



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2025 – 01:06 pm BST

PDB ID : 9QYG / pdb_00009qyg
Title : PARP9 Macro Domain 2 Free form
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Deposited on : 2025-04-17
Resolution : 2.70 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

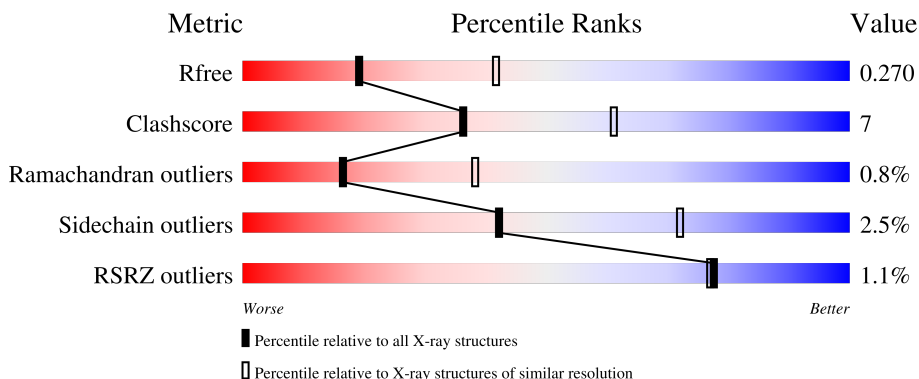
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	197	 70% 20% 11%
1	B	197	 77% 16% .. 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2941 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.

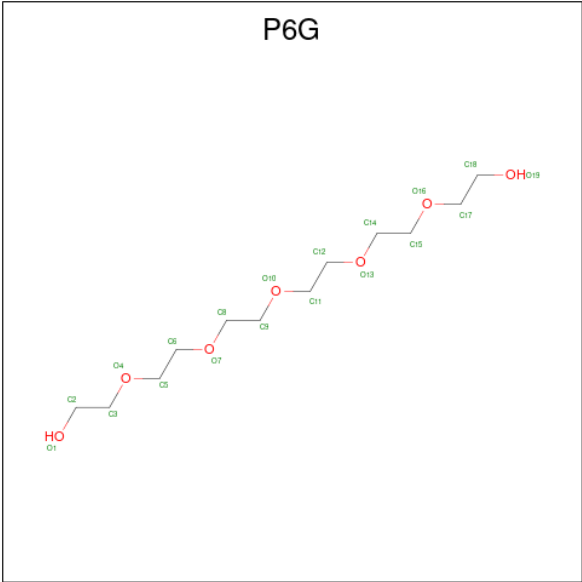
- Molecule 1 is a protein called Protein mono-ADP-ribosyltransferase PARP9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1400	907	231	253	9			
1	B	186	Total	C	N	O	S	0	0	0
			1479	959	243	268	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	GLY	-	expression tag	UNP Q8IXQ6
A	302	ALA	-	expression tag	UNP Q8IXQ6
A	303	MET	-	expression tag	UNP Q8IXQ6
A	304	ALA	-	expression tag	UNP Q8IXQ6
B	301	GLY	-	expression tag	UNP Q8IXQ6
B	302	ALA	-	expression tag	UNP Q8IXQ6
B	303	MET	-	expression tag	UNP Q8IXQ6
B	304	ALA	-	expression tag	UNP Q8IXQ6

- Molecule 2 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	12	7		
2	A	1	Total	C	O	0	0
			19	12	7		
2	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.48Å 73.29Å 58.07Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	43.65 – 2.70 43.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.65-2.70) 94.1 (43.65-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.183 , 0.264 0.198 , 0.270	Depositor DCC
R_{free} test set	942 reflections (9.25%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2941	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P6G

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	0.60	0/1428	1.13	3/1928 (0.2%)
1	B	0.63	0/1509	1.14	3/2039 (0.1%)
All	All	0.62	0/2937	1.13	6/3967 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	PRO	N-CA-C	-7.11	97.82	112.47
1	B	309	PHE	CA-CB-CG	6.39	120.19	113.80
1	B	438	LYS	CB-CA-C	6.02	118.88	109.84
1	A	344	THR	CA-CB-OG1	-5.29	101.67	109.60
1	B	448	ASP	CB-CA-C	5.07	119.47	110.85
1	A	384	PHE	CB-CA-C	5.06	120.49	110.42

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	1400	0	1436	25	2
1	B	1479	0	1509	21	2
2	A	38	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	19	0	26	3	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
All	All	2941	0	3023	42	2

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 7.

