



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:01 PM UTC

PDB ID : 6BC1 / pdb_00006bc1
Title : A Complex between PH Domain of p190RhoGEF and Activated Rac1 Bound to a GTP Analog
Authors : Chen, Z.; Sternweis, P.C.
Deposited on : 2017-10-20
Resolution : 2.90 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

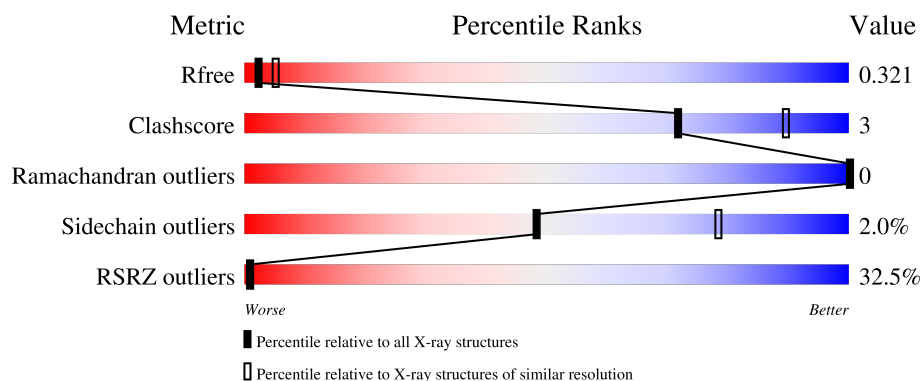
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	183	
1	B	183	
2	C	150	
2	D	150	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10469 atoms, of which 5204 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	177	Total	C	H	N	O	S	0	0	0
			2783	889	1401	228	258	7			
1	B	177	Total	C	H	N	O	S	0	0	0
			2783	889	1401	228	258	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P63000
A	178	HIS	-	expression tag	UNP P63000
A	179	HIS	-	expression tag	UNP P63000
A	180	HIS	-	expression tag	UNP P63000
A	181	HIS	-	expression tag	UNP P63000
A	182	HIS	-	expression tag	UNP P63000
A	183	HIS	-	expression tag	UNP P63000
B	1	PRO	-	expression tag	UNP P63000
B	178	HIS	-	expression tag	UNP P63000
B	179	HIS	-	expression tag	UNP P63000
B	180	HIS	-	expression tag	UNP P63000
B	181	HIS	-	expression tag	UNP P63000
B	182	HIS	-	expression tag	UNP P63000
B	183	HIS	-	expression tag	UNP P63000

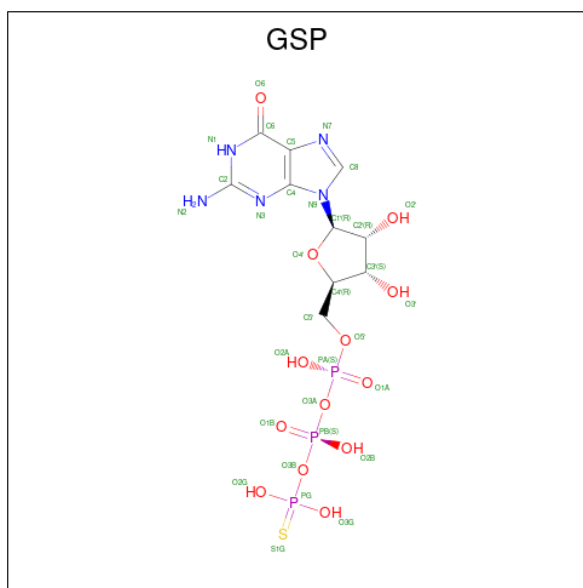
- Molecule 2 is a protein called Rho guanine nucleotide exchange factor 28.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	141	Total	C	H	N	O	S	0	0	0
			2349	742	1188	202	212	5			
2	D	141	Total	C	H	N	O	S	0	0	0
			2349	742	1188	202	212	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1045	GLY	-	expression tag	UNP Q8N1W1
C	1046	ILE	-	expression tag	UNP Q8N1W1
C	1047	LEU	-	expression tag	UNP Q8N1W1
C	1048	ASP	-	expression tag	UNP Q8N1W1
D	1045	GLY	-	expression tag	UNP Q8N1W1
D	1046	ILE	-	expression tag	UNP Q8N1W1
D	1047	LEU	-	expression tag	UNP Q8N1W1
D	1048	ASP	-	expression tag	UNP Q8N1W1

