Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 01:03 am GMT

PDB ID	:	7AJK
Title	:	Crystal structure of CRYI-B Rac1 complex
Authors	:	Yelland, T.; Anh, L.; Insall, R.; Machesky, L.; Ismail, S.
Deposited on	:	2020-09-29
Resolution	:	3.10 Å(reported)

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

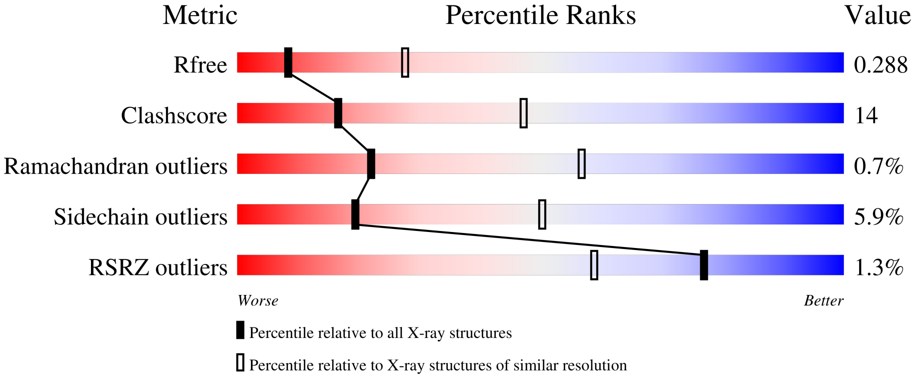
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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

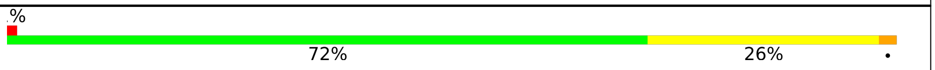
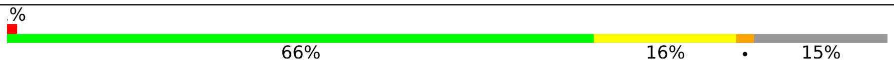
The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 chain
1	BBB	180	
2	CCC	325	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3612 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 Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BBB	180	1381	888	225	261	7	1	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-2	GLY	-	expression tag	UNP P63000
BBB	-1	SER	-	expression tag	UNP P63000
BBB	0	ALA	-	expression tag	UNP P63000
BBB	1	GLY	-	expression tag	UNP P63000
BBB	61	LEU	GLN	conflict	UNP P63000

- Molecule 2 is a protein called CYFIP-related Rac1 interactor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	CCC	276	2186	1381	383	409	13	0	0	0

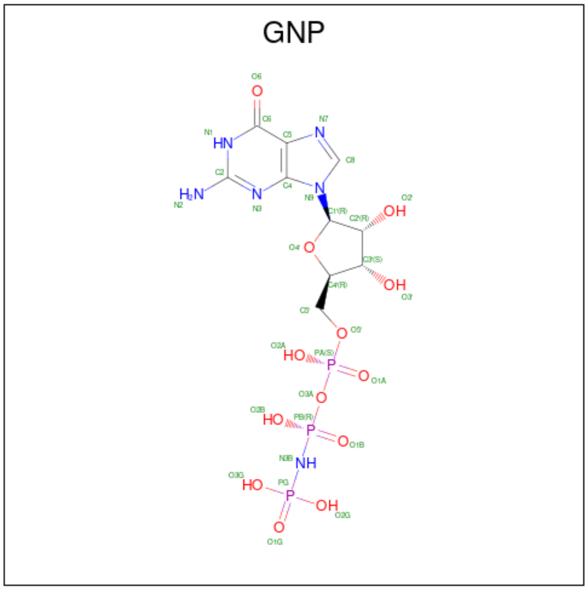
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	300	GLY	-	expression tag	UNP Q9NUQ9

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	BBB	1	1	1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	BBB	1	32	10	6	13	3	0	0

- Molecule 5 is water.