All (42) 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:402:LYS:HG2	1:A:435:MET:HE3	1.70	0.73
1:A:330:THR:HG21	1:B:331:ALA:C	2.15	0.72
1:B:487:SER:HB2	1:B:492:LEU:HD22	1.78	0.66
1:A:359:GLU:CD	1:A:359:GLU:H	2.06	0.64
1:B:359:GLU:H	1:B:359:GLU:CD	2.07	0.63
1:A:331:ALA:C	1:B:330:THR:HG21	2.23	0.62
1:A:439:LYS:HE2	1:A:474:GLU:HB3	1.81	0.61
2:B:501:P6G:O16	2:B:501:P6G:H22	2.00	0.60
1:A:406:LEU:HD11	1:A:446:LEU:HD11	1.84	0.59
1:B:406:LEU:HD11	1:B:446:LEU:HD11	1.85	0.58
1:A:448:ASP:OD1	1:A:486:ARG:NH2	2.35	0.58
1:A:313:VAL:HG23	1:B:313:VAL:HG23	1.86	0.56
1:A:451:LEU:HD12	1:A:486:ARG:HH11	1.71	0.55
1:A:316:ASN:OD1	1:A:461:GLN:HG3	2.10	0.52
1:A:318:THR:HG21	1:B:318:THR:HG21	1.92	0.51
1:B:485:LYS:HA	1:B:488:LYS:HD2	1.93	0.51
1:B:387:PHE:CZ	2:B:501:P6G:H82	2.48	0.49
1:B:370:LYS:O	1:B:371:GLN:HB2	2.12	0.49
1:A:312:MET:HE2	1:A:319:LEU:HD23	1.94	0.48
1:B:420:GLN:HB2	1:B:422:ILE:HG12	1.95	0.48
1:A:402:LYS:HD2	1:A:435:MET:HB3	1.95	0.47
1:B:387:PHE:CE1	2:B:501:P6G:H82	2.50	0.47
1:B:312:MET:SD	1:B:492:LEU:HD11	2.56	0.46
1:B:332:ASP:HB2	1:B:424:SER:O	2.16	0.46
1:A:451:LEU:HD12	1:A:486:ARG:NH1	2.30	0.45
1:B:323:GLN:HG2	1:B:476:TYR:CD1	2.51	0.45
1:B:379:LEU:C	1:B:379:LEU:HD23	2.41	0.45
1:A:379:LEU:HD23	1:A:379:LEU:C	2.41	0.45
1:A:320:GLN:NE2	1:A:465:LYS:HE2	2.32	0.45
1:B:487:SER:HA	1:B:492:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LYS:N	1:A:403:PRO:CD	2.80	0.44
1:B:402:LYS:N	1:B:403:PRO:CD	2.81	0.44
1:A:435:MET:O	1:A:436:GLU:HB3	2.18	0.43
1:A:469:PHE:HA	1:A:470:PRO:HD3	1.85	0.43
1:A:325:HIS:HB3	1:A:327:GLU:OE1	2.20	0.42
1:B:325:HIS:HB3	1:B:327:GLU:OE1	2.20	0.42
1:A:330:THR:HG21	1:B:331:ALA:CA	2.50	0.41
1:A:332:ASP:HB2	1:A:424:SER:O	2.21	0.41
1:A:359:GLU:CD	1:A:359:GLU:N	2.76	0.41
1:A:337:SER:OG	1:A:396:TRP:NE1	2.48	0.41
1:A:402:LYS:HG2	1:A:435:MET:CE	2.47	0.40
1:B:359:GLU:CD	1:B:359:GLU:N	2.77	0.40