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

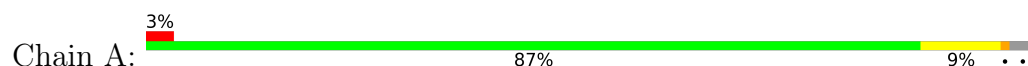


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total 34	O 34	0	0
5	C	41	Total 41	O 41	0	0
5	B	22	Total 22	O 22	0	0
5	D	16	Total 16	O 16	0	0

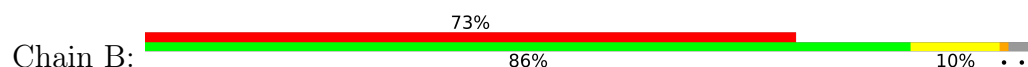
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

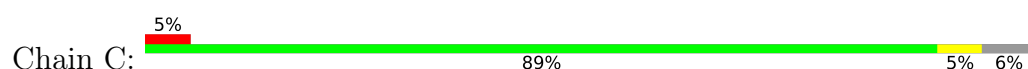
- Molecule 1: Ras-related C3 botulinum toxin substrate 1



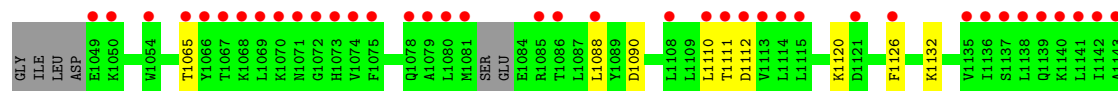
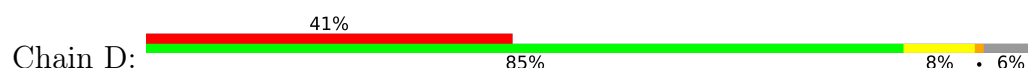
- Molecule 1: Ras-related C3 botulinum toxin substrate 1

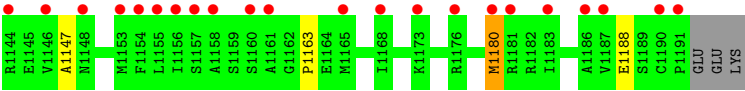


- Molecule 2: Rho guanine nucleotide exchange factor 28



- Molecule 2: Rho guanine nucleotide exchange factor 28





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.33Å 96.33Å 189.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.90 48.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.17-2.90) 99.9 (48.17-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.278 , 0.323 0.275 , 0.321	Depositor DCC
R_{free} test set	959 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10469	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.89% 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: MG, GSP

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	0.15	0/1413	0.32	0/1923
1	B	0.20	0/1413	0.31	0/1923
2	C	0.12	0/1180	0.31	0/1585
2	D	0.12	0/1180	0.31	0/1585
All	All	0.15	0/5186	0.31	0/7016

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1110	LEU	Peptide
2	D	1110	LEU	Peptide

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	1382	1401	1401	13	0
1	B	1382	1401	1402	12	1
2	C	1161	1188	1188	3	0
2	D	1161	1188	1188	8	1
3	A	32	13	12	0	0
3	B	32	13	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	34	0	0	4	0
5	B	22	0	0	0	0
5	C	41	0	0	1	0
5	D	16	0	0	3	0
All	All	5265	5204	5203	34	1

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 3.

