



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 09:28 pm GMT

PDB ID : 7NYM
Title : Mutant V517A - SH3 domain of JNK-interacting Protein 1 (JIP1)
Authors : Perez, L.M.; Ielasi, F.S.; Palencia, A.; Jensen, M.R.
Deposited on : 2021-03-23
Resolution : 1.61 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 : 4.02b-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

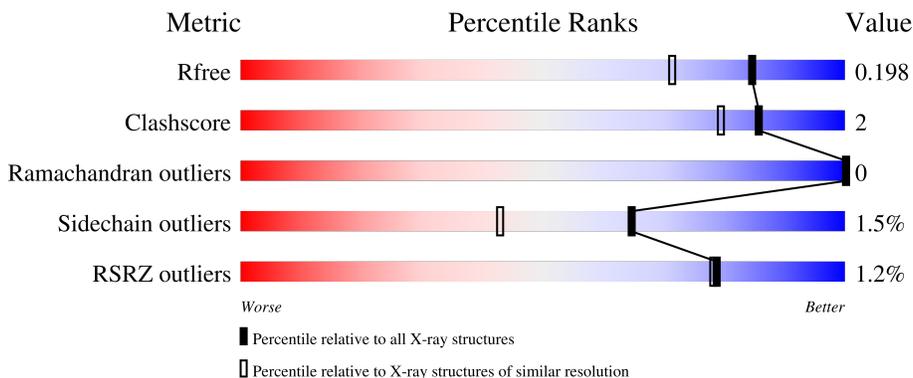
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	AAA	63	 2% 86% 6% 8%
1	BBB	63	 2% 92% 5% ..
1	CCC	63	 2% 81% 13% 6%
1	DDD	63	 95% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2350 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.

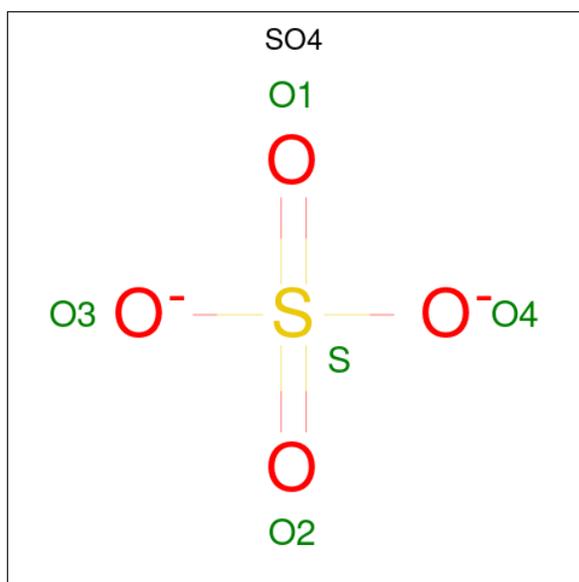
- Molecule 1 is a protein called SH3 domain of JNK-interacting Protein 1 (JIP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	58	Total 497	C 319	N 84	O 93	S 1	0	1	0
1	BBB	62	Total 525	C 336	N 87	O 99	S 3	0	1	0
1	CCC	59	Total 504	C 323	N 82	O 98	S 1	0	1	0
1	DDD	62	Total 529	C 340	N 87	O 100	S 2	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

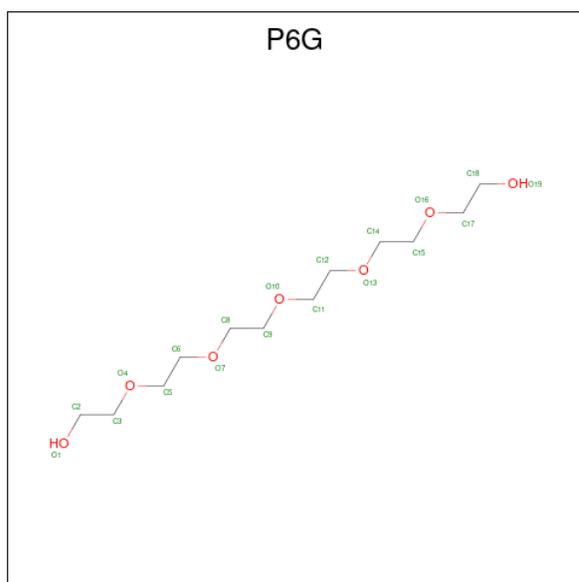
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	487	GLY	-	expression tag	UNP Q9UQF2
AAA	488	HIS	-	expression tag	UNP Q9UQF2
AAA	489	MET	-	expression tag	UNP Q9UQF2
AAA	517	ALA	VAL	engineered mutation	UNP Q9UQF2
BBB	-2	GLY	-	expression tag	UNP Q9UQF2
BBB	-1	HIS	-	expression tag	UNP Q9UQF2
BBB	0	MET	-	expression tag	UNP Q9UQF2
BBB	28	ALA	VAL	engineered mutation	UNP Q9UQF2
CCC	487	GLY	-	expression tag	UNP Q9UQF2
CCC	488	HIS	-	expression tag	UNP Q9UQF2
CCC	489	MET	-	expression tag	UNP Q9UQF2
CCC	517	ALA	VAL	engineered mutation	UNP Q9UQF2
DDD	-2	GLY	-	expression tag	UNP Q9UQF2
DDD	-1	HIS	-	expression tag	UNP Q9UQF2
DDD	0	MET	-	expression tag	UNP Q9UQF2
DDD	517	ALA	VAL	engineered mutation	UNP Q9UQF2

