



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:05 AM EDT

PDB ID : 2I66 / pdb_00002i66
Title : Structural Basis for the Mechanistic Understanding Human CD38 Controlled Multiple Catalysis
Authors : Liu, Q.; Kriksunov, I.A.; Graeff, R.; Munshi, C.; Lee, H.C.; Hao, Q.
Deposited on : 2006-08-28
Resolution : 1.70 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

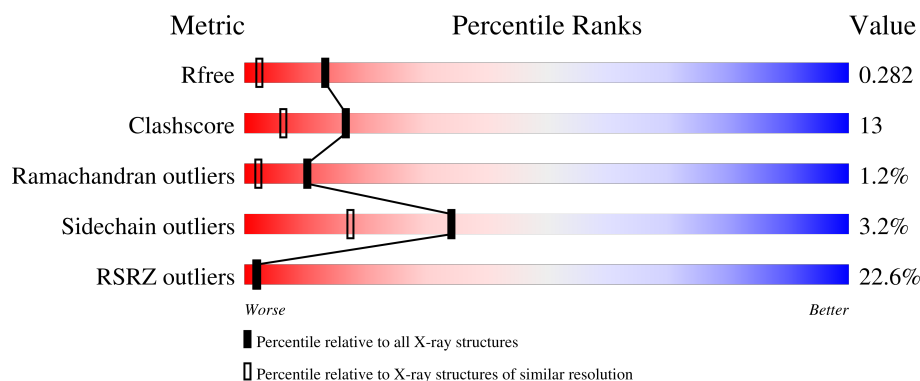
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	262	
1	B	262	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G1R	A	301	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4690 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 ADP-ribosyl cyclase 1.

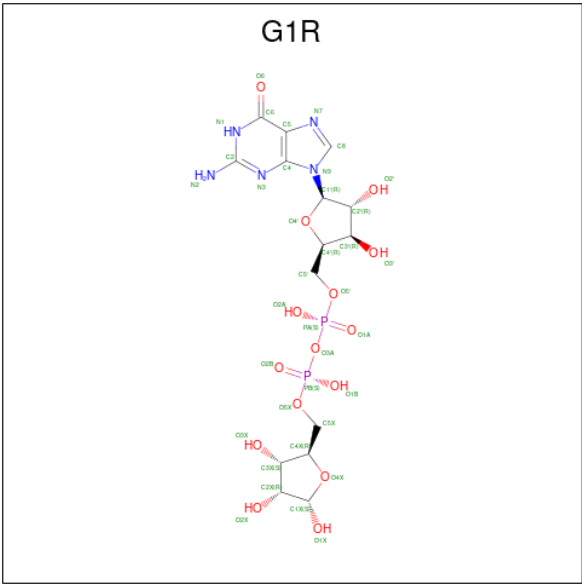
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

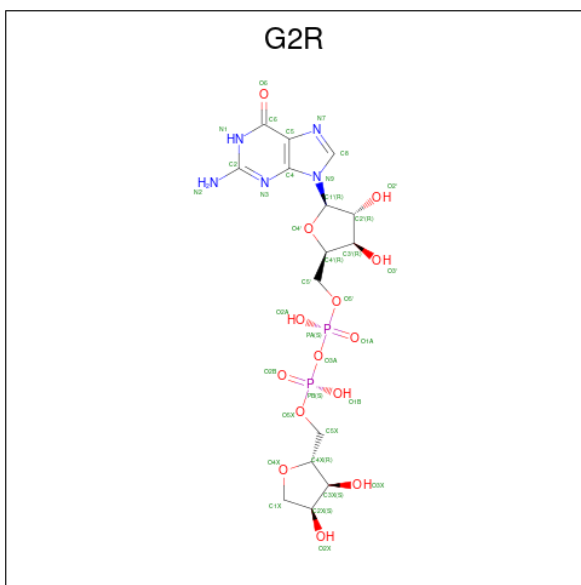
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	cloning artifact	UNP P28907
A	40	ARG	-	cloning artifact	UNP P28907
A	41	GLU	-	cloning artifact	UNP P28907
A	42	ALA	-	cloning artifact	UNP P28907
A	43	GLU	-	cloning artifact	UNP P28907
A	44	ALA	-	cloning artifact	UNP P28907
A	49	THR	GLN	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
B	39	LYS	-	cloning artifact	UNP P28907
B	40	ARG	-	cloning artifact	UNP P28907
B	41	GLU	-	cloning artifact	UNP P28907
B	42	ALA	-	cloning artifact	UNP P28907
B	43	GLU	-	cloning artifact	UNP P28907
B	44	ALA	-	cloning artifact	UNP P28907
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907

- Molecule 2 is [(2R,3R,4R,5R)-5-(2-AMINO-6-OXO-1,6-DIHYDRO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4R,5S)-3,4,5-TRIHYDRO

XYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (CCD ID: G1R) (formula: C₁₅H₂₃N₅O₁₅P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 36	C 15	N 5	O 14	P 2	0	0

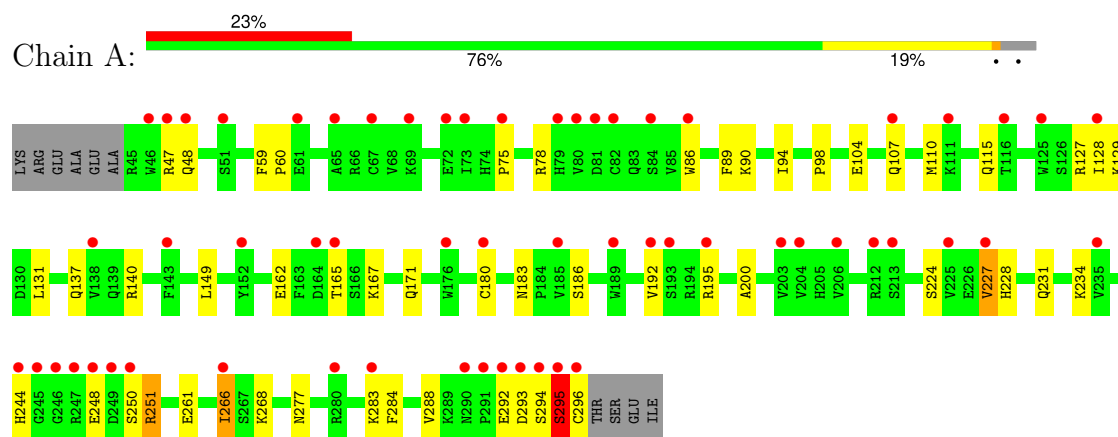
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	235	Total O 235 235	0	0
4	B	209	Total O 209 209	0	0