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)
2:D:1180:MET:SD	5:D:1212:HOH:O	2.42	0.77
2:C:1049:GLU:N	5:C:1201:HOH:O	2.23	0.71
1:A:177:LEU:O	5:A:301:HOH:O	2.08	0.71
1:A:92:ASN:OD1	5:A:302:HOH:O	2.10	0.69
2:D:1090:ASP:OD1	5:D:1201:HOH:O	2.16	0.62
2:D:1120:LYS:O	5:D:1202:HOH:O	2.16	0.62
1:A:127:GLU:N	5:A:305:HOH:O	2.35	0.59
1:B:33:ILE:O	1:B:33:ILE:HG22	2.04	0.57
2:C:1112:ASP:OD1	2:C:1112:ASP:N	2.38	0.56
2:C:1065:THR:HG21	2:C:1126:PHE:H	1.72	0.54
1:B:17:THR:OG1	3:B:201:GSP:O1B	2.25	0.54
1:B:105:CYS:O	1:B:108:THR:OG1	2.26	0.53
1:A:105:CYS:O	1:A:108:THR:OG1	2.26	0.53
1:A:33:ILE:HG22	1:A:33:ILE:O	2.10	0.52
1:A:139:TYR:HB3	1:A:140:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:OE1	1:A:94:ARG:NH1	2.48	0.47
1:A:72:TYR:N	1:A:73:PRO:CD	2.78	0.47
1:B:41:SER:HB3	2:D:1147:ALA:HB1	1.96	0.47
1:B:67:LEU:HB2	2:D:1163:PRO:HG2	1.97	0.46
1:A:11:ASP:O	1:A:16:LYS:NZ	2.49	0.46
1:A:11:ASP:OD2	1:A:92:ASN:ND2	2.41	0.46
2:D:1088:LEU:HD11	2:D:1111:THR:HG23	2.00	0.44
2:D:1111:THR:HA	2:D:1112:ASP:HA	1.85	0.43
2:D:1065:THR:HG21	2:D:1126:PHE:H	1.82	0.43
1:B:139:TYR:HB3	1:B:140:PRO:HD3	2.00	0.43
1:B:139:TYR:C	1:B:139:TYR:CD1	2.97	0.42
1:B:155:LEU:HD13	1:B:168:VAL:HA	2.01	0.42
1:B:91:GLU:OE1	1:B:94:ARG:NH1	2.53	0.42
1:A:139:TYR:C	1:A:139:TYR:CD1	2.98	0.41
1:A:139:TYR:C	1:A:139:TYR:HD1	2.29	0.41
1:B:105:CYS:HB3	1:B:108:THR:HG21	2.03	0.41
1:B:72:TYR:N	1:B:73:PRO:CD	2.84	0.41
1:A:128:LYS:N	5:A:305:HOH:O	2.31	0.41
1:B:120:ARG:NH1	1:B:156:GLU:OE2	2.43	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TYR:HH	2:D:1188:GLU:OE1[1_455]	1.53	0.07

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	175/183 (96%)	169 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	175/183 (96%)	167 (95%)	8 (5%)	0	100	100
2	C	137/150 (91%)	128 (93%)	9 (7%)	0	100	100
2	D	137/150 (91%)	129 (94%)	8 (6%)	0	100	100
All	All	624/666 (94%)	593 (95%)	31 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	153/159 (96%)	150 (98%)	3 (2%)	48	78
1	B	153/159 (96%)	150 (98%)	3 (2%)	48	78
2	C	126/134 (94%)	123 (98%)	3 (2%)	43	75
2	D	126/134 (94%)	124 (98%)	2 (2%)	55	83
All	All	558/586 (95%)	547 (98%)	11 (2%)	48	78

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

Mol	Chain	Res	Type
1	A	71	SER
1	A	111	ILE
1	A	139	TYR
2	C	1058	LEU
2	C	1132	LYS
2	C	1160	SER
1	B	6	CYS
1	B	77	VAL
1	B	139	TYR
2	D	1132	LYS
2	D	1180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	61	GLN
1	B	61	GLN
1	B	74	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GSP	A	201	4	33,34,34	1.91	4 (12%)	47,54,54	1.71	10 (21%)
3	GSP	B	201	4	33,34,34	1.89	3 (9%)	47,54,54	1.72	10 (21%)