All (2) 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:A:441:THR:CG2	1:B:489:MET:CE[2_545]	2.05	0.15
1:A:434:ASN:OD1	1:B:419:GLU:OE2[2_645]	2.17	0.03

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	172/197 (87%)	164 (95%)	8 (5%)	0	100	100
1	B	182/197 (92%)	172 (94%)	7 (4%)	3 (2%)	8	21
All	All	354/394 (90%)	336 (95%)	15 (4%)	3 (1%)	16	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	B	492	LEU
1	B	433	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	157/175 (90%)	154 (98%)	3 (2%)	52	79
1	B	166/175 (95%)	161 (97%)	5 (3%)	36	65
All	All	323/350 (92%)	315 (98%)	8 (2%)	42	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	ILE
1	A	472	ASP
1	A	473	LEU
1	B	418	ILE
1	B	473	LEU
1	B	489	MET
1	B	491	SER
1	B	492	LEU

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	329	GLN
1	A	397	HIS
1	B	329	GLN
1	B	397	HIS

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 ⓘ

3 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	P6G	A	501	-	18,18,18	0.41	0	17,17,17	0.26	0
2	P6G	A	502	-	18,18,18	0.34	0	17,17,17	0.24	0
2	P6G	B	501	-	18,18,18	0.21	0	17,17,17	0.23	0

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	P6G	A	501	-	-	10/16/16/16	-
2	P6G	A	502	-	-	9/16/16/16	-
2	P6G	B	501	-	-	9/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	P6G	O7-C8-C9-O10
2	B	501	P6G	O10-C11-C12-O13
2	A	502	P6G	O13-C14-C15-O16
2	B	501	P6G	O13-C14-C15-O16
2	A	501	P6G	O10-C11-C12-O13
2	A	501	P6G	O4-C5-C6-O7
2	B	501	P6G	O16-C17-C18-O19
2	A	502	P6G	O4-C5-C6-O7
2	A	501	P6G	O7-C8-C9-O10
2	A	502	P6G	O16-C17-C18-O19
2	A	501	P6G	O1-C2-C3-O4
2	A	501	P6G	O16-C17-C18-O19
2	A	502	P6G	O10-C11-C12-O13
2	A	501	P6G	C11-C12-O13-C14
2	B	501	P6G	O1-C2-C3-O4
2	B	501	P6G	C14-C15-O16-C17
2	A	501	P6G	C8-C9-O10-C11
2	B	501	P6G	C9-C8-O7-C6
2	B	501	P6G	C11-C12-O13-C14
2	B	501	P6G	C2-C3-O4-C5
2	A	502	P6G	C12-C11-O10-C9
2	A	502	P6G	C11-C12-O13-C14
2	A	501	P6G	C6-C5-O4-C3
2	B	501	P6G	C5-C6-O7-C8
2	A	502	P6G	C2-C3-O4-C5
2	A	501	P6G	O13-C14-C15-O16
2	A	501	P6G	C18-C17-O16-C15
2	A	502	P6G	C8-C9-O10-C11