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	DDD	1	Total O S 5 4 1	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



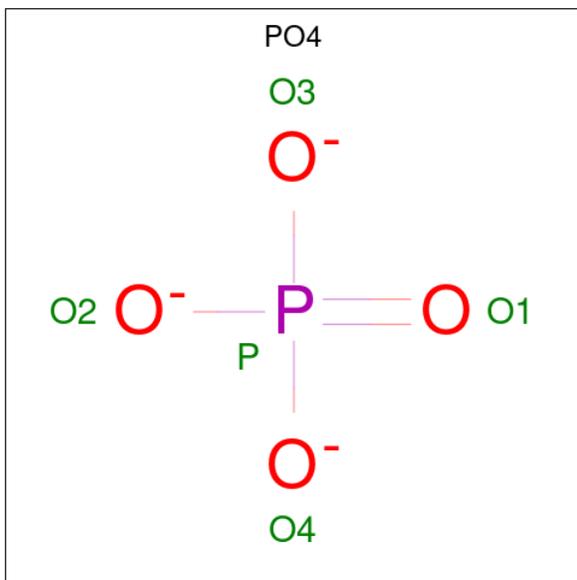
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 19 12 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			19	12	7		
3	CCC	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	47	Total	O	0	0
			47	47		
5	BBB	63	Total	O	0	0
			63	63		
5	CCC	56	Total	O	0	0
			56	56		
5	DDD	52	Total	O	0	0
			52	52		

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.

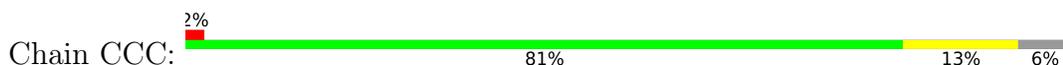
- Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)



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- Molecule 1: SH3 domain of JNK-interacting Protein 1 (JIP1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.12Å 84.25Å 98.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.98 – 1.61 63.98 – 1.61	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.98-1.61) 100.0 (63.98-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.62Å)	Xtrriage
Refinement program	REFMAC 7.0.078	Depositor
R, R_{free}	0.131 , 0.198 0.132 , 0.198	Depositor DCC
R_{free} test set	1815 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2350	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 31.17 % 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 1.1578e-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: SO4, PO4, 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	AAA	0.82	0/514	0.90	0/699
1	BBB	0.99	3/543 (0.6%)	0.87	1/737 (0.1%)
1	CCC	0.88	1/521 (0.2%)	0.96	2/709 (0.3%)
1	DDD	0.83	1/548 (0.2%)	0.92	0/745
All	All	0.88	5/2126 (0.2%)	0.91	3/2890 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	547	VAL	C-N	10.11	1.57	1.34
1	BBB	0[A]	MET	C-N	9.17	1.55	1.34
1	BBB	0[B]	MET	C-N	9.17	1.55	1.34
1	DDD	0	MET	C-N	8.92	1.54	1.34
1	BBB	58	VAL	C-N	8.14	1.52	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	CCC	547	VAL	O-C-N	-7.99	109.91	122.70
1	BBB	9	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	CCC	494	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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	AAA	497	0	464	3	0
1	BBB	525	0	488	0	0
1	CCC	504	0	463	4	0
1	DDD	529	0	488	0	0
2	AAA	5	0	0	0	0
2	BBB	5	0	0	0	0
2	DDD	5	0	0	0	0
3	BBB	38	0	52	2	0
3	CCC	19	0	26	0	0
4	BBB	5	0	0	0	0
5	AAA	47	0	0	0	0
5	BBB	63	0	0	1	0
5	CCC	56	0	0	1	0
5	DDD	52	0	0	0	0
All	All	2350	0	1981	9	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 2.

