



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:13 PM UTC

PDB ID : 1K8R / pdb_00001k8r
Title : Crystal structure of Ras-Bry2RBD complex
Authors : Scheffzek, K.; Gruenewald, P.; Wohlgemuth, S.; Kabsch, W.; Tu, H.; Wigler, M.; Wittinghofer, A.; Herrmann, C.
Deposited on : 2001-10-25
Resolution : 3.00 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

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

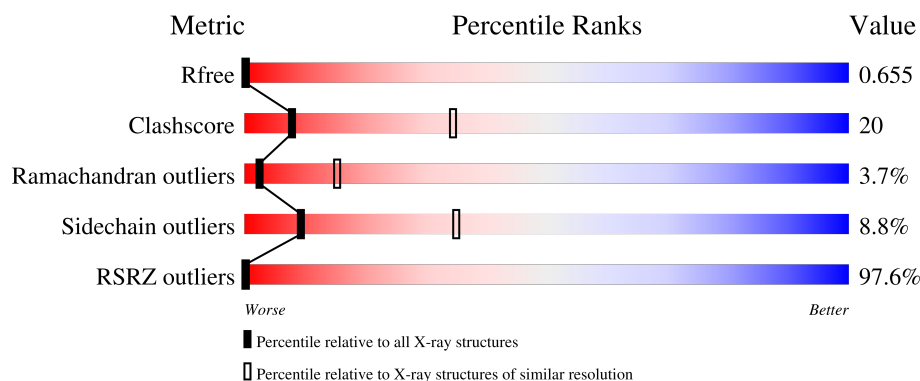
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 ≥ 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	166	96% 58% 37% 5%
2	B	110	75% 34% 36% 5% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2012 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 Transforming protein P21/H-RAS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1319	822	228	263	6			

- Molecule 2 is a protein called Protein kinase byr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			660	416	119	121	4			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

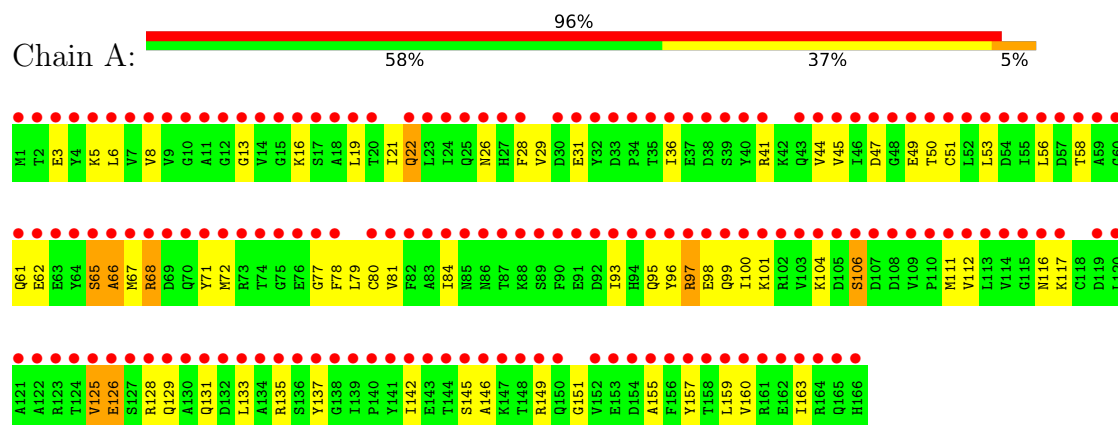


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	32	10	6	13	3	0	0

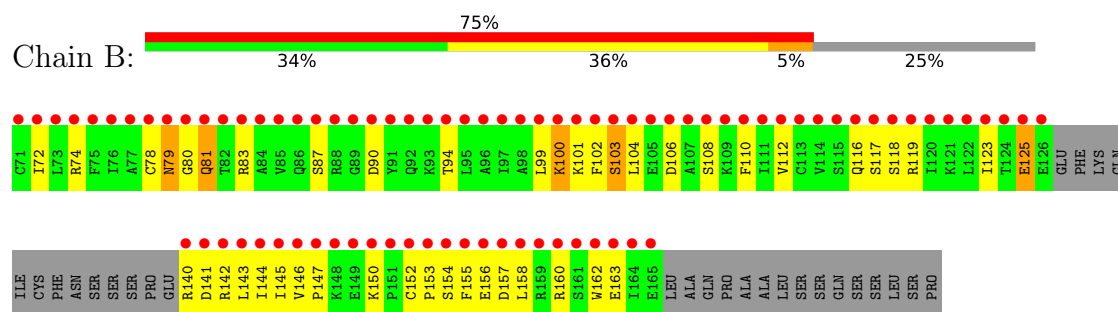
3 Residue-property plots

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: Transforming protein P21/H-RAS-1