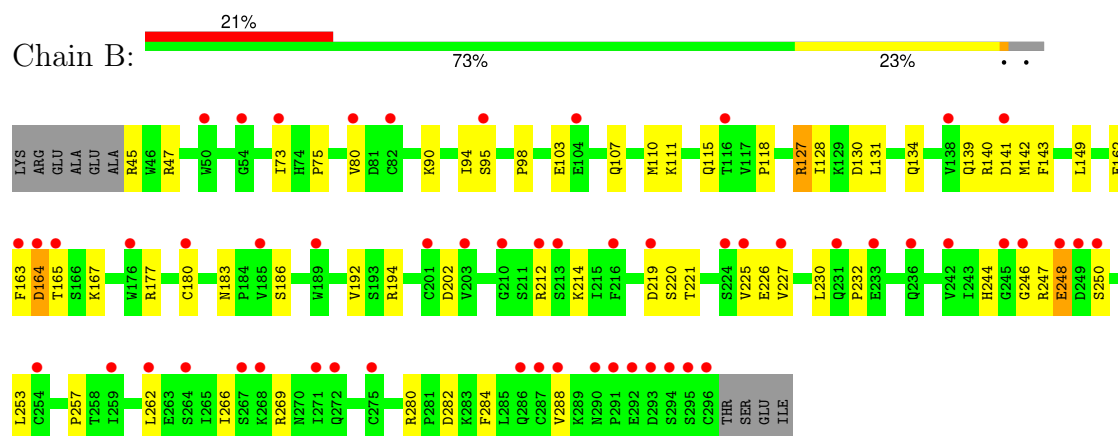
3 Residue-property plots [i](#)

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: ADP-ribosyl cyclase 1



• Molecule 1: ADP-ribosyl cyclase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.71Å 52.81Å 65.42Å 105.93° 91.80° 95.22°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.70) 96.7 (20.00-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.229 0.246 , 0.282	Depositor DCC
R_{free} test set	2857 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4690	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% 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: G1R, G2R

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	0.86	1/2101 (0.0%)	0.99	5/2846 (0.2%)
1	B	0.82	0/2101	0.98	5/2846 (0.2%)
All	All	0.84	1/4202 (0.0%)	0.98	10/5692 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	295	SER	C-N	-7.22	1.23	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	SER	N-CA-C	6.89	117.60	107.88
1	B	280	ARG	CA-C-N	6.78	126.58	119.05
1	B	280	ARG	C-N-CA	6.78	126.58	119.05
1	A	266	ILE	CB-CG1-CD1	-6.40	100.35	113.80
1	A	295	SER	O-C-N	-5.94	114.69	122.59
1	B	164	ASP	N-CA-CB	-5.76	101.44	110.30
1	A	89	PHE	N-CA-C	-5.63	105.06	111.14
1	B	262	LEU	N-CA-C	-5.20	105.51	111.07
1	A	295	SER	CA-C-N	5.05	130.79	121.70
1	A	295	SER	C-N-CA	5.05	130.79	121.70

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	A	2050	0	1976	40	0
1	B	2050	0	1976	48	0
2	A	73	0	39	13	0
2	B	37	0	21	11	0
3	B	36	0	21	6	0
4	A	235	0	0	7	0
4	B	209	0	0	4	0
All	All	4690	0	4033	105	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 13.