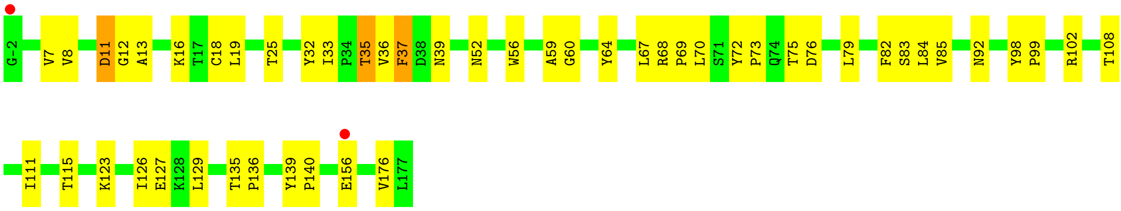
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	BBB	7	7	7	0	0
5	CCC	5	5	5	0	0

3 Residue-property plots ⓘ

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

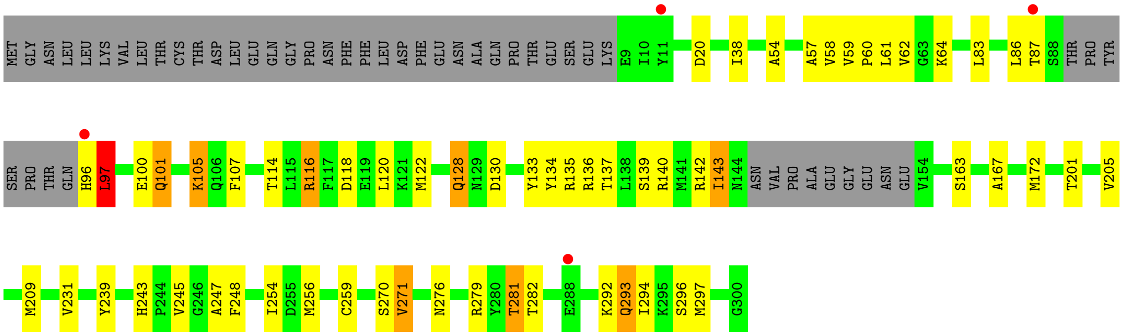
- Molecule 1: Ras-related C3 botulinum toxin substrate 1

Chain BBB:



- Molecule 2: CYFIP-related Rac1 interactor B

Chain CCC:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	81.87Å 81.87Å 355.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.38 – 3.10 59.31 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (59.38-3.10) 97.9 (59.31-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.249 , 0.282 0.251 , 0.288	Depositor DCC
R_{free} test set	672 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	88.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3612	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GNP

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	BBB	0.63	0/1411	0.65	0/1923
2	CCC	0.63	0/2221	0.67	0/2995
All	All	0.63	0/3632	0.66	0/4918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	BBB	1381	0	1384	50	0
2	CCC	2186	0	2203	58	0
3	BBB	1	0	0	0	0
4	BBB	32	0	13	8	0
5	BBB	7	0	0	2	0
5	CCC	5	0	0	0	0
All	All	3612	0	3600	102	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 14.

