OD2	5:B:2404:HOH:O	2.22	0.41
1:C:95:ILE:HB	1:C:96:PRO:CD	2.51	0.41
1:F:69:LEU:CD1	2:B:2303:MET:HE2	2.51	0.40
1:C:70:ARG:HB3	1:C:71:PRO:HD3	2.03	0.40
1:F:20:CYS:SG	1:F:31:PRO:HG2	2.61	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	C	177/185 (96%)	171 (97%)	6 (3%)	0	100	100
1	F	177/185 (96%)	171 (97%)	6 (3%)	0	100	100
2	A	135/151 (89%)	131 (97%)	4 (3%)	0	100	100
2	B	135/151 (89%)	131 (97%)	4 (3%)	0	100	100
All	All	624/672 (93%)	604 (97%)	20 (3%)	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	C	156/160 (98%)	155 (99%)	1 (1%)	86	90
1	F	156/160 (98%)	154 (99%)	2 (1%)	69	74
2	A	126/137 (92%)	124 (98%)	2 (2%)	62	67
2	B	127/137 (93%)	121 (95%)	6 (5%)	26	22
All	All	565/594 (95%)	554 (98%)	11 (2%)	57	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	41	ASN
1	F	68	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	2314	HIS
2	A	2329	GLN
2	B	2208	THR
2	B	2238	VAL
2	B	2248	LYS
2	B	2273	SER
2	B	2275	ASP
2	B	2314	HIS
1	C	150	ARG

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

Mol	Chain	Res	Type
2	A	2314	HIS
2	B	2314	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
4	GSP	F	202	3	26,34,34	1.38	3 (11%)	27,54,54	1.28	3 (11%)
4	GSP	C	202	3	26,34,34	1.51	4 (15%)	27,54,54	1.51	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GSP	F	202	3	-	1/17/38/38	0/3/3/3
4	GSP	C	202	3	-	1/17/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	202	GSP	C5-C6	-3.74	1.39	1.47
4	C	202	GSP	PG-S1G	-3.30	1.83	1.90
4	F	202	GSP	PG-S1G	-3.28	1.83	1.90
4	C	202	GSP	C5-C6	-2.57	1.42	1.47
4	C	202	GSP	PA-O1A	-2.50	1.42	1.50
4	F	202	GSP	C2-N3	2.50	1.39	1.33
4	C	202	GSP	C2-N3	2.38	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	GSP	C8-N7-C5	4.47	111.51	102.99
4	F	202	GSP	C8-N7-C5	3.32	109.31	102.99
4	C	202	GSP	N2-C2-N1	2.83	122.73	116.71
4	F	202	GSP	C2-N1-C6	-2.65	120.22	125.10
4	F	202	GSP	C5-C6-N1	2.62	118.58	113.95
4	C	202	GSP	C2-N1-C6	-2.46	120.57	125.10
4	C	202	GSP	C5-C6-N1	2.10	117.66	113.95

There are no chirality outliers.

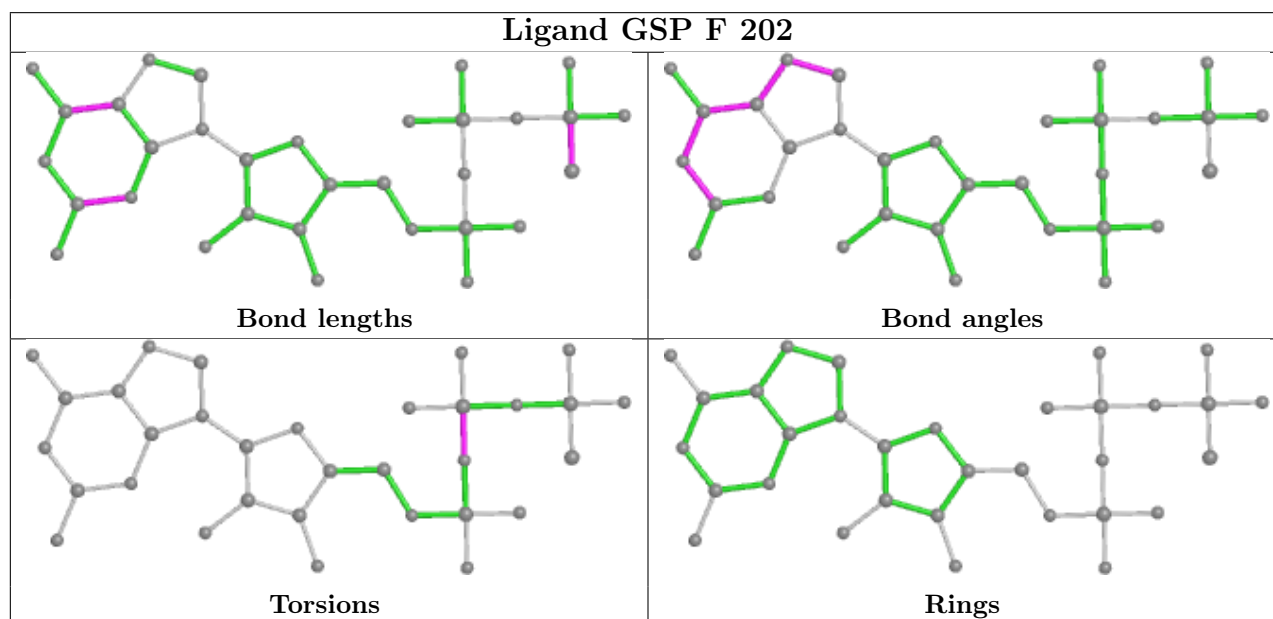
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	202	GSP	PA-O3A-PB-O2B
4	F	202	GSP	PA-O3A-PB-O2B