• Molecule 2: Protein kinase byr2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	139.03Å 139.03Å 112.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (25.00-3.00) 39.1 (25.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.46 (at 1.73Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.305 0.643 , 0.655	Depositor DCC
R_{free} test set	1181 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	4.4	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.04	EDS
Total number of atoms	2012	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4336e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	A	0.57	0/1338	0.96	2/1807 (0.1%)
2	B	0.48	0/668	1.05	4/894 (0.4%)
All	All	0.54	0/2006	0.99	6/2701 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	PHE	N-CA-C	7.08	120.50	109.52
1	A	81	VAL	N-CA-C	6.82	117.72	108.17
1	A	28	PHE	N-CA-C	6.35	118.52	108.67
2	B	150	LYS	CA-C-N	6.12	127.49	119.84
2	B	150	LYS	C-N-CA	6.12	127.49	119.84
2	B	108	SER	N-CA-C	-5.84	106.19	113.55

There are no chirality outliers.

There are no planarity outliers.

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	1319	0	1289	53	0
2	B	660	0	680	33	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	13	1	0
All	All	2012	0	1982	79	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 20.

All (79) 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:41:ARG:HG2	2:B:81:GLN:HE21	1.38	0.89
1:A:41:ARG:HH21	2:B:80:GLY:HA3	1.47	0.79
1:A:6:LEU:HG	1:A:159:LEU:HD12	1.64	0.77
1:A:8:VAL:HG22	1:A:79:LEU:HD21	1.68	0.75
2:B:146:VAL:HG22	2:B:147:PRO:HD2	1.68	0.74
1:A:68:ARG:HA	1:A:71:TYR:CZ	2.23	0.74
1:A:112:VAL:HG23	1:A:159:LEU:HD23	1.71	0.70
1:A:41:ARG:HG2	2:B:81:GLN:NE2	2.11	0.66
1:A:68:ARG:NH1	1:A:99:GLN:HG2	2.14	0.62
1:A:41:ARG:H	2:B:81:GLN:HE22	1.46	0.61
1:A:26:ASN:C	1:A:26:ASN:HD22	2.07	0.60
2:B:146:VAL:CG2	2:B:147:PRO:HD2	2.32	0.59
2:B:160:ARG:O	2:B:163:GLU:HG2	2.02	0.59
2:B:144:ILE:HG21	2:B:153:PRO:HB3	1.85	0.59
1:A:157:TYR:O	1:A:160:VAL:HG22	2.03	0.58
1:A:68:ARG:HH22	1:A:99:GLN:HB3	1.68	0.57
1:A:101:LYS:HB2	1:A:106:SER:O	2.04	0.57
2:B:154:SER:HB3	2:B:157:ASP:OD2	2.04	0.57
2:B:162:TRP:HD1	2:B:163:GLU:N	2.02	0.56
2:B:162:TRP:CD1	2:B:163:GLU:N	2.74	0.56
1:A:72:MET:HE2	1:A:100:ILE:HA	1.87	0.55
2:B:78:CYS:O	2:B:79:ASN:HB2	2.08	0.54
2:B:102:PHE:O	2:B:103:SER:HB2	2.08	0.54
1:A:41:ARG:N	2:B:81:GLN:HE22	2.06	0.53
1:A:21:ILE:HD12	1:A:29:VAL:HG21	1.90	0.53
1:A:80:CYS:HB3	1:A:93:ILE:HD12	1.91	0.53
1:A:97:ARG:HG2	1:A:97:ARG:HH21	1.73	0.53