All (102) 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:CCC:270:SER:O	2:CCC:271:VAL:HG22	1.34	1.25
1:BBB:39:ASN:HD22	2:CCC:167:ALA:HB2	1.14	1.08
1:BBB:39:ASN:ND2	2:CCC:167:ALA:HB2	1.78	0.96
2:CCC:61:LEU:HD23	2:CCC:130:ASP:OD2	1.75	0.86
2:CCC:142:ARG:HB3	2:CCC:142:ARG:NH1	1.96	0.81
2:CCC:270:SER:O	2:CCC:271:VAL:CG2	2.25	0.79
1:BBB:36:VAL:HA	1:BBB:59:ALA:HB2	1.64	0.77
2:CCC:293:GLN:HE21	2:CCC:293:GLN:HA	1.50	0.76
2:CCC:293:GLN:HE21	2:CCC:293:GLN:CA	1.99	0.75
2:CCC:59:VAL:HB	2:CCC:60:PRO:HD3	1.69	0.74
1:BBB:32:TYR:CD1	4:BBB:202:GNP:H5'2	2.24	0.73
1:BBB:39:ASN:HD22	2:CCC:167:ALA:CB	1.99	0.72
2:CCC:97:LEU:O	2:CCC:97:LEU:HD23	1.91	0.70
1:BBB:36:VAL:HG13	1:BBB:64:TYR:CD1	2.29	0.68
1:BBB:72:TYR:N	1:BBB:73:PRO:HD2	2.09	0.67
1:BBB:52:ASN:HB2	5:BBB:305:HOH:O	1.94	0.67
1:BBB:129:LEU:HD12	1:BBB:136:PRO:HG3	1.75	0.67
1:BBB:85:VAL:HG12	1:BBB:85:VAL:O	1.95	0.66
1:BBB:19:LEU:C	1:BBB:19:LEU:HD12	2.15	0.66
2:CCC:139:SER:O	2:CCC:142:ARG:HB2	1.96	0.66
1:BBB:67:LEU:HD12	1:BBB:70:LEU:HD23	1.79	0.65
2:CCC:116:ARG:CG	2:CCC:116:ARG:HH11	2.10	0.64
1:BBB:35:THR:HG21	5:BBB:303:HOH:O	1.98	0.63
1:BBB:70:LEU:HD12	1:BBB:70:LEU:C	2.21	0.61
1:BBB:139:TYR:HB3	1:BBB:140:PRO:HD3	1.83	0.61
1:BBB:39:ASN:ND2	2:CCC:167:ALA:CB	2.61	0.60
1:BBB:68:ARG:N	1:BBB:69:PRO:HD2	2.16	0.60
2:CCC:54:ALA:O	2:CCC:58:VAL:HG23	2.02	0.59
2:CCC:143:ILE:O	2:CCC:143:ILE:HG22	2.03	0.59
1:BBB:76:ASP:HB3	1:BBB:176:VAL:HG11	1.83	0.59
2:CCC:248:PHE:HZ	2:CCC:282:THR:HG21	1.65	0.59
1:BBB:37:PHE:CD1	1:BBB:37:PHE:O	2.56	0.59
2:CCC:59:VAL:O	2:CCC:62:VAL:HG22	2.02	0.59
2:CCC:116:ARG:HH11	2:CCC:116:ARG:HG2	1.69	0.57
2:CCC:142:ARG:HB3	2:CCC:142:ARG:HH11	1.70	0.57
2:CCC:62:VAL:HG11	2:CCC:134:TYR:CD1	2.40	0.56
2:CCC:281:THR:HG23	2:CCC:281:THR:O	2.05	0.55
1:BBB:32:TYR:HD1	4:BBB:202:GNP:H5'2	1.69	0.55
1:BBB:102:ARG:NH2	1:BBB:108:THR:O	2.40	0.54
2:CCC:116:ARG:NH2	2:CCC:120:LEU:HD21	2.23	0.54
2:CCC:133:TYR:O	2:CCC:137:THR:HG23	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:CCC:142:ARG:HB3	2:CCC:142:ARG:CZ	2.38	0.54
1:BBB:37:PHE:CD1	1:BBB:37:PHE:C	2.82	0.53
2:CCC:100:GLU:O	2:CCC:100:GLU:HG2	2.09	0.53
1:BBB:36:VAL:CA	1:BBB:59:ALA:HB2	2.38	0.52
2:CCC:293:GLN:HA	2:CCC:293:GLN:NE2	2.18	0.52
1:BBB:12:GLY:HA2	4:BBB:202:GNP:HNB3	1.74	0.52
2:CCC:38:ILE:HG23	2:CCC:133:TYR:CD1	2.44	0.52
1:BBB:82:PHE:C	1:BBB:82:PHE:CD1	2.82	0.52
2:CCC:256:MET:O	2:CCC:259:CYS:N	2.44	0.51
1:BBB:8:VAL:HG22	1:BBB:79:LEU:HB2	1.93	0.51
1:BBB:11:ASP:OD2	1:BBB:92:ASN:ND2	2.43	0.51
1:BBB:33:ILE:HD13	2:CCC:140:ARG:HB2	1.93	0.51