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	GSP	A	201	4	-	2/21/38/38	0/3/3/3
3	GSP	B	201	4	-	0/21/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GSP	PG-S1G	-9.29	1.70	1.90
3	B	201	GSP	PG-S1G	-9.24	1.70	1.90
3	A	201	GSP	C2-N3	2.24	1.38	1.33
3	B	201	GSP	C2-N3	2.22	1.38	1.33
3	A	201	GSP	PA-O3A	2.18	1.61	1.59
3	B	201	GSP	PB-O3B	2.12	1.61	1.59
3	A	201	GSP	PB-O3B	2.07	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	GSP	C5-C4-N3	-5.16	120.17	128.39
3	A	201	GSP	C5-C4-N3	-5.10	120.28	128.39
3	B	201	GSP	C2-N3-C4	4.77	120.52	112.30
3	A	201	GSP	C2-N3-C4	4.72	120.43	112.30
3	B	201	GSP	PB-O3B-PG	-3.34	120.94	133.17
3	A	201	GSP	PB-O3B-PG	-3.17	121.56	133.17
3	A	201	GSP	N9-C4-N3	3.08	132.12	125.95
3	B	201	GSP	N9-C4-N3	3.08	132.10	125.95
3	B	201	GSP	C2-N1-C6	-2.88	119.88	125.11
3	A	201	GSP	C2-N1-C6	-2.88	119.89	125.11
3	B	201	GSP	C8-N7-C5	2.62	108.92	104.26
3	A	201	GSP	C8-N7-C5	2.58	108.86	104.26
3	B	201	GSP	N9-C8-N7	-2.55	108.66	113.40
3	A	201	GSP	N9-C8-N7	-2.55	108.67	113.40
3	A	201	GSP	C5-C6-N1	2.47	119.54	113.25
3	B	201	GSP	C5-C6-N1	2.43	119.45	113.25
3	B	201	GSP	C3'-C2'-C1'	2.29	105.80	101.46
3	A	201	GSP	O6-C6-C5	-2.28	120.52	126.53
3	B	201	GSP	O6-C6-C5	-2.20	120.73	126.53
3	A	201	GSP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

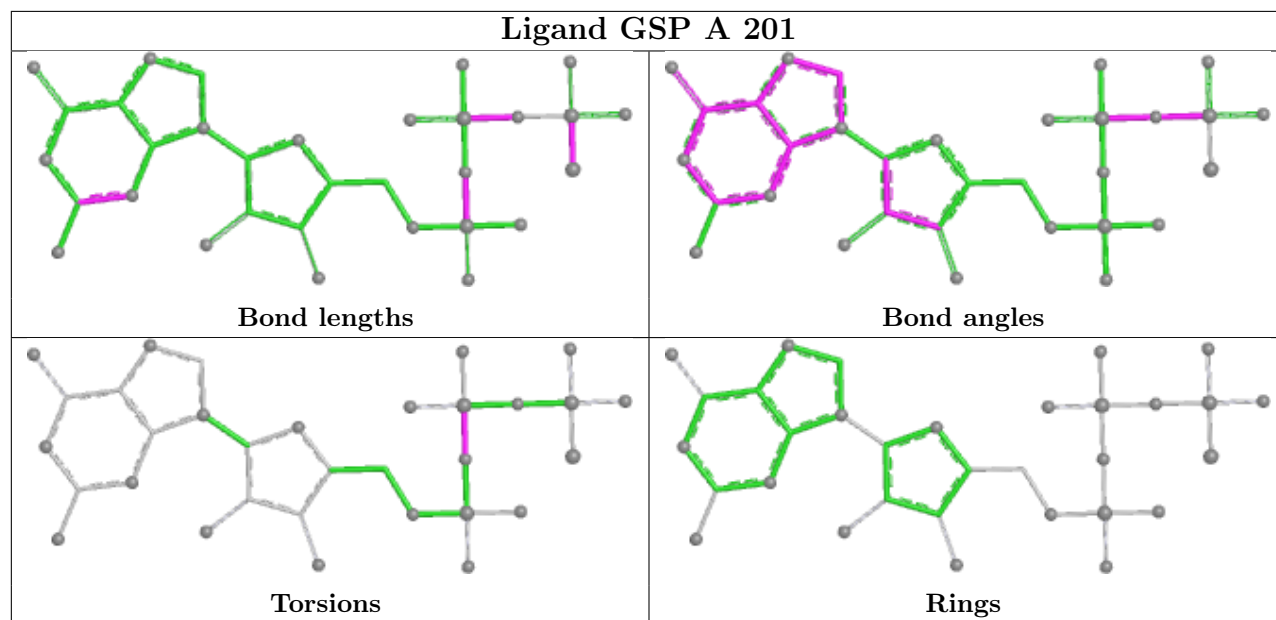
Mol	Chain	Res	Type	Atoms
3	A	201	GSP	PA-O3A-PB-O1B
3	A	201	GSP	PA-O3A-PB-O2B