All (105) 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:301:G1R:O6	3:B:302:G2R:H1X1	1.33	1.23
2:A:302:G1R:H5'1	2:A:302:G1R:C8	1.76	1.16
2:A:302:G1R:H5'1	2:A:302:G1R:H8	1.28	1.14
1:A:165:THR:HG23	1:A:167:LYS:H	1.24	1.02
2:A:302:G1R:H8	2:A:302:G1R:C5'	1.91	0.99
1:B:103:GLU:CD	1:B:194:ARG:HH22	1.71	0.98
1:B:219:ASP:O	3:B:302:G2R:H8	1.67	0.93
1:B:165:THR:HG23	1:B:167:LYS:H	1.37	0.89
1:B:232:PRO:HD3	1:B:269:ARG:HH12	1.35	0.89
2:B:301:G1R:O6	3:B:302:G2R:C1X	2.22	0.88
1:B:115:GLN:HE22	1:B:149:LEU:H	1.20	0.87
1:A:115:GLN:HE22	1:A:149:LEU:H	1.24	0.85
2:A:301:G1R:H8	2:A:302:G1R:O4'	1.82	0.80
1:A:231:GLN:HG3	4:A:535:HOH:O	1.82	0.78
1:B:221:THR:O	1:B:225:VAL:HG12	1.84	0.77
1:B:227:VAL:HG23	1:B:266:ILE:HD11	1.72	0.71
2:A:302:G1R:C8	2:A:302:G1R:C5'	2.59	0.70
1:B:230:LEU:O	1:B:269:ARG:NH1	2.24	0.69
2:A:302:G1R:O2A	2:A:302:G1R:O3'	2.10	0.69
1:A:195:ARG:HD3	4:A:447:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HG2	1:A:94:ILE:HG13	1.79	0.64
1:B:103:GLU:CD	1:B:194:ARG:NH2	2.52	0.64
2:B:301:G1R:PA	2:B:301:G1R:HO3'	2.21	0.64
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.79	0.64
1:B:177:ARG:HH11	1:B:177:ARG:HB3	1.64	0.63
1:A:183:ASN:ND2	1:A:186:SER:H	1.97	0.62
1:A:162:GLU:HG2	4:A:486:HOH:O	1.98	0.62
1:B:202:ASP:HB3	4:B:373:HOH:O	2.00	0.62
1:B:232:PRO:HD3	1:B:269:ARG:NH1	2.13	0.62
2:B:301:G1R:PA	2:B:301:G1R:O3'	2.58	0.61
1:A:268:LYS:NZ	1:B:95:SER:O	2.25	0.61
1:A:294:SER:O	1:A:296:CYS:N	2.34	0.60
1:B:127:ARG:NH2	3:B:302:G2R:H4'	2.15	0.60
1:B:183:ASN:ND2	1:B:186:SER:H	1.99	0.60
1:A:140:ARG:NH2	4:A:417:HOH:O	2.31	0.60
1:B:177:ARG:HB3	1:B:177:ARG:NH1	2.17	0.59
1:B:45:ARG:HG3	4:B:453:HOH:O	2.03	0.58
1:B:212:ARG:HH22	2:B:301:G1R:H5X1	1.69	0.57
1:A:48:GLN:NE2	1:A:171:GLN:HB3	2.19	0.57
1:B:127:ARG:HH21	2:B:301:G1R:PA	2.26	0.57
1:B:115:GLN:NE2	1:B:149:LEU:H	1.95	0.56
1:B:221:THR:O	1:B:225:VAL:CG1	2.52	0.56
1:A:104:GLU:OE1	1:B:177:ARG:NH2	2.38	0.56
1:A:75:PRO:HA	1:A:78:ARG:HG3	1.87	0.56
1:B:103:GLU:OE1	1:B:194:ARG:NH2	2.40	0.55
1:B:127:ARG:NH2	2:B:301:G1R:O3A	2.35	0.55
1:A:180:CYS:HB2	4:A:470:HOH:O	2.06	0.54
1:A:104:GLU:HA	1:A:107:GLN:HG2	1.90	0.54
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.90	0.54
1:B:118:PRO:HD2	1:B:143:PHE:CE2	2.42	0.54
1:B:73:ILE:O	1:B:75:PRO:HD3	2.08	0.53
2:B:301:G1R:O1A	3:B:302:G2R:H4'	2.09	0.53
1:B:269:ARG:HH11	1:B:269:ARG:HB3	1.74	0.53
1:A:183:ASN:HD21	1:A:186:SER:H	1.56	0.52
1:B:212:ARG:C	1:B:214:LYS:H	2.15	0.52
1:A:251:ARG:H	1:A:251:ARG:HD3	1.75	0.52
2:A:301:G1R:H8	2:A:302:G1R:C1'	2.40	0.52
1:A:224:SER:OG	2:A:302:G1R:H3X	2.09	0.52
1:A:244:HIS:CD2	1:A:250:SER:HB3	2.45	0.51
1:B:220:SER:HB2	3:B:302:G2R:O2B	2.11	0.51
2:B:301:G1R:O3'	2:B:301:G1R:O5'	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:G1R:C8	2:A:302:G1R:H3'	2.41	0.50
1:B:244:HIS:CE1	1:B:253:LEU:HD12	2.46	0.50
1:A:110:MET:HE1	1:A:192:VAL:HG12	1.94	0.49
1:B:47:ARG:HD2	4:B:424:HOH:O	2.13	0.48
1:A:283:LYS:NZ	1:A:295:SER:O	2.44	0.48
1:A:231:GLN:HB2	1:A:234:LYS:HD3	1.95	0.47
1:B:227:VAL:CG2	1:B:266:ILE:HD11	2.44	0.47
1:A:244:HIS:HD2	1:A:250:SER:HB3	1.79	0.46
1:A:47:ARG:O	1:A:47:ARG:HG3	2.16	0.46
1:A:98:PRO:O	1:A:183:ASN:HA	2.16	0.46
1:A:227:VAL:HG13	1:A:228:HIS:CD2	2.51	0.46
1:B:246:GLY:C	1:B:248:GLU:H	2.24	0.46
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.98	0.46
1:A:293:ASP:HB2	4:A:532:HOH:O	2.15	0.46
2:A:301:G1R:C1X	2:A:302:G1R:C6	2.75	0.45
1:B:90:LYS:HG3	1:B:94:ILE:HG13	1.97	0.45
1:A:86:TRP:NE1	1:A:90:LYS:HE2	2.30	0.45
1:A:110:MET:HE1	1:A:192:VAL:CG1	2.47	0.45
1:A:115:GLN:NE2	1:A:149:LEU:H	2.03	0.44
1:B:180:CYS:HB2	4:B:310:HOH:O	2.17	0.44
1:B:225:VAL:HG13	1:B:226:GLU:HG3	1.99	0.44
1:B:246:GLY:O	1:B:248:GLU:N	2.51	0.44
1:A:284:PHE:O	1:A:288:VAL:HG23	2.18	0.44
1:B:225:VAL:HG13	1:B:226:GLU:N	2.32	0.44
1:A:200:ALA:O	1:A:234:LYS:HE2	2.17	0.43
1:A:251:ARG:H	1:A:251:ARG:CD	2.30	0.43
1:A:165:THR:HG23	1:A:167:LYS:N	2.08	0.43
2:A:302:G1R:H8	2:A:302:G1R:C4'	2.47	0.43
1:B:284:PHE:O	1:B:288:VAL:HG23	2.18	0.43
1:B:130:ASP:O	1:B:134:GLN:HG3	2.19	0.43
1:A:137:GLN:NE2	4:A:498:HOH:O	2.52	0.43
1:B:110:MET:SD	1:B:192:VAL:HG12	2.59	0.43
2:A:302:G1R:H5'1	2:A:302:G1R:N9	2.23	0.42
1:A:261:GLU:HG3	1:B:163:PHE:HZ	1.84	0.41
1:A:127:ARG:N	1:A:127:ARG:HD2	2.34	0.41
2:B:301:G1R:O3'	2:B:301:G1R:O1A	2.39	0.41
1:B:139:GLN:HG2	1:B:142:MET:HG3	2.02	0.41
1:B:139:GLN:C	1:B:141:ASP:H	2.28	0.41
1:B:162:GLU:HB2	1:B:165:THR:HG22	2.03	0.41
1:B:244:HIS:C	1:B:246:GLY:H	2.29	0.41
1:B:221:THR:HG23	1:B:225:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:G1R:C8	2:A:302:G1R:C4'	2.99	0.40
2:B:301:G1R:H8	2:B:301:G1R:H2'	1.81	0.40
1:B:98:PRO:O	1:B:183:ASN:HA	2.21	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	250/262 (95%)	236 (94%)	11 (4%)	3 (1%)	10	2
1	B	250/262 (95%)	236 (94%)	11 (4%)	3 (1%)	10	2
All	All	500/524 (95%)	472 (94%)	22 (4%)	6 (1%)	10	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	248	GLU
1	A	292	GLU
1	B	248	GLU
1	B	247	ARG
1	B	128	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/241 (97%)	227 (97%)	6 (3%)	40	23
1	B	233/241 (97%)	224 (96%)	9 (4%)	28	12
All	All	466/482 (97%)	451 (97%)	15 (3%)	34	17

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	129	LYS
1	A	131	LEU
1	A	227	VAL
1	A	251	ARG
1	A	266	ILE
1	B	80	VAL
1	B	107	GLN
1	B	111	LYS
1	B	127	ARG
1	B	131	LEU
1	B	140	ARG
1	B	164	ASP
1	B	257	PRO
1	B	282	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	183	ASN
1	A	244	HIS
1	A	290	ASN
1	B	48	GLN
1	B	74	HIS
1	B	83	GLN
1	B	115	GLN
1	B	183	ASN
1	B	231	GLN
1	B	270	ASN
1	B	272	GLN