1:A:41:ARG:HH21	2:B:80:GLY:CA	2.21	0.52
1:A:84:ILE:HA	1:A:125:VAL:CG1	2.40	0.52
2:B:125:GLU:HA	2:B:125:GLU:OE1	2.11	0.51
2:B:74:ARG:HD2	2:B:141:ASP:O	2.11	0.51
2:B:142:ARG:O	2:B:143:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ILE:HG23	2:B:72:ILE:O	2.10	0.51
2:B:90:ASP:OD2	2:B:90:ASP:C	2.55	0.50
1:A:135:ARG:HG2	1:A:135:ARG:HH21	1.77	0.50
2:B:99:LEU:HD22	2:B:104:LEU:HB2	1.95	0.49
1:A:45:VAL:HG13	1:A:45:VAL:O	2.13	0.48
1:A:16:LYS:HE3	1:A:58:THR:HG22	1.95	0.48
1:A:22:GLN:O	1:A:26:ASN:HA	2.13	0.48
1:A:5:LYS:C	1:A:6:LEU:HD12	2.39	0.48
1:A:77:GLY:HA3	1:A:163:ILE:HD11	1.96	0.48
1:A:5:LYS:O	1:A:6:LEU:HD12	2.15	0.47
1:A:126:GLU:N	1:A:129:GLN:OE1	2.40	0.47
1:A:56:LEU:CD2	1:A:71:TYR:HB2	2.45	0.47
1:A:97:ARG:HH21	1:A:97:ARG:CG	2.28	0.46
1:A:47:ASP:C	1:A:49:GLU:H	2.23	0.46
1:A:98:GLU:CD	1:A:101:LYS:HE2	2.41	0.46
1:A:128:ARG:HD2	1:A:131:GLN:OE1	2.16	0.46
1:A:13:GLY:H	4:A:167:GNP:HNB3	1.63	0.46
1:A:19:LEU:HD23	1:A:146:ALA:HB2	1.98	0.46
1:A:41:ARG:HA	1:A:53:LEU:O	2.15	0.46
1:A:65:SER:O	1:A:66:ALA:C	2.58	0.45
1:A:71:TYR:CE1	1:A:72:MET:HG3	2.52	0.45
1:A:96:TYR:O	1:A:100:ILE:HG13	2.17	0.44
2:B:116:GLN:O	2:B:118:SER:N	2.49	0.44
2:B:118:SER:O	2:B:119:ARG:HB3	2.18	0.44
1:A:128:ARG:NH2	1:A:131:GLN:OE1	2.51	0.44
1:A:6:LEU:HG	1:A:159:LEU:CD1	2.41	0.44
1:A:8:VAL:HG22	1:A:79:LEU:CD2	2.42	0.44
2:B:112:VAL:O	2:B:123:ILE:HG22	2.18	0.44
2:B:162:TRP:CD1	2:B:162:TRP:C	2.95	0.44
1:A:116:ASN:CG	1:A:117:LYS:N	2.76	0.44
1:A:53:LEU:O	1:A:53:LEU:HD12	2.17	0.44
2:B:81:GLN:H	2:B:81:GLN:HG2	1.54	0.44
1:A:68:ARG:HA	1:A:71:TYR:CE2	2.53	0.43
2:B:83:ARG:HD2	2:B:101:LYS:HE3	2.01	0.43
2:B:99:LEU:HD21	2:B:145:ILE:HG21	2.00	0.43
1:A:26:ASN:C	1:A:26:ASN:ND2	2.76	0.43
1:A:145:SER:O	1:A:149:ARG:N	2.51	0.43
2:B:100:LYS:O	2:B:100:LYS:HD3	2.18	0.43
1:A:142:ILE:HD12	1:A:155:ALA:HA	2.00	0.42
1:A:78:PHE:O	1:A:111:MET:HA	2.19	0.42
2:B:87:SER:HB2	2:B:94:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HG	1:A:137:TYR:CE2	2.55	0.42
1:A:36:ILE:HG21	2:B:72:ILE:HD11	2.01	0.41
1:A:116:ASN:CG	1:A:117:LYS:H	2.29	0.41
2:B:152:CYS:HA	2:B:153:PRO:HD2	1.91	0.41
2:B:155:PHE:CE1	2:B:156:GLU:CD	2.99	0.41
1:A:72:MET:HE3	1:A:100:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/166 (99%)	145 (88%)	15 (9%)	4 (2%)	4	24
2	B	78/110 (71%)	60 (77%)	13 (17%)	5 (6%)	1	6
All	All	242/276 (88%)	205 (85%)	28 (12%)	9 (4%)	2	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ALA
2	B	106	ASP
1	A	65	SER
2	B	81	GLN
2	B	117	SER
2	B	79	ASN
1	A	67	MET
2	B	103	SER
1	A	151	GLY