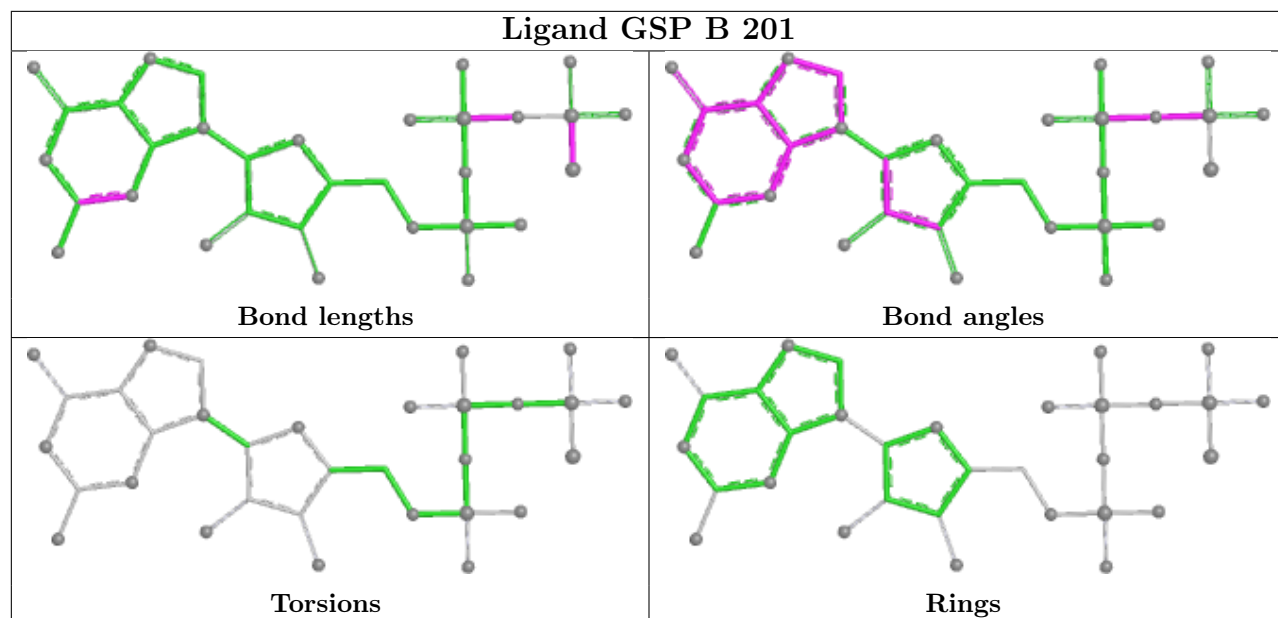
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	GSP	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	177/183 (96%)	0.34	5 (2%) 55 46	14, 37, 81, 100	0
1	B	177/183 (96%)	2.90	134 (75%) 0 0	51, 84, 128, 178	0
2	C	141/150 (94%)	0.23	7 (4%) 34 27	14, 32, 63, 91	0
2	D	141/150 (94%)	1.90	61 (43%) 0 0	24, 73, 117, 136	0
All	All	636/666 (95%)	1.37	207 (32%) 1 1	14, 55, 115, 178	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	PHE	7.6
1	B	111	ILE	7.6
1	B	7	VAL	6.2
1	B	169	PHE	5.9
1	B	9	VAL	5.5
1	B	164	GLY	5.4
1	B	154	TYR	5.3
1	B	51	VAL	5.2
1	B	110	ILE	5.0
1	B	81	CYS	4.9
2	D	1144	ARG	4.9
1	B	113	VAL	4.8
1	B	42	ALA	4.8
2	D	1142	ILE	4.7
1	B	165	LEU	4.7
2	D	1075	PHE	4.7
1	B	172	ALA	4.7
2	D	1154	PHE	4.6
2	D	1111	THR	4.6
2	D	1187	VAL	4.6
1	B	167	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	1080	LEU	4.5
1	B	80	ILE	4.5
1	B	84	LEU	4.5
2	D	1138	LEU	4.4
1	B	136	PRO	4.4
1	B	55	LEU	4.3
2	D	1136	ILE	4.3
2	D	1191	PRO	4.3
2	D	1114	LEU	4.3
2	D	1081	MET	4.3
2	D	1069	LEU	4.3
2	D	1073	HIS	4.2
1	B	43	ASN	4.2
1	B	115	THR	4.2
1	B	175	ALA	4.2
1	B	146	ALA	4.2
2	D	1112	ASP	4.2
2	D	1158	ALA	4.1
1	B	171	GLU	4.1
1	B	135	THR	4.1
1	B	53	LEU	4.0
1	B	82	PHE	4.0
1	B	112	LEU	4.0
1	B	44	VAL	3.9
1	B	131	GLU	3.9
2	D	1141	LEU	3.9
1	B	37	PHE	3.9
2	D	1066	TYR	3.9
1	B	121	ASP	3.9
1	B	134	LEU	3.9
2	D	1153	MET	3.9
2	D	1148	ASN	3.8
1	B	12	GLY	3.8
2	D	1155	LEU	3.8
1	B	46	VAL	3.8
2	D	1054	TRP	3.8
1	B	39	ASN	3.8
1	B	173	ILE	3.7
1	B	161	THR	3.7
1	B	77	VAL	3.7
1	B	93	VAL	3.7
2	D	1074	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	159	ALA	3.6
1	B	65	ASP	3.6
1	B	29	PRO	3.6
1	B	85	VAL	3.6
2	D	1135	VAL	3.5
2	D	1140	LYS	3.5
1	B	155	LEU	3.5
1	B	87	PRO	3.5
1	B	26	ASN	3.5
1	B	91	GLU	3.5
1	B	97	TRP	3.5
1	B	35	THR	3.5
2	D	1078	GLN	3.4
2	D	1180	MET	3.4
1	B	40	TYR	3.4
1	B	48	GLY	3.4
1	B	83	SER	3.3
1	B	79	LEU	3.3
1	B	89	SER	3.3
2	D	1113	VAL	3.3
1	B	90	PHE	3.3
1	B	157	CYS	3.3
2	D	1156	ILE	3.2
1	B	176	VAL	3.2
1	B	30	GLY	3.2
2	D	1072	GLY	3.2
1	B	56	TRP	3.2
1	B	45	MET	3.2