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Mol	Chain	Res	Type
1	B	286	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	G1R	A	302	2	40,40,40	1.54	7 (17%)	58,62,62	2.24	14 (24%)
2	G1R	B	301	-	40,40,40	1.52	7 (17%)	58,62,62	1.27	7 (12%)
2	G1R	A	301	2	39,39,40	1.47	4 (10%)	55,60,62	2.12	14 (25%)
3	G2R	B	302	-	39,39,39	1.03	2 (5%)	55,60,60	1.74	8 (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
2	G1R	A	302	2	-	8/22/54/54	0/4/4/4
2	G1R	B	301	-	-	9/22/54/54	0/4/4/4
2	G1R	A	301	2	2/2/9/10	8/22/51/54	0/4/4/4
3	G2R	B	302	-	-	5/22/51/51	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	G1R	C1'-N9	-4.60	1.34	1.47
2	A	301	G1R	PB-O3A	4.25	1.64	1.59
2	B	301	G1R	PA-O3A	4.17	1.64	1.59
2	B	301	G1R	PB-O3A	4.02	1.63	1.59
2	B	301	G1R	O4X-C1X	3.56	1.47	1.43
2	A	302	G1R	C5-N7	-3.46	1.32	1.39
2	A	302	G1R	C1'-N9	3.33	1.57	1.47
2	A	302	G1R	PA-O3A	3.33	1.63	1.59
2	A	302	G1R	C6-N1	-3.15	1.32	1.38
2	B	301	G1R	C5-N7	-3.04	1.33	1.39
2	A	301	G1R	C5-N7	-2.92	1.33	1.39
3	B	302	G2R	C5-N7	-2.92	1.33	1.39
3	B	302	G2R	PB-O3A	2.58	1.62	1.59
2	B	301	G1R	C1X-C2X	2.49	1.55	1.52
2	A	302	G1R	C5'-C4'	2.40	1.58	1.51
2	A	302	G1R	O1X-C1X	2.26	1.46	1.39
2	B	301	G1R	C4-N9	-2.24	1.32	1.38
2	A	302	G1R	O4'-C1'	2.23	1.47	1.42
2	B	301	G1R	C5-C6	-2.09	1.36	1.44
2	A	301	G1R	O4'-C1'	-2.07	1.37	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	G1R	O4'-C1'-N9	6.96	124.12	108.36
2	A	302	G1R	C2'-C1'-N9	6.88	132.39	113.25
2	A	302	G1R	O4'-C1'-N9	-6.74	93.09	108.36
2	A	301	G1R	C2-N3-C4	5.57	121.90	112.30
2	A	301	G1R	C5-C4-N3	-5.49	119.65	128.39
2	A	302	G1R	C5-C4-N3	-5.44	119.73	128.39
3	B	302	G2R	C5-C4-N3	-5.34	119.89	128.39
3	B	302	G2R	C2-N3-C4	5.34	121.50	112.30
2	A	302	G1R	C5'-C4'-C3'	-5.11	96.81	115.21
2	A	301	G1R	C2'-C1'-N9	4.22	124.99	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	G1R	O6-C6-C5	-4.15	115.57	126.53
2	A	301	G1R	N9-C4-N3	4.00	133.96	125.95
3	B	302	G2R	N9-C4-N3	3.99	133.93	125.95
2	A	302	G1R	C2-N3-C4	3.55	118.42	112.30
2	A	302	G1R	O4'-C4'-C3'	-3.50	98.20	105.15
2	A	301	G1R	O2X-C2X-C3X	-3.43	104.67	111.43
2	B	301	G1R	C5-C4-N3	-3.43	122.94	128.39
2	A	301	G1R	C2-N1-C6	-3.40	118.95	125.11
3	B	302	G2R	C4'-O4'-C1'	-3.37	102.03	109.47
2	A	302	G1R	N9-C4-N3	3.34	132.63	125.95
2	A	302	G1R	O6-C6-N1	3.15	126.04	120.11
2	A	302	G1R	O4'-C4'-C5'	3.12	119.33	109.33
3	B	302	G2R	C2-N1-C6	-3.09	119.51	125.11
2	B	301	G1R	N9-C4-N3	3.04	132.04	125.95
2	A	302	G1R	O2'-C2'-C3'	-2.86	102.64	111.82
2	A	302	G1R	O4'-C1'-C2'	-2.76	100.70	106.62
2	A	301	G1R	O1B-PB-O2B	2.74	125.19	112.44
3	B	302	G2R	O4'-C1'-C2'	-2.59	101.06	106.62
2	B	301	G1R	O6-C6-C5	-2.59	119.69	126.53
2	A	302	G1R	C4'-O4'-C1'	-2.52	103.90	109.47
2	A	302	G1R	C2-N1-C6	-2.46	120.65	125.11
2	A	301	G1R	O6-C6-C5	-2.44	120.10	126.53
2	B	301	G1R	C2-N3-C4	2.43	116.48	112.30
3	B	302	G2R	O6-C6-C5	-2.31	120.44	126.53
3	B	302	G2R	C5-C6-N1	2.28	119.05	113.25
2	B	301	G1R	N9-C8-N7	-2.23	109.27	113.40
2	A	301	G1R	O2X-C2X-C1X	-2.18	104.09	110.89
2	A	301	G1R	C5'-C4'-C3'	-2.17	107.39	115.21
2	B	301	G1R	C2-N1-C6	-2.17	121.18	125.11
2	A	301	G1R	O3A-PB-O2B	-2.16	104.20	110.70
2	B	301	G1R	C4'-O4'-C1'	-2.13	104.77	109.47
2	A	301	G1R	O5X-C5X-C4X	2.11	116.18	108.99
2	A	301	G1R	C5-C6-N1	2.11	118.62	113.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	G1R	C3'
2	A	301	G1R	C1'