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	143/144 (99%)	128 (90%)	15 (10%)	6	27
2	B	74/100 (74%)	70 (95%)	4 (5%)	20	53
All	All	217/244 (89%)	198 (91%)	19 (9%)	9	35

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	22	GLN
1	A	31	GLU
1	A	44	VAL
1	A	50	THR
1	A	51	CYS
1	A	61	GLN
1	A	62	GLU
1	A	68	ARG
1	A	95	GLN
1	A	97	ARG
1	A	104	LYS
1	A	106	SER
1	A	125	VAL
1	A	126	GLU
2	B	100	LYS
2	B	125	GLU
2	B	140	ARG
2	B	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	GLN
1	A	26	ASN

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Mol	Chain	Res	Type
1	A	70	GLN
1	A	95	GLN
1	A	165	GLN
2	B	81	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 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	A	167	3	34,34,34	1.44	4 (11%)	47,54,54	1.05	3 (6%)

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	A	167	3	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	167	GNP	PB-O2B	-4.41	1.45	1.56
4	A	167	GNP	PG-O2G	-4.33	1.45	1.56
4	A	167	GNP	C2-N3	2.44	1.39	1.33
4	A	167	GNP	C4-N3	2.39	1.39	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	167	GNP	O3G-PG-O1G	-4.35	102.56	113.45
4	A	167	GNP	O1G-PG-N3B	2.67	115.69	111.77
4	A	167	GNP	O1B-PB-N3B	2.30	115.15	111.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