1	B	177	LEU	3.1
2	D	1157	SER	3.1
1	B	33	ILE	3.1
1	B	139	TYR	3.1
1	B	126	ILE	3.1
2	D	1190	CYS	3.1
1	B	2	GLN	3.1
1	B	60	GLY	3.1
1	B	127	GLU	3.1
1	B	163	ARG	3.1
1	B	132	LYS	3.1
1	A	114	GLY	3.0
1	B	96	LYS	3.0
1	B	156	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	13	ALA	3.0
2	D	1079	ALA	3.0
1	B	32	TYR	3.0
1	B	124	ASP	3.0
1	B	20	LEU	3.0
2	D	1108	LEU	3.0
1	B	61	GLN	3.0
1	B	27	ALA	2.9
1	B	10	GLY	2.9
1	B	28	PHE	2.9
1	B	36	VAL	2.9
2	D	1067	THR	2.9
1	B	88	ALA	2.9
1	B	125	THR	2.9
2	C	1064	LYS	2.9
1	B	170	ASP	2.9
2	D	1126	PHE	2.9
1	B	149	ILE	2.9
1	B	1	PRO	2.8
1	B	137	ILE	2.8
1	B	153	LYS	2.8
1	B	100	GLU	2.8
2	D	1143	ALA	2.8
2	D	1121	ASP	2.8
2	D	1086	THR	2.8
1	B	15	GLY	2.8
1	B	23	TYR	2.8
1	B	114	GLY	2.8
1	B	3	ALA	2.8
1	B	98	TYR	2.8
2	C	1111	THR	2.8
1	B	86	SER	2.8
1	B	158	SER	2.8
1	B	69	PRO	2.7
1	B	174	ARG	2.7
1	B	67	LEU	2.7
1	B	147	LYS	2.7
2	D	1085	ARG	2.7
2	D	1168	ILE	2.6
1	B	6	CYS	2.6
1	B	72	TYR	2.6
1	B	18	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	31	GLU	2.6
2	D	1183	ILE	2.6
2	C	1181	ARG	2.6
2	D	1065	THR	2.6
1	B	142	GLY	2.5
2	D	1110	LEU	2.5
1	B	168	VAL	2.5
2	D	1137	SER	2.5
1	B	21	ILE	2.5
1	B	120	ARG	2.5
1	B	41	SER	2.4
2	D	1050	LYS	2.4
1	B	14	VAL	2.4
1	B	95	ALA	2.4
2	D	1161	ALA	2.4
2	C	1191	PRO	2.4
1	B	38	ASP	2.4
2	D	1139	GLN	2.4
1	A	85	VAL	2.3
1	B	57	ASP	2.3
1	B	71	SER	2.3
1	B	49	LYS	2.3
2	C	1158	ALA	2.3
2	D	1068	LYS	2.3
1	B	117	LEU	2.3
2	D	1088	LEU	2.3
1	B	104	HIS	2.3
2	D	1173	LYS	2.3
1	B	34	PRO	2.3
1	B	119	LEU	2.3
1	B	143	LEU	2.3
1	B	5	LYS	2.3
2	D	1146	VAL	2.3
1	B	59	ALA	2.2
1	B	70	LEU	2.2
1	B	133	LYS	2.2
1	B	145	MET	2.2
2	D	1186	ALA	2.2
1	A	134	LEU	2.2
1	B	17	THR	2.2
2	D	1160	SER	2.2
2	D	1071	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	PRO	2.2
2	D	1070	LYS	2.2
1	B	19	LEU	2.2
1	B	166	LYS	2.2
2	C	1065	THR	2.1
2	C	1049	GLU	2.1
1	B	50	PRO	2.1
1	B	138	THR	2.1
2	D	1049	GLU	2.1
1	B	106	PRO	2.1
1	A	131	GLU	2.1
1	B	122	ASP	2.1
2	D	1176	ARG	2.1
2	D	1165	MET	2.0
2	D	1181	ARG	2.0
1	B	62	GLU	2.0
2	D	1115	LEU	2.0
1	B	64	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](#)