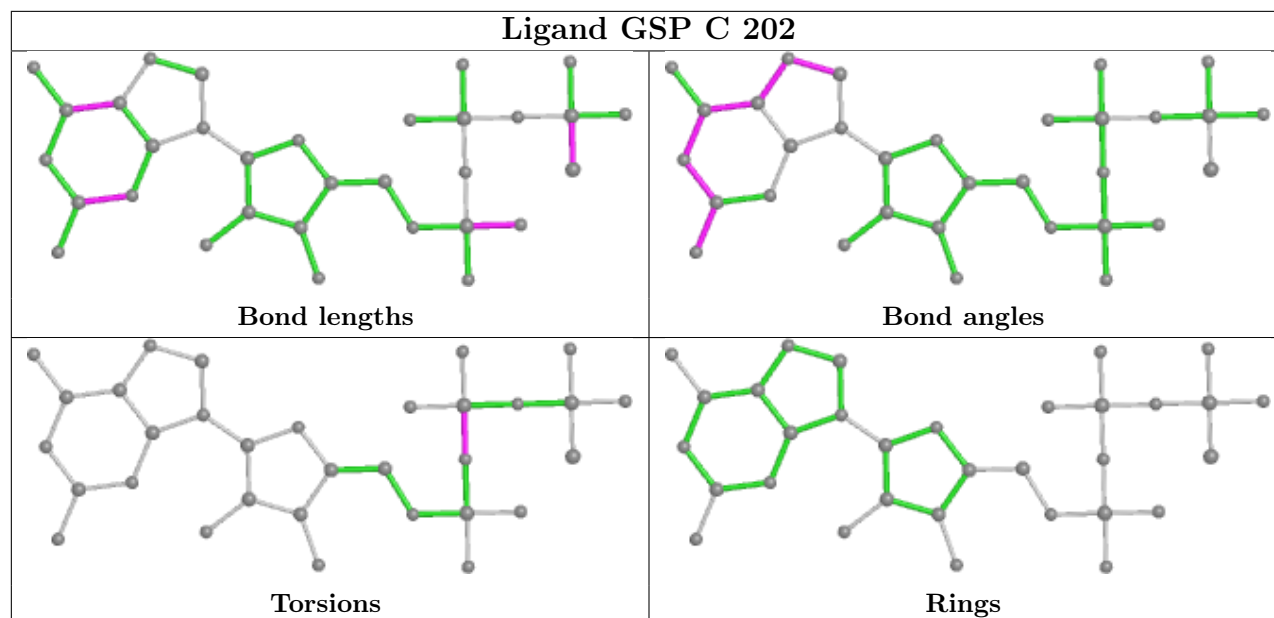
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	179/185 (96%)	0.47	9 (5%) 28 28	10, 15, 38, 47	0
1	F	179/185 (96%)	0.46	6 (3%) 45 44	10, 15, 35, 51	0
2	A	139/151 (92%)	0.24	5 (3%) 42 42	12, 21, 42, 51	0
2	B	139/151 (92%)	0.37	5 (3%) 42 42	12, 23, 46, 55	0
All	All	636/672 (94%)	0.39	25 (3%) 39 38	10, 18, 40, 55	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2195	TYR	5.7
1	F	181	ALA	4.8
2	B	2267	GLN	4.0
1	C	181	ALA	3.6
2	B	2266	ASP	3.0
1	C	49	ASP	2.8
2	A	2266	ASP	2.8
1	C	129	ARG	2.8
2	B	2335	HIS	2.5
1	F	48	VAL	2.5
1	C	3	ALA	2.5
1	C	175	THR	2.5
2	A	2228	LYS	2.5
2	A	2267	GLN	2.5
2	A	2246	ARG	2.4
1	C	52	GLN	2.4
1	F	52	GLN	2.3
1	F	34	TYR	2.2
1	C	132	ALA	2.2
2	A	2247	LEU	2.2
1	F	114	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	155	GLY	2.2
2	B	2201	LEU	2.1
1	C	34	TYR	2.1
1	F	20	CYS	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](#)