1:BBB:82:PHE:HE1	1:BBB:84:LEU:HD23	1.76	0.50
1:BBB:98:TYR:HB3	1:BBB:99:PRO:HD3	1.94	0.50
1:BBB:36:VAL:HG13	1:BBB:64:TYR:CE1	2.46	0.50
2:CCC:116:ARG:CG	2:CCC:116:ARG:NH1	2.73	0.49
1:BBB:13:ALA:H	4:BBB:202:GNP:HNB3	1.59	0.49
2:CCC:118:ASP:O	2:CCC:122:MET:HB2	2.12	0.49
2:CCC:97:LEU:O	2:CCC:97:LEU:CD2	2.60	0.49
1:BBB:123:LYS:HA	1:BBB:126:ILE:HG22	1.95	0.49
2:CCC:97:LEU:O	2:CCC:97:LEU:CG	2.60	0.49
2:CCC:243:HIS:CD2	2:CCC:245:VAL:HG22	2.47	0.49
2:CCC:140:ARG:O	2:CCC:143:ILE:HB	2.15	0.47
2:CCC:83:LEU:O	2:CCC:86:LEU:HB2	2.14	0.47
2:CCC:247:ALA:CB	2:CCC:254:ILE:HG13	2.44	0.47
1:BBB:67:LEU:HD12	1:BBB:70:LEU:CD2	2.43	0.47
2:CCC:116:ARG:HA	2:CCC:116:ARG:HD2	1.64	0.46
1:BBB:72:TYR:N	1:BBB:73:PRO:CD	2.77	0.46
1:BBB:39:ASN:ND2	2:CCC:163:SER:O	2.46	0.46
1:BBB:68:ARG:N	1:BBB:69:PRO:CD	2.78	0.46
2:CCC:292:LYS:HA	2:CCC:292:LYS:HD3	1.78	0.46
2:CCC:114:THR:HG23	2:CCC:172:MET:HB3	1.98	0.45
2:CCC:239:TYR:CD1	2:CCC:254:ILE:HD11	2.52	0.45
2:CCC:248:PHE:CZ	2:CCC:282:THR:HG21	2.49	0.45
1:BBB:60:GLY:N	4:BBB:202:GNP:O1G	2.50	0.44
2:CCC:209:MET:CE	2:CCC:231:VAL:HG11	2.46	0.44
2:CCC:279:ARG:HG2	2:CCC:297:MET:HE3	1.99	0.44
1:BBB:16:LYS:HB2	4:BBB:202:GNP:O2B	2.17	0.44
2:CCC:86:LEU:HD12	2:CCC:86:LEU:HA	1.86	0.44
1:BBB:7:VAL:HG22	1:BBB:56:TRP:HB2	1.99	0.43
1:BBB:37:PHE:C	1:BBB:37:PHE:HD1	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:85:VAL:O	1:BBB:85:VAL:CG1	2.65	0.43
1:BBB:82:PHE:CD1	1:BBB:82:PHE:O	2.72	0.43
2:CCC:281:THR:O	2:CCC:281:THR:CG2	2.67	0.43
1:BBB:98:TYR:CE1	1:BBB:102:ARG:HG3	2.54	0.43
2:CCC:57:ALA:O	2:CCC:60:PRO:HD2	2.20	0.42
1:BBB:83:SER:HA	1:BBB:115:THR:OG1	2.19	0.42
1:BBB:19:LEU:C	1:BBB:19:LEU:CD1	2.88	0.42
2:CCC:276:ASN:O	2:CCC:279:ARG:HB2	2.20	0.42
1:BBB:12:GLY:HA2	4:BBB:202:GNP:N3B	2.35	0.42
2:CCC:128:GLN:HE21	2:CCC:128:GLN:HB3	1.56	0.42
2:CCC:133:TYR:CZ	2:CCC:137:THR:HG21	2.54	0.42
2:CCC:60:PRO:O	2:CCC:64:LYS:HG3	2.19	0.42
2:CCC:101:GLN:O	2:CCC:105:LYS:HB2	2.20	0.42
1:BBB:18:CYS:SG	4:BBB:202:GNP:H2'	2.61	0.41
1:BBB:35:THR:O	1:BBB:59:ALA:HA	2.20	0.41
2:CCC:201:THR:O	2:CCC:205:VAL:HG23	2.20	0.41
2:CCC:101:GLN:HE21	2:CCC:101:GLN:HB2	1.71	0.41
2:CCC:100:GLU:O	2:CCC:100:GLU:CG	2.68	0.41
1:BBB:79:LEU:CD2	1:BBB:111:ILE:HB	2.51	0.40
2:CCC:142:ARG:CZ	2:CCC:142:ARG:CB	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	BBB	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
2	CCC	270/325 (83%)	250 (93%)	17 (6%)	3 (1%)	14	46
All	All	448/505 (89%)	417 (93%)	28 (6%)	3 (1%)	22	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	97	LEU
2	CCC	271	VAL
2	CCC	296	SER