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	G1R	C5'-O5'-PA-O1A
2	A	301	G1R	C5'-O5'-PA-O2A
2	A	301	G1R	C5'-O5'-PA-O3A
2	A	302	G1R	C3'-C4'-C5'-O5'
2	A	302	G1R	C4'-C5'-O5'-PA
2	A	302	G1R	C5X-O5X-PB-O3A
2	B	301	G1R	C5'-O5'-PA-O1A
2	B	301	G1R	C5'-O5'-PA-O2A
2	B	301	G1R	C5'-O5'-PA-O3A
2	B	301	G1R	PB-O3A-PA-O5'
2	B	301	G1R	C5X-O5X-PB-O3A
2	A	302	G1R	O4'-C4'-C5'-O5'
2	B	301	G1R	C4X-C5X-O5X-PB
2	A	301	G1R	C3'-C4'-C5'-O5'
2	A	301	G1R	O4'-C4'-C5'-O5'
2	A	301	G1R	C4'-C5'-O5'-PA
2	A	302	G1R	PB-O3A-PA-O5'
2	A	302	G1R	PA-O3A-PB-O5X
3	B	302	G2R	PB-O3A-PA-O5'
2	A	302	G1R	C5X-O5X-PB-O2B
2	B	301	G1R	C5X-O5X-PB-O2B
2	A	301	G1R	C4X-C5X-O5X-PB
3	B	302	G2R	C4X-C5X-O5X-PB
3	B	302	G2R	C3X-C4X-C5X-O5X
2	A	301	G1R	C3X-C4X-C5X-O5X
3	B	302	G2R	O4X-C4X-C5X-O5X
2	B	301	G1R	C2'-C1'-N9-C8
3	B	302	G2R	PA-O3A-PB-O1B
2	B	301	G1R	C2'-C1'-N9-C4
2	A	302	G1R	PA-O3A-PB-O1B

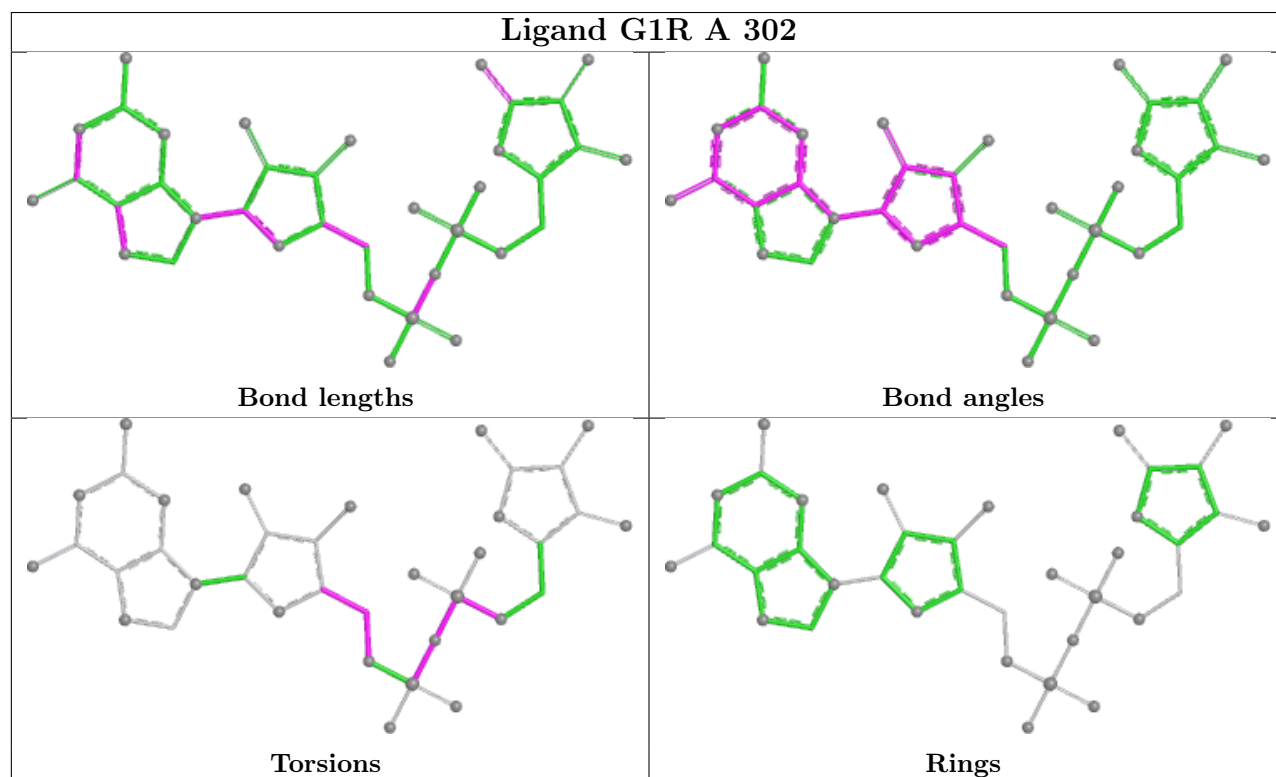
There are no ring outliers.