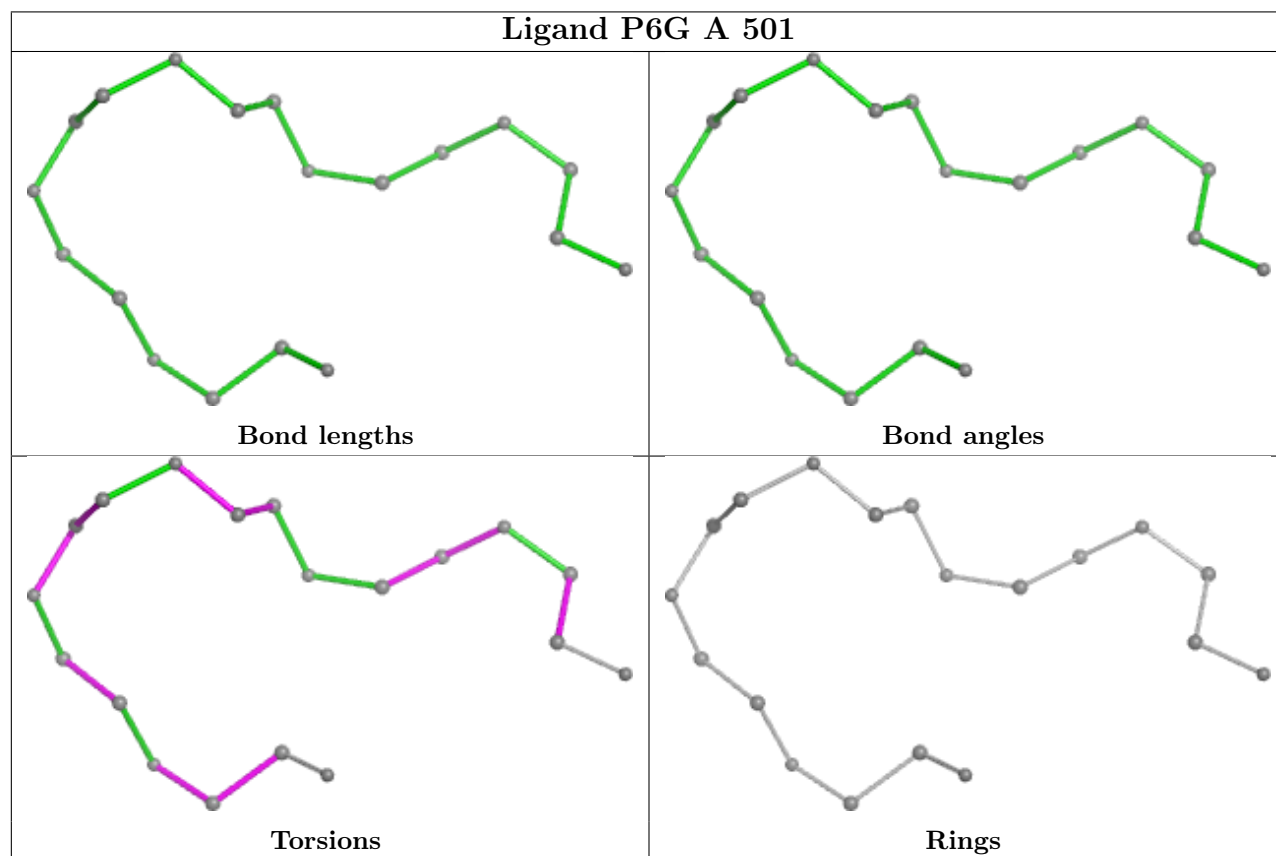
There are no ring outliers.

1 monomer is involved in 3 short contacts:

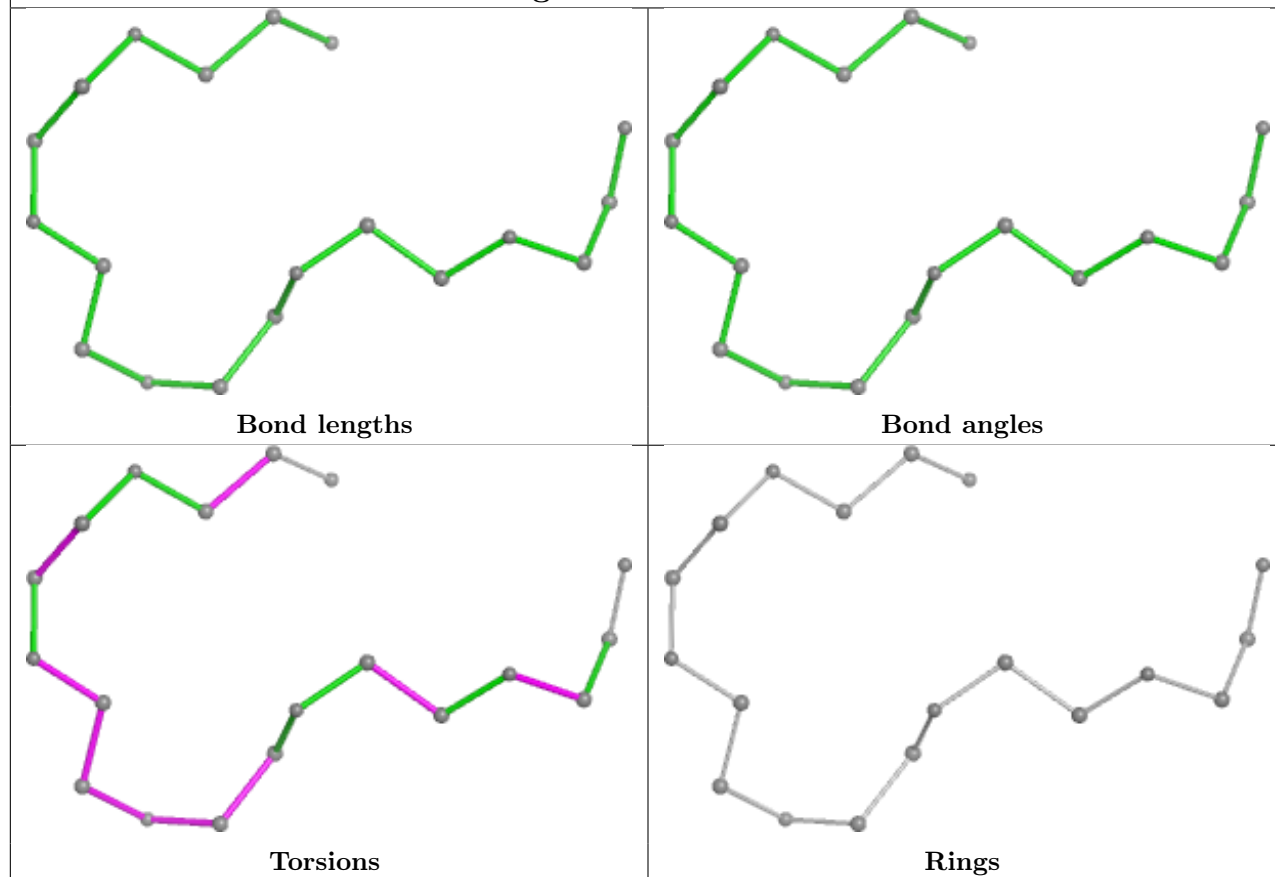
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	P6G	3	0