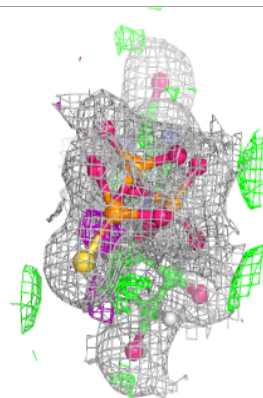
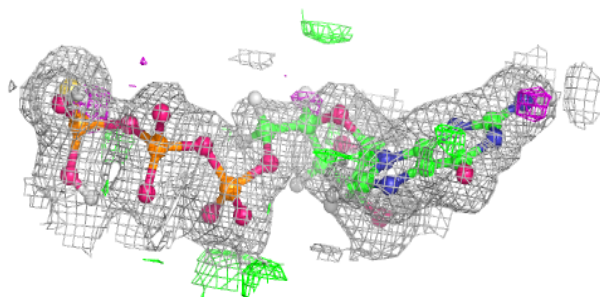
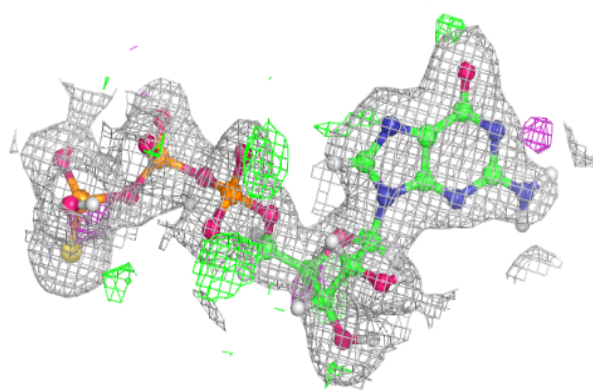
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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	MG	F	201	1/1	0.97	0.11	10,10,10,10	0
4	GSP	F	202	32/32	0.97	0.14	9,11,14,16	0
4	GSP	C	202	32/32	0.97	0.14	10,12,15,18	0
3	MG	C	201	1/1	0.99	0.15	10,10,10,10	0

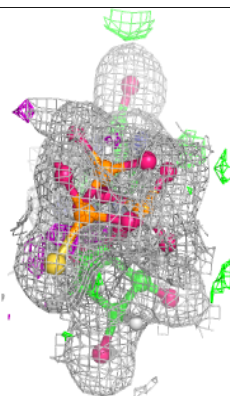
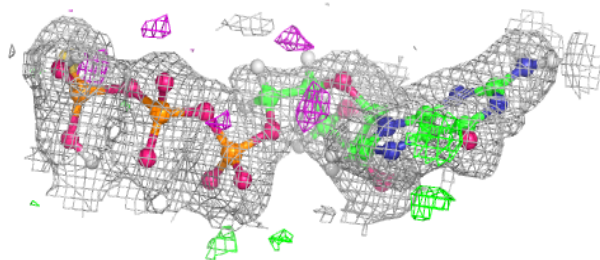
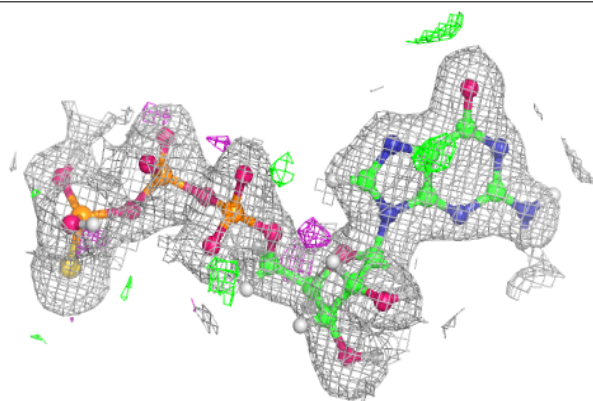
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GSP F 202:**

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

**Electron density around GSP C 202:**

$2mF_o-DF_c$  (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.