All (9) 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:AAA:547:VAL:O	1:AAA:548:THR:HG23	1.82	0.79
1:AAA:547:VAL:O	1:AAA:548:THR:CG2	2.42	0.67
1:CCC:490:GLU:O	1:CCC:516:LEU:CD2	2.57	0.51
1:CCC:498:ARG:CZ	1:CCC:510[A]:GLU:OE2	2.58	0.51
3:BBB:102:P6G:H62	5:BBB:208:HOH:O	2.13	0.48
3:BBB:102:P6G:H122	5:CCC:740:HOH:O	2.16	0.45
1:CCC:526:TYR:O	1:CCC:538:VAL:HA	2.19	0.42
1:AAA:491:GLN:HA	1:AAA:516:LEU:HD23	2.02	0.41
1:CCC:490:GLU:O	1:CCC:516:LEU:HD22	2.21	0.41

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	AAA	57/63 (90%)	55 (96%)	2 (4%)	0	100	100
1	BBB	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
1	CCC	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
1	DDD	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
All	All	237/252 (94%)	231 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	50/53 (94%)	50 (100%)	0	100	100
1	BBB	53/53 (100%)	50 (94%)	3 (6%)	20	4
1	CCC	51/53 (96%)	51 (100%)	0	100	100
1	DDD	53/53 (100%)	52 (98%)	1 (2%)	57	32
All	All	207/212 (98%)	203 (98%)	4 (2%)	65	32

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	0[A]	MET
1	BBB	0[B]	MET

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Mol	Chain	Res	Type
1	BBB	23	ASP
1	DDD	512	ASP

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SO4	AAA	601	-	4,4,4	0.34	0	6,6,6	0.06	0
3	P6G	BBB	103	-	18,18,18	0.80	0	17,17,17	0.59	0
4	PO4	BBB	104	-	4,4,4	0.59	0	6,6,6	0.69	0
2	SO4	BBB	101	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	DDD	601	-	4,4,4	0.35	0	6,6,6	0.06	0
3	P6G	CCC	601	-	18,18,18	0.37	0	17,17,17	0.96	1 (5%)
3	P6G	BBB	102	-	18,18,18	0.47	0	17,17,17	0.49	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
3	P6G	BBB	102	-	-	8/16/16/16	-
3	P6G	CCC	601	-	-	6/16/16/16	-
3	P6G	BBB	103	-	-	10/16/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	601	P6G	C8-O7-C6	-2.46	102.61	113.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	103	P6G	C2-C3-O4-C5
3	BBB	103	P6G	O13-C14-C15-O16
3	BBB	103	P6G	O7-C8-C9-O10
3	BBB	102	P6G	O13-C14-C15-O16
3	BBB	103	P6G	O10-C11-C12-O13
3	BBB	102	P6G	O10-C11-C12-O13
3	BBB	103	P6G	O16-C17-C18-O19
3	BBB	102	P6G	O7-C8-C9-O10
3	BBB	102	P6G	O1-C2-C3-O4
3	BBB	102	P6G	O16-C17-C18-O19
3	CCC	601	P6G	O1-C2-C3-O4
3	CCC	601	P6G	C15-C14-O13-C12
3	BBB	102	P6G	C11-C12-O13-C14
3	CCC	601	P6G	O16-C17-C18-O19
3	BBB	103	P6G	C11-C12-O13-C14
3	BBB	102	P6G	C9-C8-O7-C6
3	CCC	601	P6G	C18-C17-O16-C15
3	CCC	601	P6G	C11-C12-O13-C14
3	BBB	102	P6G	O4-C5-C6-O7
3	BBB	103	P6G	C9-C8-O7-C6
3	CCC	601	P6G	C2-C3-O4-C5
3	BBB	103	P6G	C18-C17-O16-C15
3	BBB	103	P6G	C14-C15-O16-C17