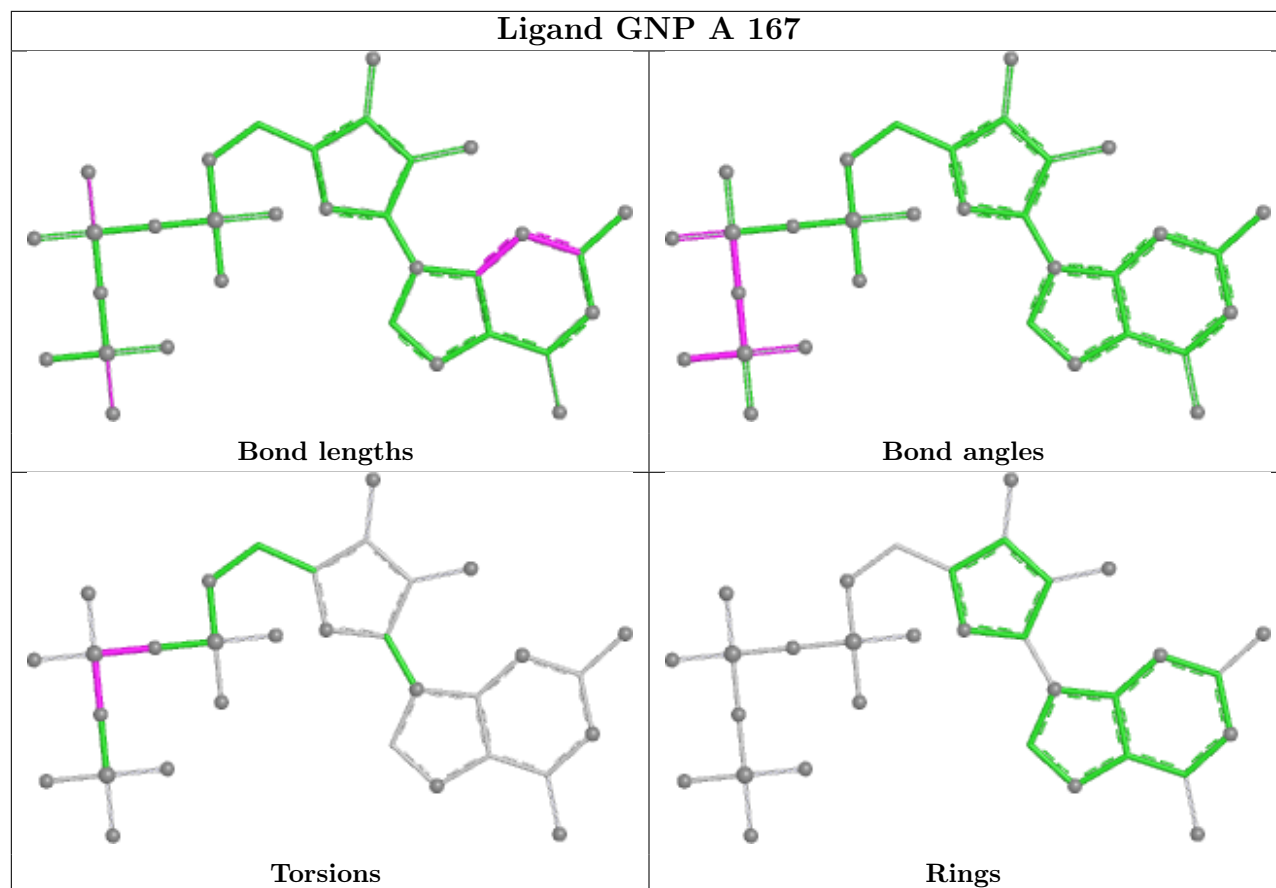
Mol	Chain	Res	Type	Atoms
4	A	167	GNP	PG-N3B-PB-O1B
4	A	167	GNP	PA-O3A-PB-O2B
4	A	167	GNP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	167	GNP	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	166/166 (100%)	5.16	160 (96%)  	14, 44, 76, 82	0
2	B	82/110 (74%)	5.15	82 (100%)  	35, 63, 79, 86	0
All	All	248/276 (89%)	5.16	242 (97%)  	14, 51, 77, 86	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	113	CYS	17.2
1	A	47	ASP	14.2
1	A	31	GLU	14.0
1	A	95	GLN	12.4
2	B	116	GLN	11.9
1	A	140	PRO	11.9
1	A	143	GLU	11.5
1	A	159	LEU	11.3
1	A	8	VAL	11.1
1	A	59	ALA	10.8
2	B	105	GLU	10.7
1	A	88	LYS	10.4
2	B	117	SER	10.1
1	A	39	SER	10.0
2	B	111	ILE	9.6
2	B	72	ILE	9.6
1	A	112	VAL	9.3
2	B	95	LEU	8.9
1	A	58	THR	8.9
2	B	163	GLU	8.5
1	A	24	ILE	8.5
1	A	111	MET	8.5
1	A	80	CYS	8.3
2	B	110	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	THR	8.1
2	B	108	SER	7.8
1	A	72	MET	7.7
1	A	13	GLY	7.7
1	A	145	SER	7.7
2	B	88	ARG	7.6
1	A	30	ASP	7.5
2	B	106	ASP	7.5
1	A	60	GLY	7.4
2	B	104	LEU	7.3
1	A	135	ARG	7.3
1	A	55	ILE	7.3
1	A	90	PHE	7.1
2	B	84	ALA	7.1
1	A	70	GLN	7.1
1	A	74	THR	7.0
2	B	118	SER	7.0
1	A	71	TYR	7.0
2	B	92	GLN	7.0
1	A	18	ALA	7.0
1	A	133	LEU	7.0
2	B	81	GLN	6.9
1	A	87	THR	6.9
1	A	138	GLY	6.7
1	A	11	ALA	6.6
1	A	166	HIS	6.6
2	B	124	THR	6.6
1	A	132	ASP	6.6
1	A	127	SER	6.5
2	B	112	VAL	6.5
1	A	3	GLU	6.4
2	B	115	SER	6.4
1	A	15	GLY	6.3
1	A	163	ILE	6.3
1	A	67	MET	6.3
1	A	34	PRO	6.3
1	A	110	PRO	6.2
1	A	149	ARG	6.2
2	B	121	LYS	6.2
1	A	113	LEU	6.2
1	A	153	GLU	6.1
1	A	45	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	6.0
1	A	78	PHE	6.0
1	A	119	ASP	5.9
1	A	120	LEU	5.9
1	A	76	GLU	5.9
1	A	48	GLY	5.9
1	A	92	ASP	5.9
1	A	37	GLU	5.8
1	A	141	TYR	5.8
1	A	154	ASP	5.8
2	B	125	GLU	5.8
2	B	83	ARG	5.7
1	A	105	ASP	5.7
1	A	94	HIS	5.7
1	A	14	VAL	5.7
1	A	61	GLN	5.7
1	A	137	TYR	5.6
2	B	147	PRO	5.6
2	B	151	PRO	5.6
1	A	107	ASP	5.6
2	B	86	GLN	5.5
2	B	143	LEU	5.5
1	A	98	GLU	5.5
2	B	148	LYS	5.5
2	B	126	GLU	5.5
1	A	99	GLN	5.4
1	A	62	GLU	5.4
1	A	91	GLU	5.4
1	A	116	ASN	5.4
2	B	153	PRO	5.4
1	A	25	GLN	5.3
1	A	33	ASP	5.3
1	A	115	GLY	5.2
2	B	75	PHE	5.2
1	A	136	SER	5.1
2	B	155	PHE	5.1
1	A	54	ASP	5.0
1	A	4	TYR	5.0
1	A	123	ARG	5.0
2	B	140	ARG	5.0
1	A	142	ILE	5.0
1	A	139	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	20	THR	5.0