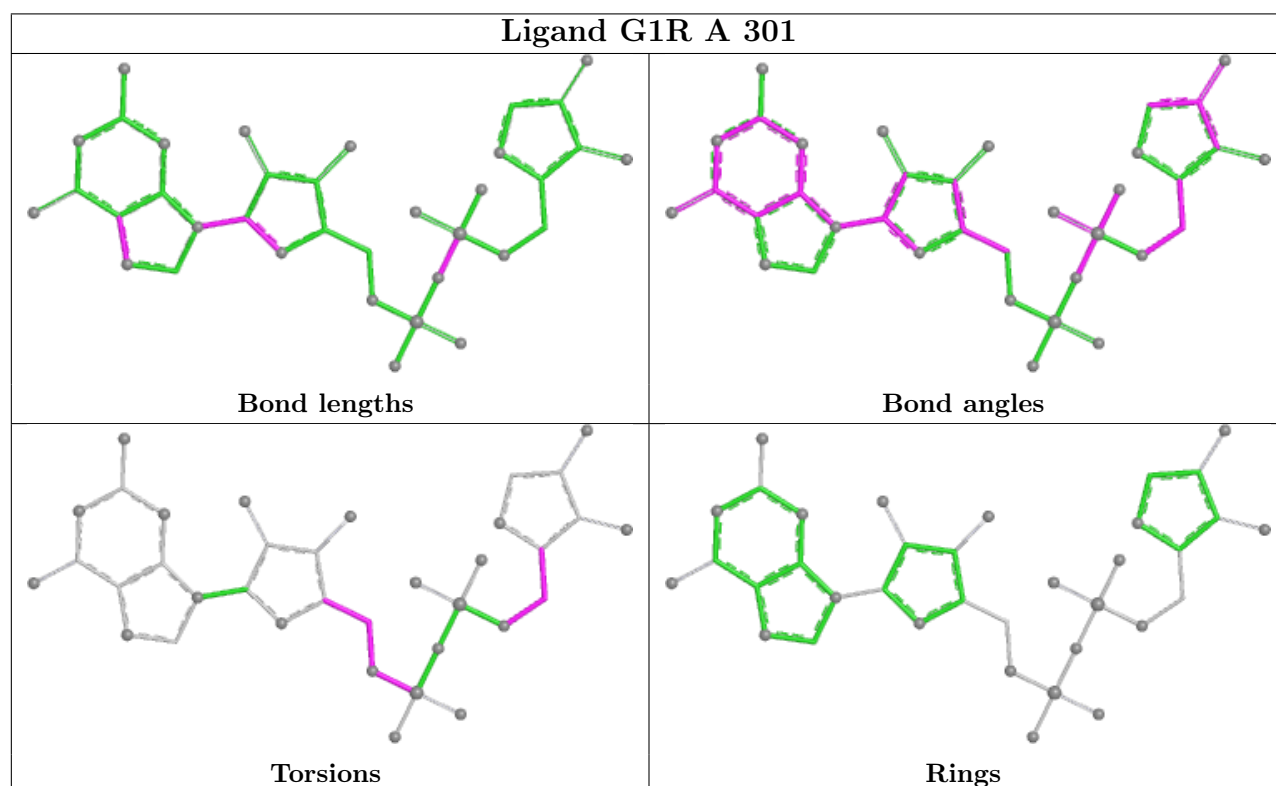
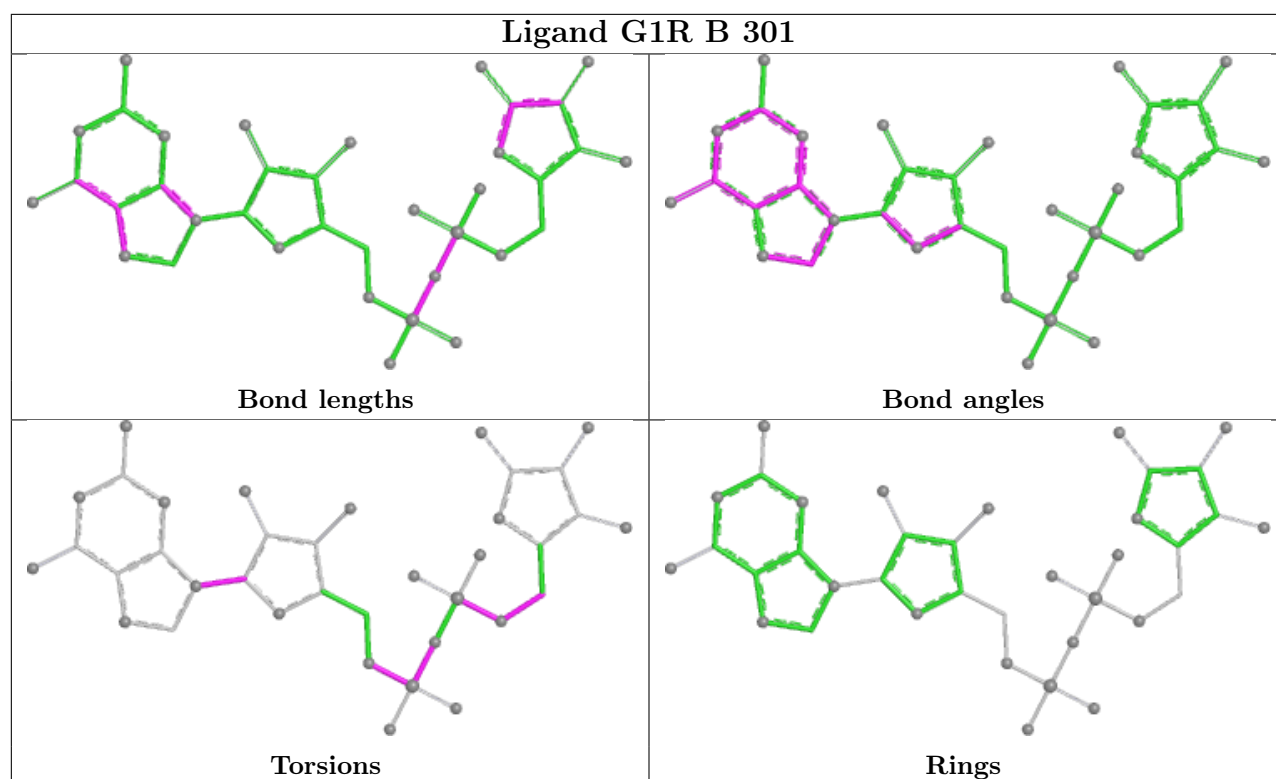
4 monomers are involved in 27 short contacts:

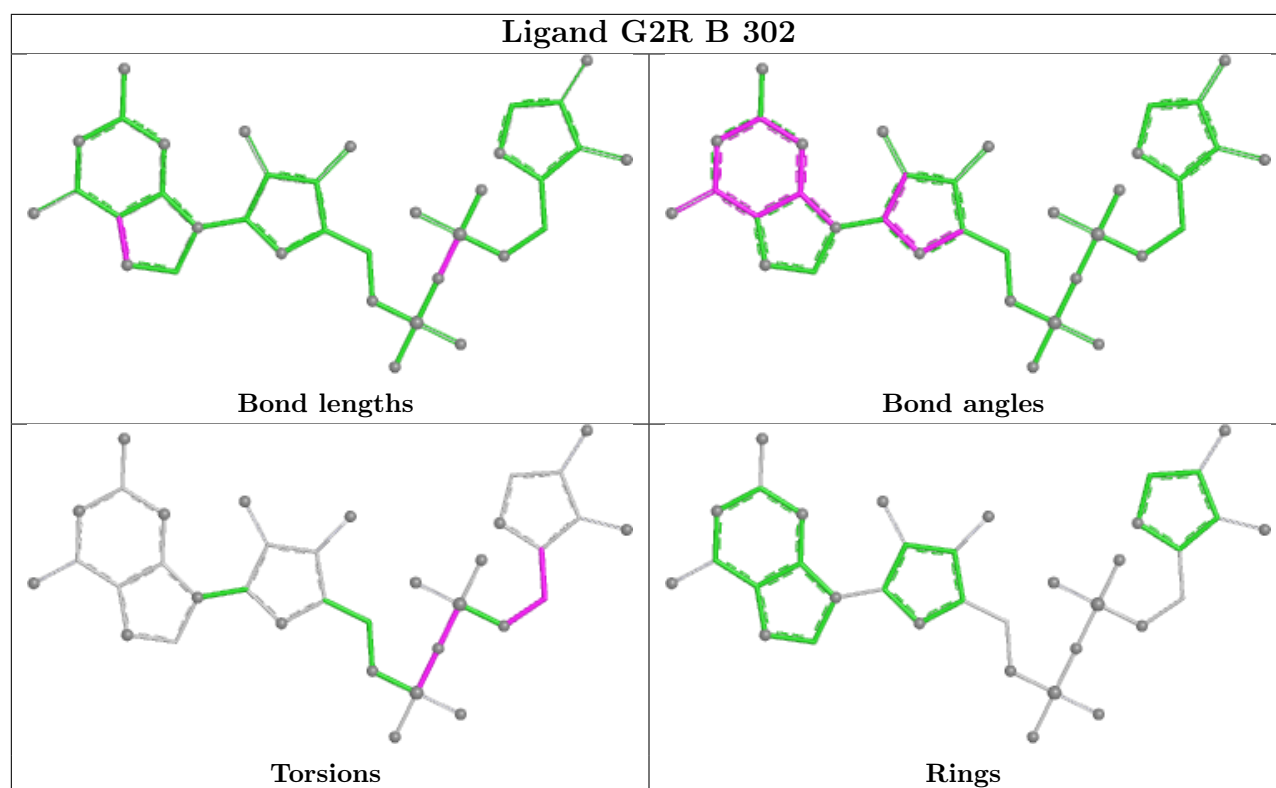
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	G1R	13	0
2	B	301	G1R	11	0
2	A	301	G1R	4	0
3	B	302	G2R	6	0