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

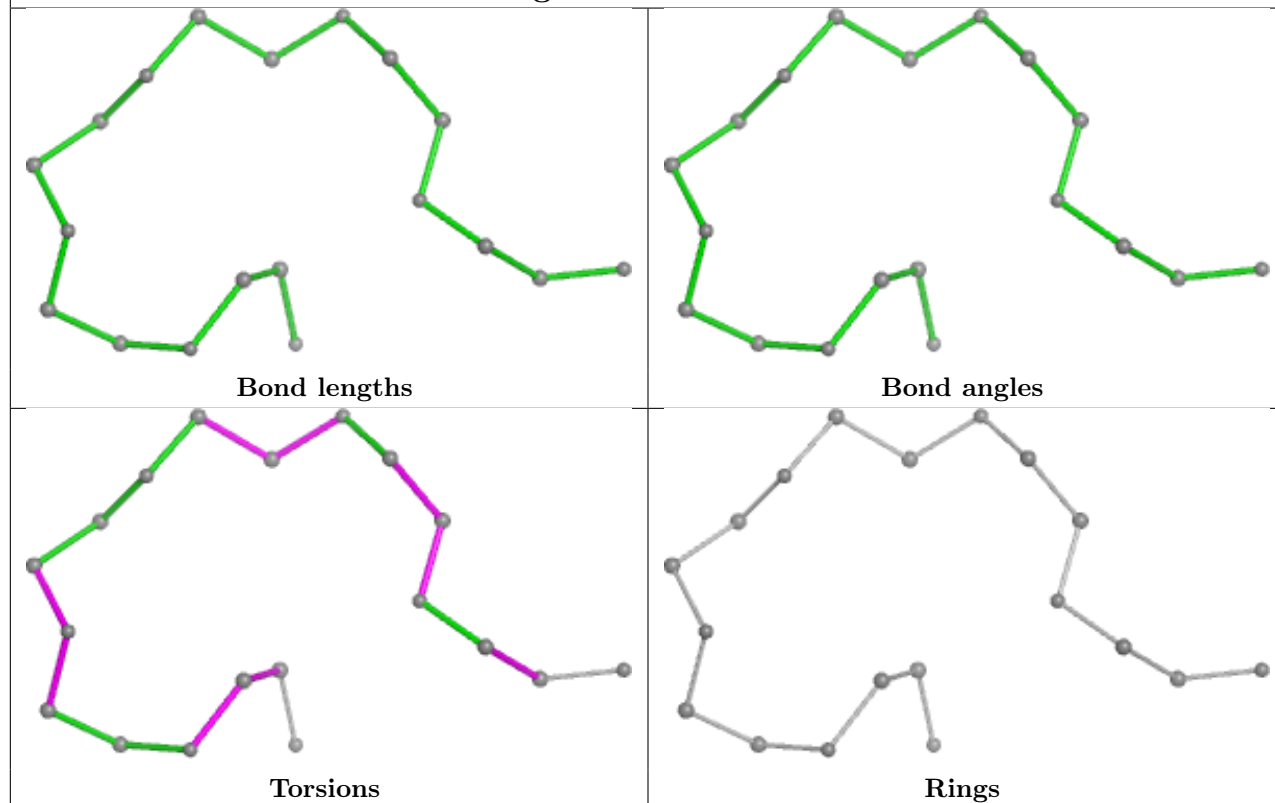
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand P6G A 502



Ligand P6G B 501



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	176/197 (89%)	-0.20	2 (1%) 77 77	40, 61, 93, 136	0
1	B	186/197 (94%)	-0.16	2 (1%) 77 77	41, 63, 108, 125	0
All	All	362/394 (91%)	-0.18	4 (1%) 77 77	40, 62, 103, 136	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ASN	3.0
1	B	309	PHE	2.9
1	B	433	GLY	2.5
1	A	473	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	P6G	A	502	19/19	0.85	0.13	61,69,76,80	0

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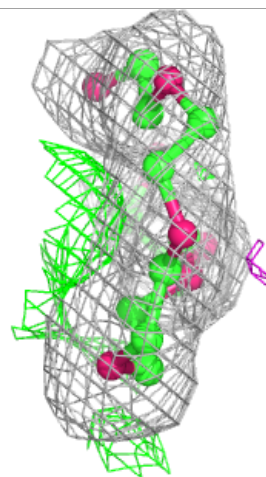
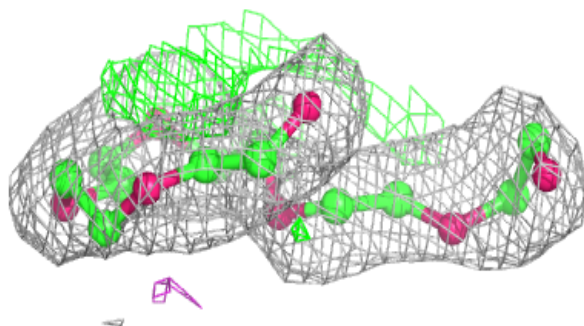
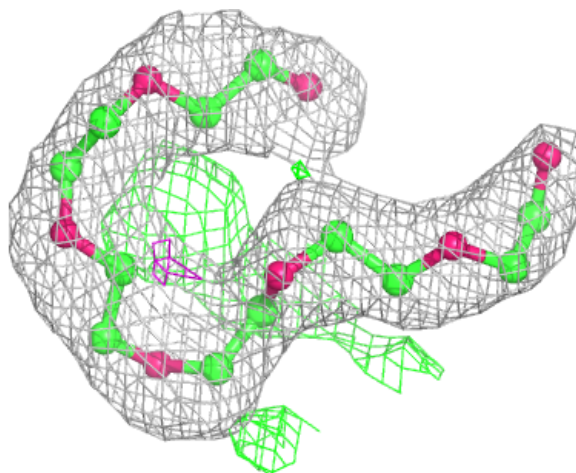
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	P6G	B	501	19/19	0.85	0.11	69,76,90,99	0
2	P6G	A	501	19/19	0.87	0.12	66,78,81,82	0

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.