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	BBB	150/153 (98%)	142 (95%)	8 (5%)	22	54
2	CCC	239/287 (83%)	224 (94%)	15 (6%)	18	48
All	All	389/440 (88%)	366 (94%)	23 (6%)	19	50

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

Mol	Chain	Res	Type
1	BBB	11	ASP
1	BBB	25	THR
1	BBB	35	THR
1	BBB	37	PHE
1	BBB	75	THR
1	BBB	127	GLU
1	BBB	135	THR
1	BBB	156	GLU
2	CCC	20	ASP
2	CCC	87	THR
2	CCC	96	HIS
2	CCC	97	LEU
2	CCC	101	GLN
2	CCC	105	LYS
2	CCC	107	PHE
2	CCC	116	ARG
2	CCC	128	GLN
2	CCC	135	ARG
2	CCC	136	ARG
2	CCC	143	ILE
2	CCC	281	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	CCC	293	GLN
2	CCC	294	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	GNP	BBB	202	3	29,34,34	1.41	6 (20%)	33,54,54	2.25	6 (18%)

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	GNP	BBB	202	3	-	8/14/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	202	GNP	C6-N1	4.00	1.40	1.33
4	BBB	202	GNP	PG-O1G	3.18	1.51	1.46
4	BBB	202	GNP	PB-O1B	2.93	1.50	1.46
4	BBB	202	GNP	PB-O2B	-2.22	1.50	1.56
4	BBB	202	GNP	PG-O3G	-2.03	1.51	1.56
4	BBB	202	GNP	PG-O2G	-2.03	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	202	GNP	C5-C6-N1	-8.78	111.42	123.43
4	BBB	202	GNP	C2-N1-C6	5.85	125.23	115.93
4	BBB	202	GNP	O2B-PB-O1B	4.20	118.73	109.92
4	BBB	202	GNP	C2-N3-C4	-2.79	112.17	115.36
4	BBB	202	GNP	N3-C2-N1	-2.70	123.62	127.22
4	BBB	202	GNP	O2G-PG-O1G	-2.13	108.10	113.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	202	GNP	PB-N3B-PG-O1G
4	BBB	202	GNP	PA-O3A-PB-O1B
4	BBB	202	GNP	C5'-O5'-PA-O1A
4	BBB	202	GNP	C5'-O5'-PA-O2A
4	BBB	202	GNP	O4'-C4'-C5'-O5'
4	BBB	202	GNP	C3'-C4'-C5'-O5'
4	BBB	202	GNP	PA-O3A-PB-O2B
4	BBB	202	GNP	C5'-O5'-PA-O3A