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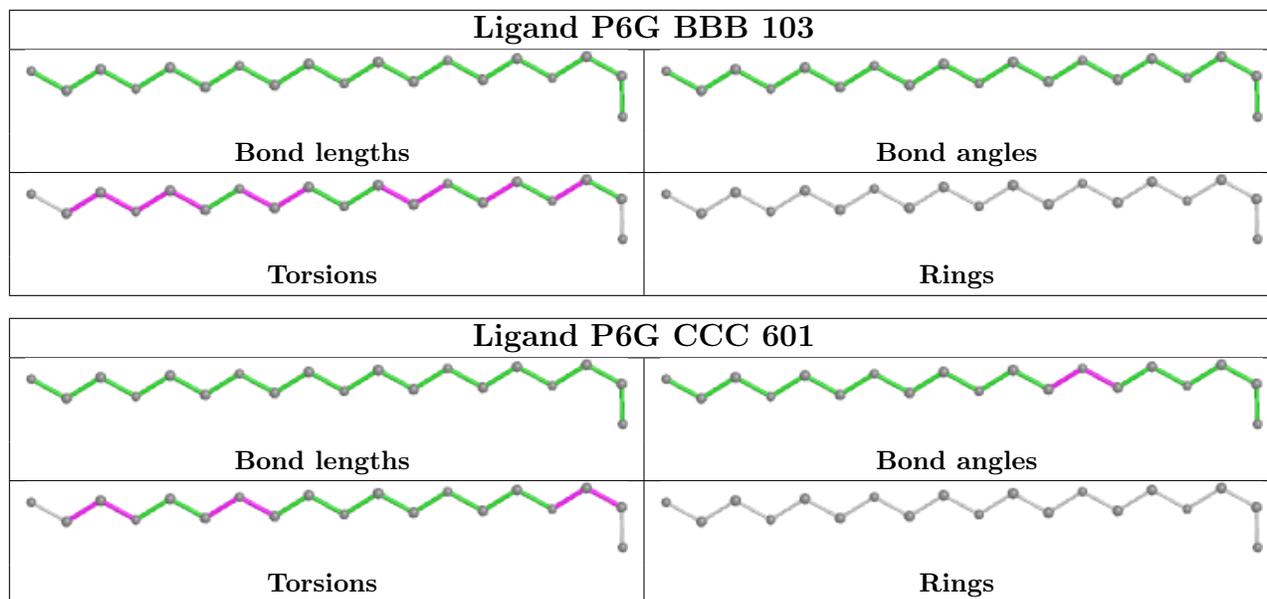
Mol	Chain	Res	Type	Atoms
3	BBB	103	P6G	O4-C5-C6-O7

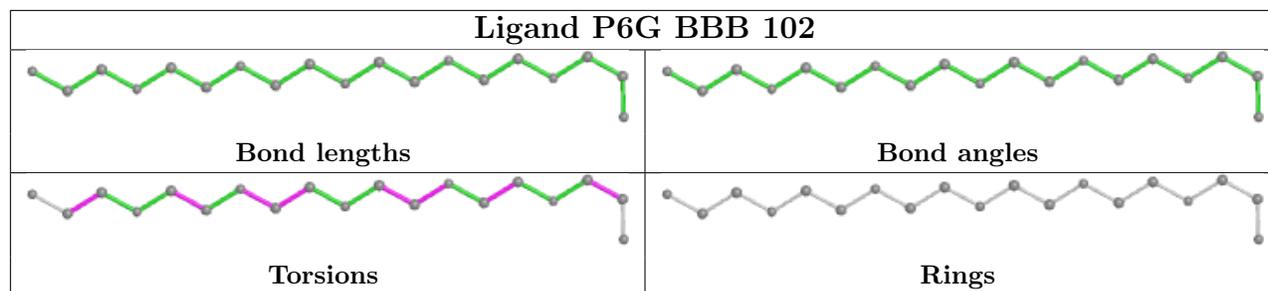
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	102	P6G	2	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 [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	AAA	58/63 (92%)	-0.44	1 (1%) 70 68	14, 18, 31, 69	0
1	BBB	62/63 (98%)	-0.47	1 (1%) 72 71	14, 19, 35, 58	0
1	CCC	59/63 (93%)	-0.48	1 (1%) 70 68	14, 19, 29, 62	0
1	DDD	62/63 (98%)	-0.48	0 100 100	14, 18, 28, 54	0
All	All	241/252 (95%)	-0.47	3 (1%) 79 78	14, 19, 31, 69	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	548	THR	4.7
1	CCC	550	THR	3.1
1	BBB	61	THR	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](#)