2	B	78	CYS	4.9
1	A	75	GLY	4.9
2	B	158	LEU	4.9
2	B	149	GLU	4.8
1	A	10	GLY	4.8
1	A	85	ASN	4.7
2	B	82	THR	4.7
1	A	50	THR	4.7
1	A	2	THR	4.7
1	A	165	GLN	4.6
2	B	99	LEU	4.6
2	B	152	CYS	4.6
1	A	12	GLY	4.6
1	A	160	VAL	4.6
2	B	93	LYS	4.5
1	A	102	ARG	4.5
1	A	26	ASN	4.4
1	A	93	ILE	4.4
2	B	154	SER	4.4
1	A	41	ARG	4.4
1	A	66	ALA	4.4
1	A	53	LEU	4.3
1	A	152	VAL	4.3
1	A	89	SER	4.3
1	A	56	LEU	4.3
2	B	162	TRP	4.3
1	A	32	TYR	4.3
1	A	64	TYR	4.3
1	A	134	ALA	4.3
2	B	150	LYS	4.3
2	B	122	LEU	4.3
2	B	109	LYS	4.3
1	A	69	ASP	4.3
1	A	97	ARG	4.3
1	A	63	GLU	4.3
1	A	9	VAL	4.2
2	B	85	VAL	4.2
1	A	128	ARG	4.2
1	A	46	ILE	4.2
2	B	77	ALA	4.1
2	B	103	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	VAL	4.1
1	A	158	THR	4.1
1	A	150	GLN	4.0
1	A	1	MET	4.0
1	A	57	ASP	4.0
2	B	141	ASP	4.0
1	A	19	LEU	4.0
1	A	27	HIS	4.0
1	A	28	PHE	3.9
1	A	155	ALA	3.9
1	A	108	ASP	3.9
2	B	74	ARG	3.8
2	B	97	ILE	3.8
2	B	98	ALA	3.8
1	A	17	SER	3.8
1	A	131	GLN	3.8
1	A	7	VAL	3.8
1	A	38	ASP	3.8
1	A	49	GLU	3.8
1	A	43	GLN	3.7
2	B	159	ARG	3.7
1	A	130	ALA	3.7
2	B	101	LYS	3.7
1	A	106	SER	3.7
2	B	91	TYR	3.7
2	B	165	GLU	3.7
1	A	40	TYR	3.6
1	A	114	VAL	3.6
1	A	124	THR	3.6
1	A	129	GLN	3.6
1	A	109	VAL	3.6
1	A	77	GLY	3.6
2	B	156	GLU	3.6
1	A	157	TYR	3.6
2	B	79	ASN	3.5
2	B	161	SER	3.5
1	A	65	SER	3.5
2	B	71	CYS	3.5
2	B	145	ILE	3.5
1	A	36	ILE	3.5
1	A	68	ARG	3.4
2	B	120	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	3.4
1	A	122	ALA	3.4
2	B	164	ILE	3.4
2	B	87	SER	3.4
2	B	123	ILE	3.4
1	A	44	VAL	3.3
1	A	82	PHE	3.3
1	A	117	LYS	3.3
2	B	94	THR	3.3
2	B	160	ARG	3.3
2	B	107	ALA	3.3
1	A	16	LYS	3.3
1	A	84	ILE	3.3
1	A	164	ARG	3.2
1	A	104	LYS	3.2
2	B	157	ASP	3.2
1	A	162	GLU	3.2
1	A	146	ALA	3.2
1	A	6	LEU	3.1
2	B	80	GLY	3.1
2	B	144	ILE	3.1
2	B	96	ALA	3.1
1	A	125	VAL	3.1
2	B	146	VAL	3.0
2	B	102	PHE	3.0
1	A	96	TYR	3.0
2	B	114	VAL	2.9
1	A	35	THR	2.9
1	A	51	CYS	2.9
2	B	142	ARG	2.9
1	A	52	LEU	2.9
1	A	156	PHE	2.8
1	A	100	ILE	2.8
1	A	86	ASN	2.8
1	A	81	VAL	2.8
2	B	76	ILE	2.8
2	B	89	GLY	2.7
1	A	126	GLU	2.7
2	B	90	ASP	2.7
1	A	73	ARG	2.7
1	A	147	LYS	2.7
2	B	119	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	73	LEU	2.6
1	A	161	ARG	2.5
1	A	5	LYS	2.5
1	A	101	LYS	2.4
1	A	144	THR	2.4
2	B	100	LYS	2.3
1	A	22	GLN	2.3
1	A	83	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