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	252/262 (96%)	1.53	59 (23%) 2 2	30, 37, 53, 62	0
1	B	252/262 (96%)	1.48	55 (21%) 2 2	29, 38, 55, 63	0
All	All	504/524 (96%)	1.51	114 (22%) 2 2	29, 37, 53, 63	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	PRO	6.0
1	A	293	ASP	5.4
1	B	287	CYS	5.2
1	B	249	ASP	5.0
1	A	247	ARG	5.0
1	B	246	GLY	4.9
1	A	143	PHE	4.6
1	A	294	SER	4.6
1	A	65	ALA	4.5
1	A	164	ASP	4.4
1	A	249	ASP	4.4
1	A	248	GLU	4.1
1	B	248	GLU	4.1
1	A	176	TRP	3.8
1	B	294	SER	3.8
1	A	79	HIS	3.7
1	B	176	TRP	3.7
1	B	254	CYS	3.7
1	A	82	CYS	3.6
1	A	296	CYS	3.4
1	B	264	SER	3.4
1	B	213	SER	3.3
1	A	81	ASP	3.3
1	A	84	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLU	3.3
1	B	141	ASP	3.2
1	A	212	ARG	3.2
1	A	180	CYS	3.1
1	B	295	SER	3.1
1	B	164	ASP	3.1
1	B	219	ASP	3.1
1	A	165	THR	3.0
1	B	210	GLY	3.0
1	B	245	GLY	3.0
1	B	236	GLN	2.9
1	A	47	ARG	2.9
1	A	193	SER	2.9
1	A	245	GLY	2.8
1	A	266	ILE	2.8
1	A	46	TRP	2.8
1	B	286	GLN	2.8
1	A	61	GLU	2.8
1	A	116	THR	2.8
1	A	227	VAL	2.8
1	A	246	GLY	2.8
1	B	296	CYS	2.7
1	B	250	SER	2.7
1	A	80	VAL	2.7
1	B	138	VAL	2.7
1	A	250	SER	2.7
1	B	275	CYS	2.7
1	B	290	ASN	2.6
1	B	80	VAL	2.6
1	B	227	VAL	2.6
1	B	259	ILE	2.6
1	B	271	ILE	2.6
1	A	235	VAL	2.6
1	B	165	THR	2.5
1	B	224	SER	2.5
1	A	225	VAL	2.5
1	B	242	VAL	2.5
1	B	116	THR	2.5
1	A	280	ARG	2.5
1	A	213	SER	2.5
1	B	212	ARG	2.5
1	B	272	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	216	PHE	2.4
1	B	233	GLU	2.4
1	B	54	GLY	2.4
1	A	203	VAL	2.4
1	A	86	TRP	2.4
1	A	189	TRP	2.4
1	A	51	SER	2.4
1	A	295	SER	2.4
1	A	138	VAL	2.4
1	A	283	LYS	2.4
1	A	290	ASN	2.3
1	B	163	PHE	2.3
1	A	291	PRO	2.3
1	A	125	TRP	2.3
1	A	204	VAL	2.3
1	B	225	VAL	2.3
1	A	69	LYS	2.3
1	A	111	LYS	2.3
1	A	195	ARG	2.3
1	B	268	LYS	2.3
1	A	73	ILE	2.3
1	A	75	PRO	2.2
1	A	244	HIS	2.2
1	A	48	GLN	2.2
1	B	185	VAL	2.2
1	B	50	TRP	2.2
1	B	95	SER	2.2
1	B	201	CYS	2.2
1	A	107	GLN	2.2
1	B	293	ASP	2.2
1	B	262	LEU	2.2
1	B	203	VAL	2.1
1	B	292	GLU	2.1
1	B	104	GLU	2.1
1	A	128	ILE	2.1
1	A	67	CYS	2.1
1	B	82	CYS	2.1
1	B	180	CYS	2.1
1	A	72	GLU	2.1
1	A	192	VAL	2.1
1	A	206	VAL	2.1
1	B	231	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	TYR	2.1
1	B	73	ILE	2.1
1	A	185	VAL	2.0
1	B	267	SER	2.0
1	B	288	VAL	2.0
1	B	189	TRP	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](#)