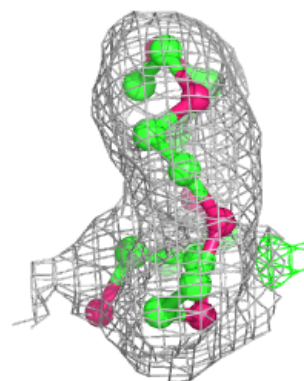
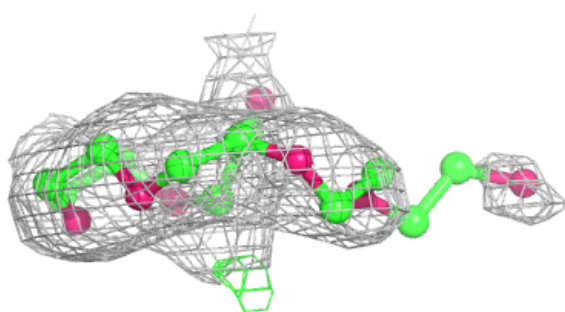
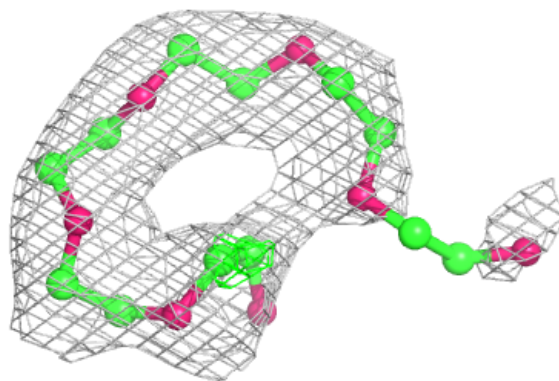
Electron density around P6G A 502:

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

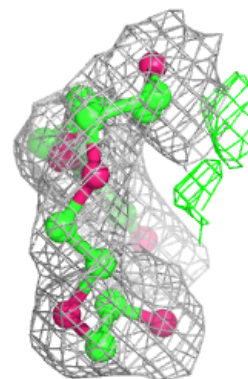
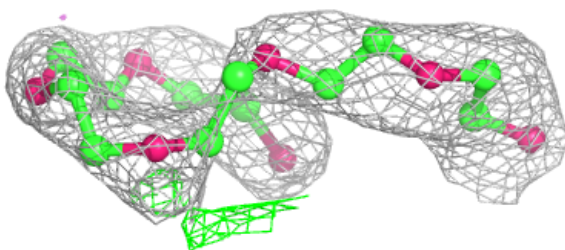
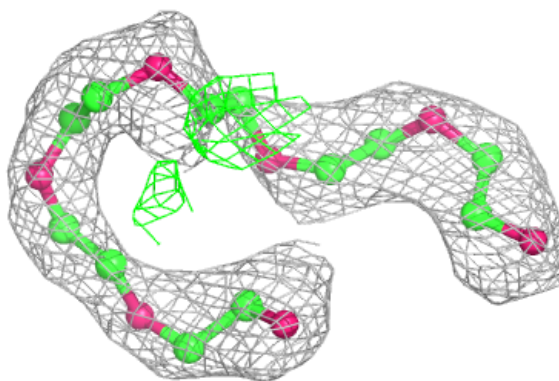


Electron density around P6G B 501:

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

**Electron density around P6G A 501:**

$2mF_o-DF_c$ (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.