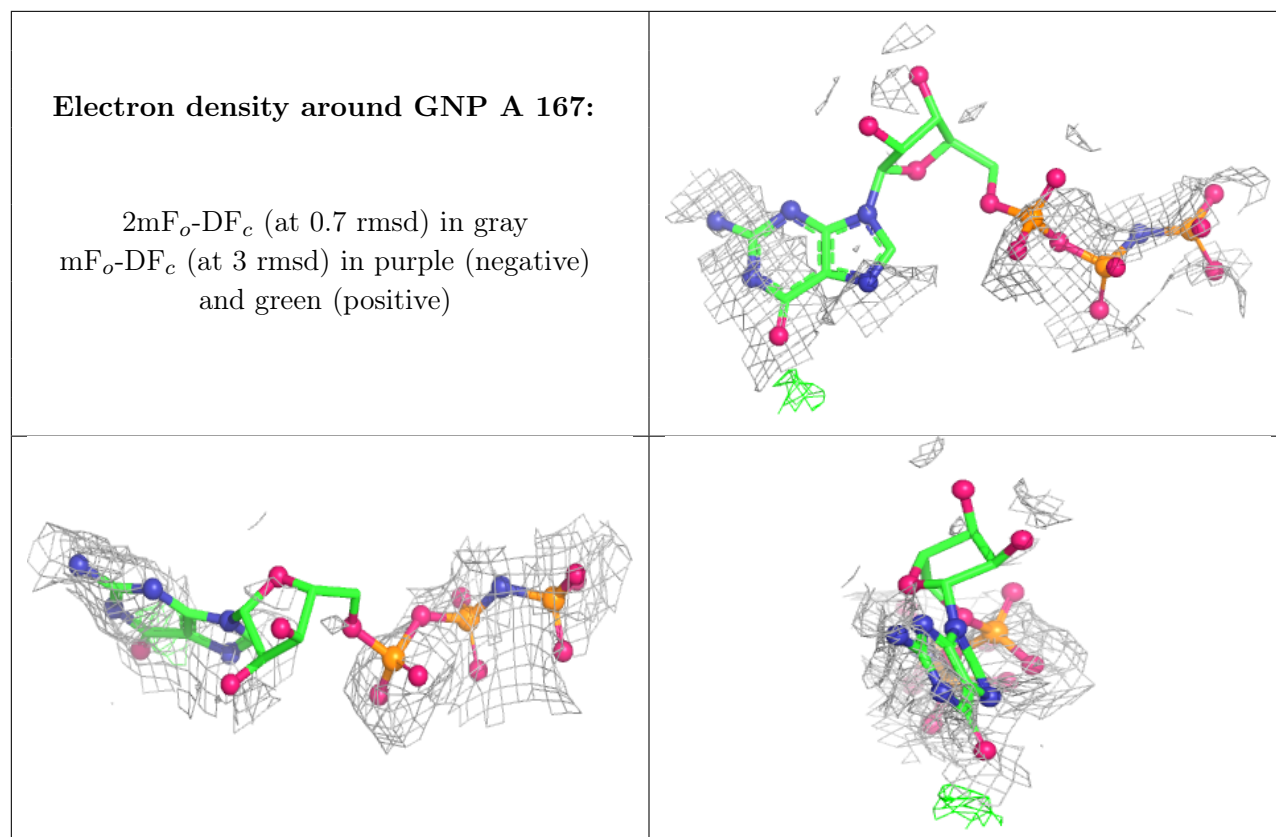
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GNP	A	167	32/32	0.33	0.25	20,23,36,37	0
3	MG	A	168	1/1	0.42	0.22	41,41,41,41	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.