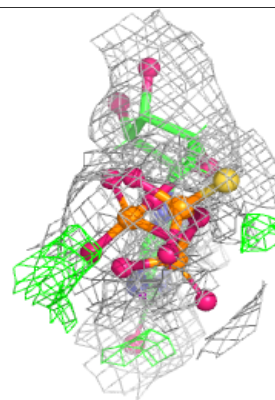
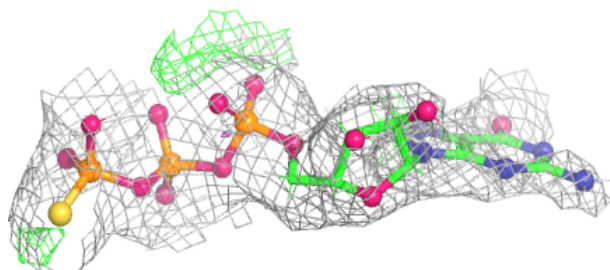
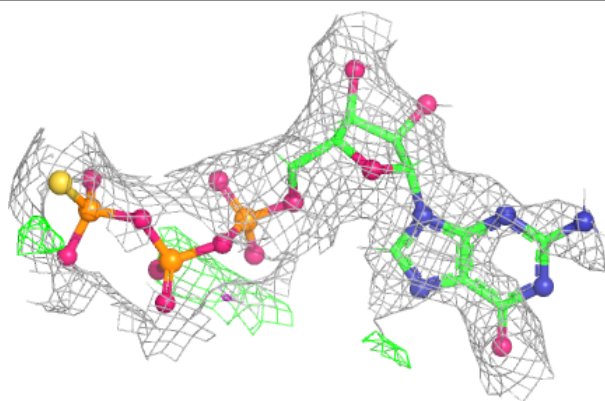
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