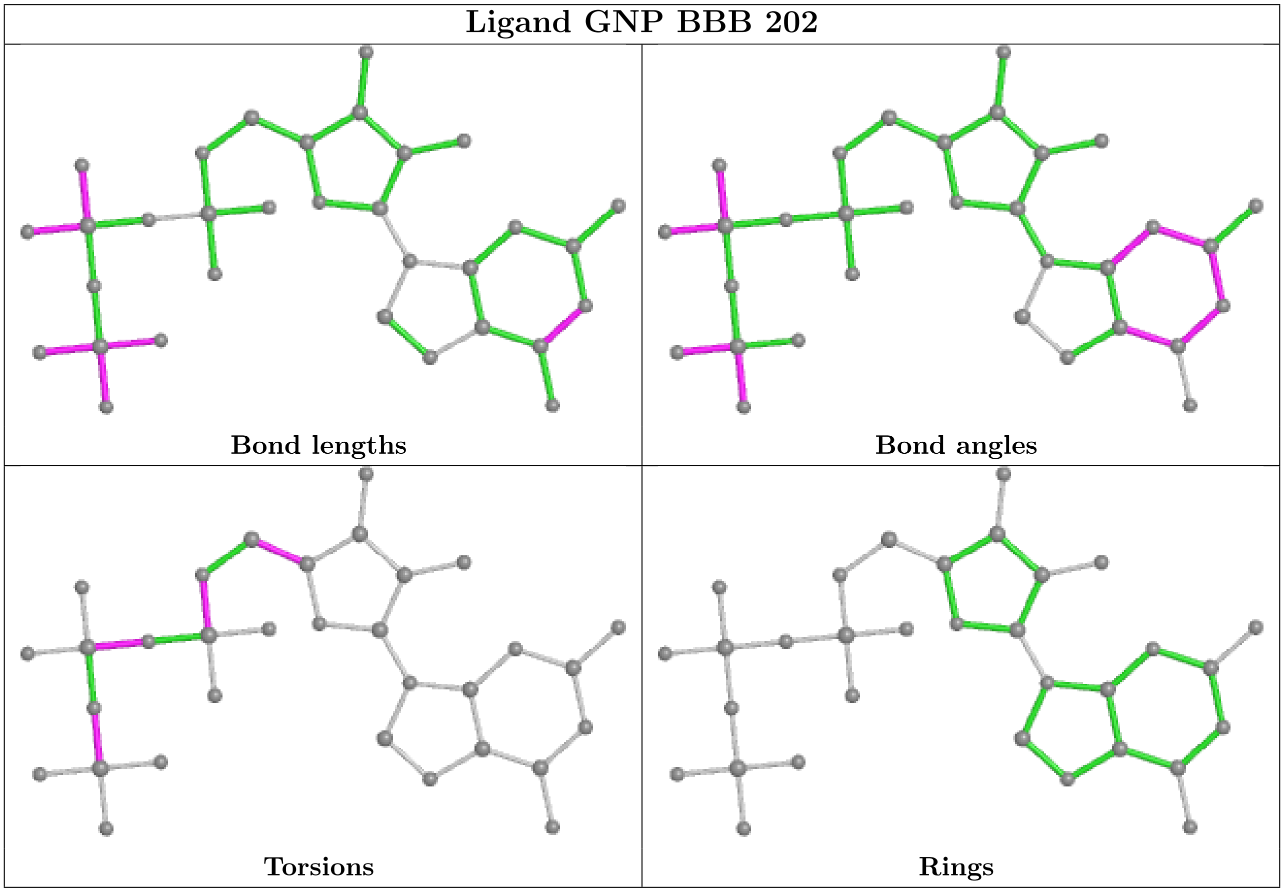
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	202	GNP	8	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.