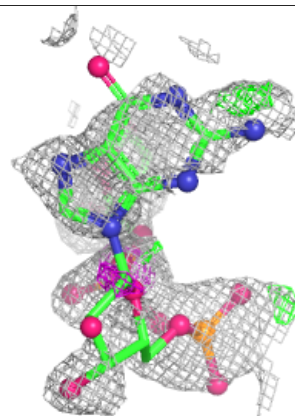
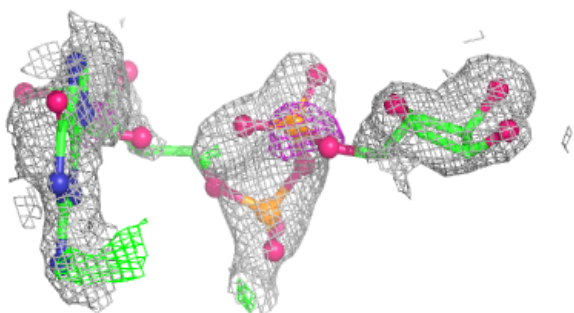
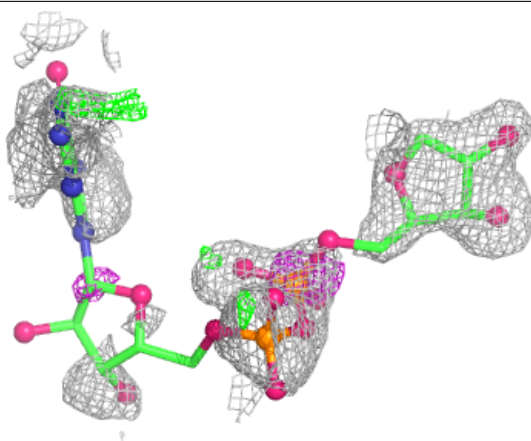
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	G2R	B	302	36/36	0.76	0.18	43,79,86,86	0
2	G1R	A	302	37/37	0.79	0.17	29,53,77,77	0
2	G1R	B	301	37/37	0.81	0.17	30,49,84,85	0
2	G1R	A	301	36/37	0.82	0.17	25,62,81,82	0

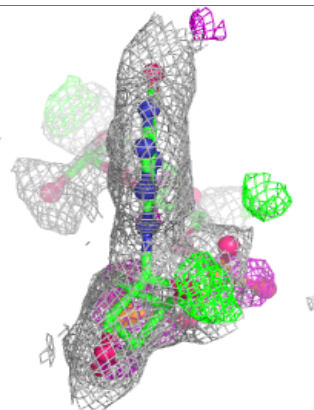
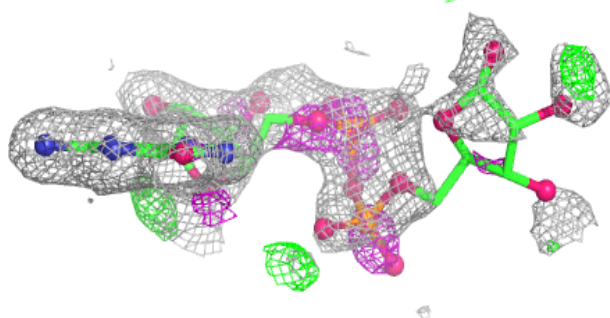
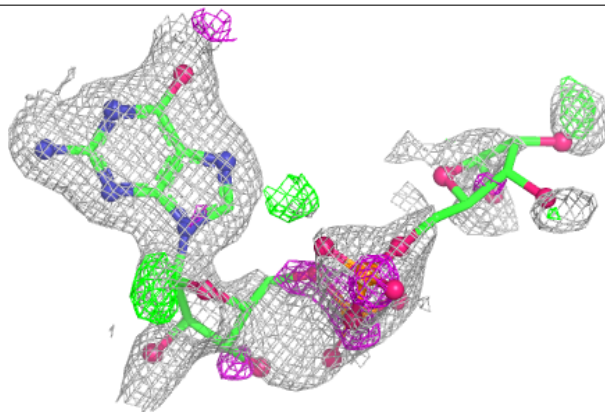
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G2R B 302:

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

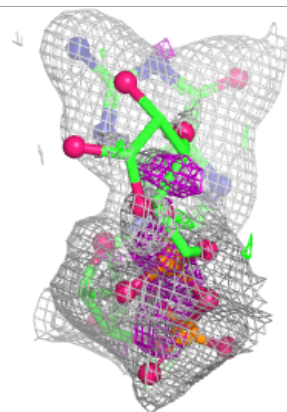
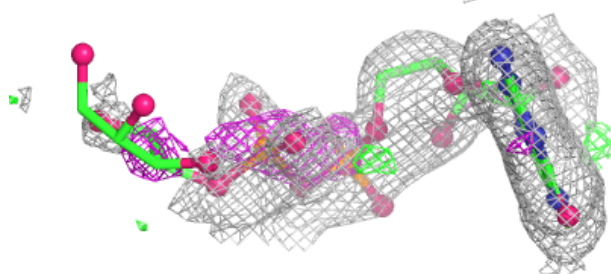
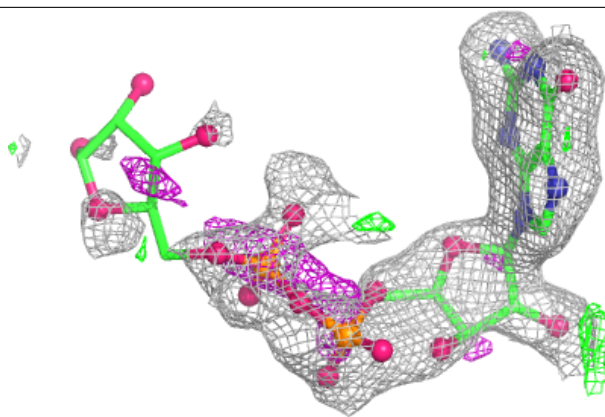
**Electron density around G1R A 302:**

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

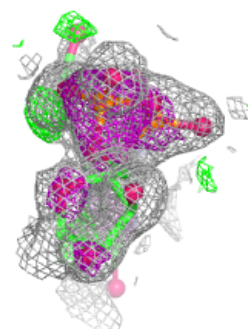
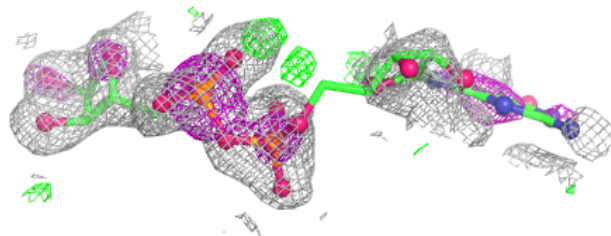
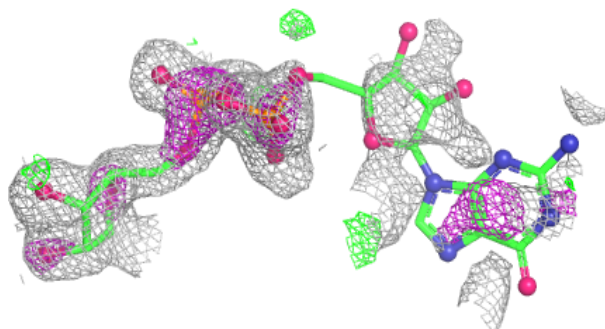


Electron density around G1R B 301:

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

**Electron density around G1R A 301:**

$2mF_o-DF_c$ (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.