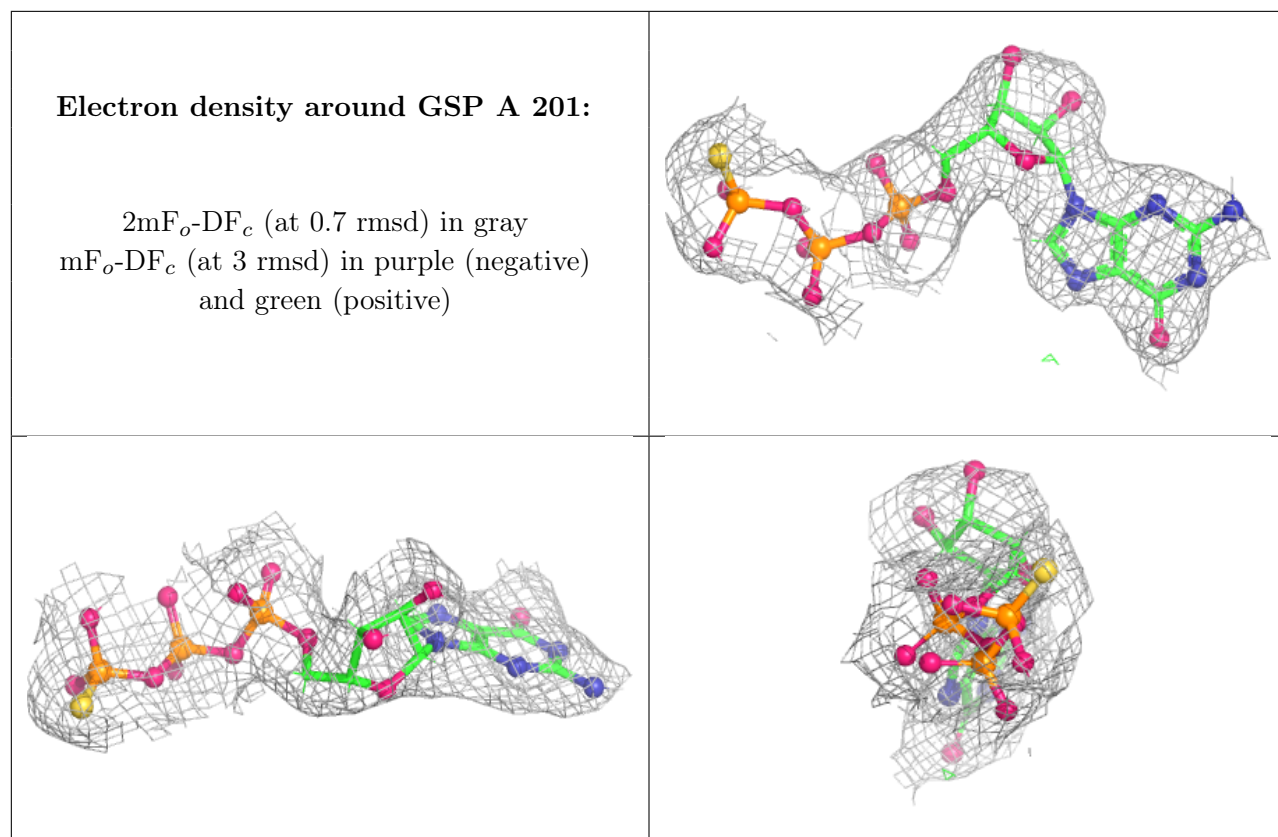
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GSP	B	201	32/32	0.83	0.15	53,97,119,144	0
4	MG	B	202	1/1	0.88	0.09	71,71,71,71	0
3	GSP	A	201	32/32	0.96	0.08	25,42,58,77	0
4	MG	A	202	1/1	0.98	0.04	39,39,39,39	0

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 B 201:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.