Ligand GNP BBB 202



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	BBB	180/180 (100%)	0.12	2 (1%)	80	64	63, 92, 120, 133	1 (0%)
2	CCC	276/325 (84%)	-0.04	4 (1%)	75	56	53, 79, 118, 138	0
All	All	456/505 (90%)	0.02	6 (1%)	77	59	53, 85, 120, 138	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	156	GLU	2.4
2	CCC	96	HIS	2.4
2	CCC	11	TYR	2.2
2	CCC	87	THR	2.2
1	BBB	-2	GLY	2.1
2	CCC	288	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

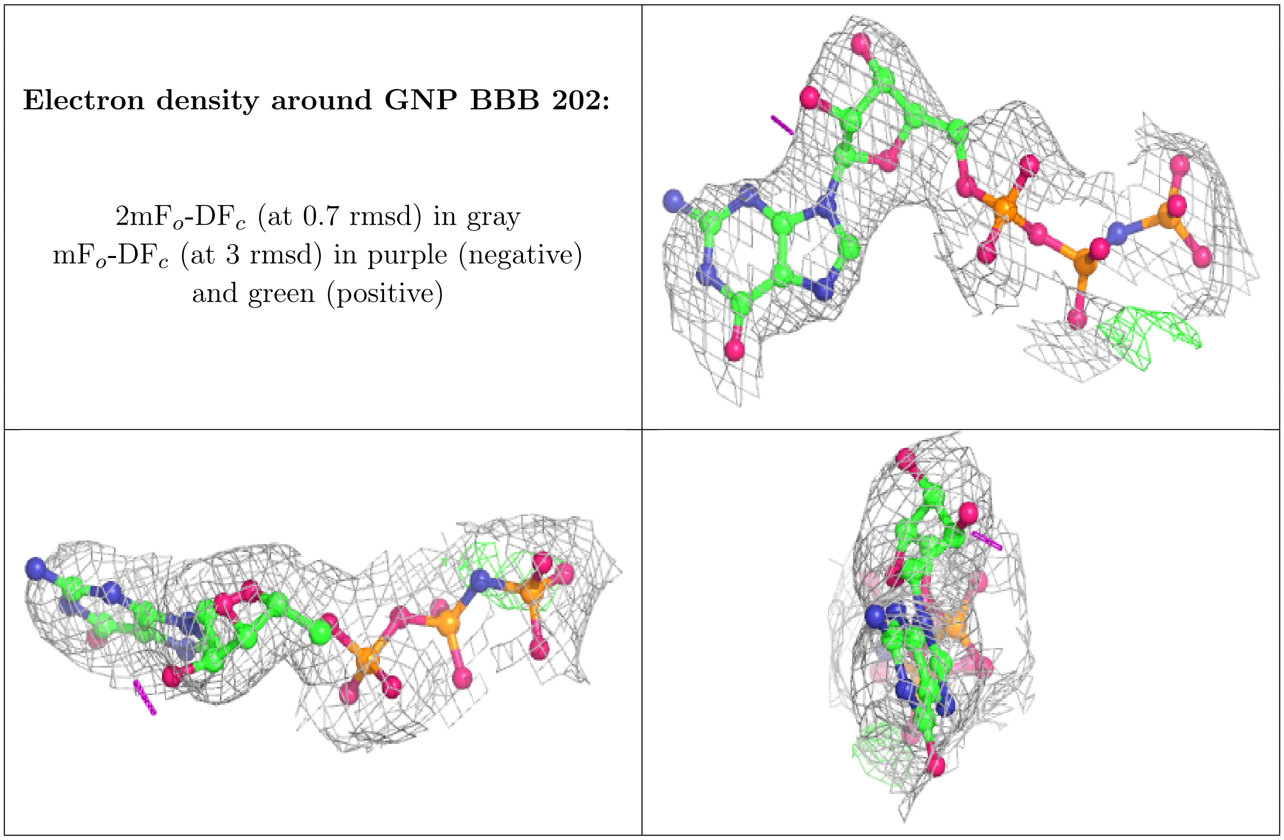
There are no monosaccharides in this entry.

6.4 Ligands

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
4	GNP	BBB	202	32/32	0.97	0.16	56,82,107,111	0
3	MG	BBB	201	1/1	0.98	0.07	59,59,59,59	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 GNP BBB 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

There are no such residues in this entry.