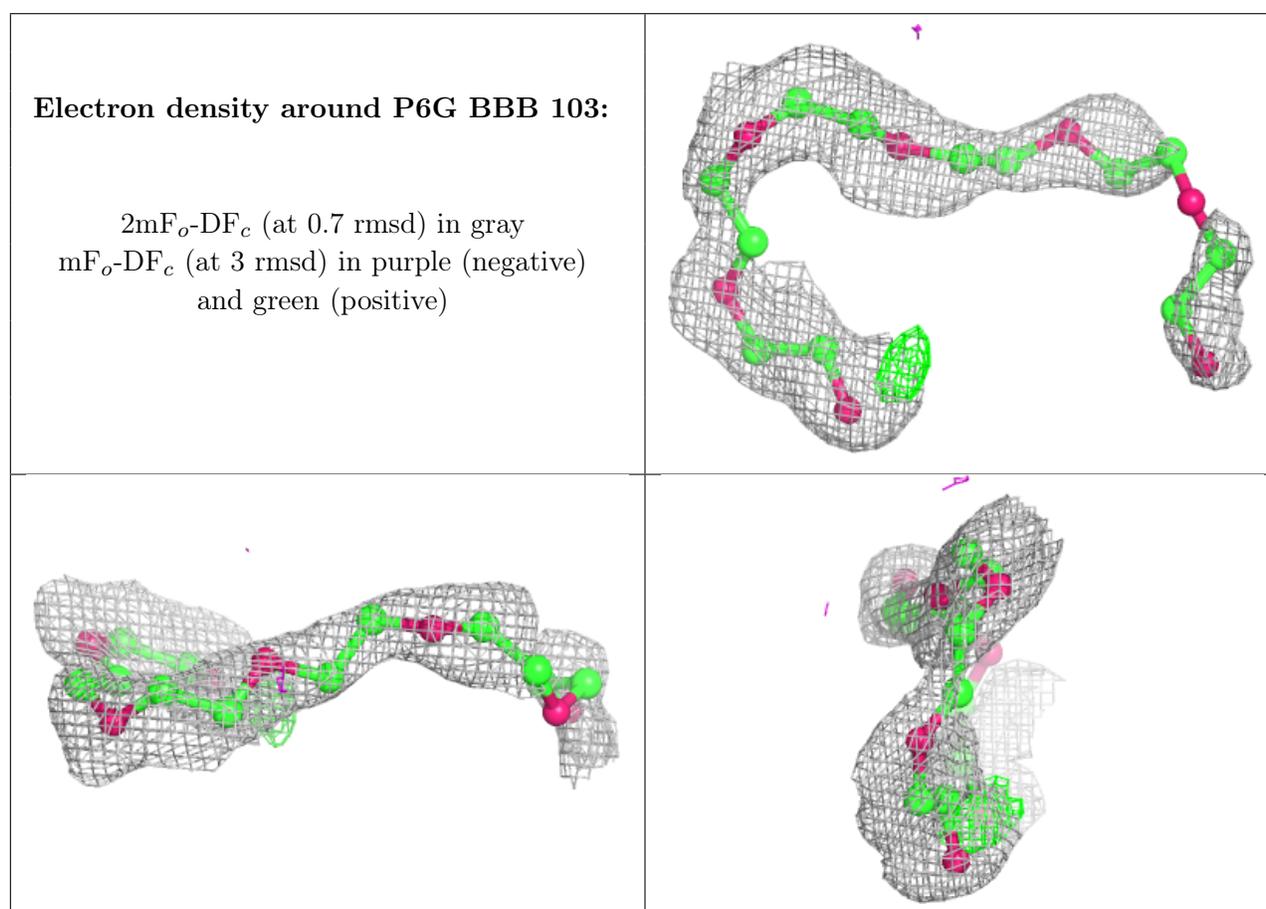
There are no monosaccharides in this entry.

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.

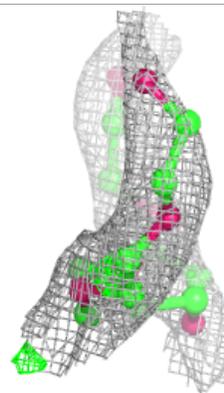
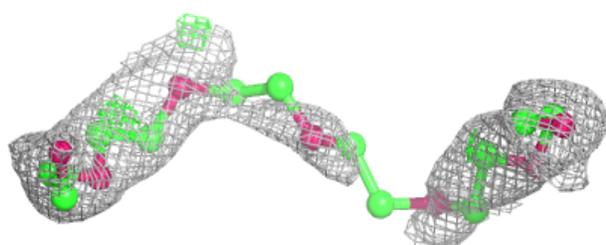
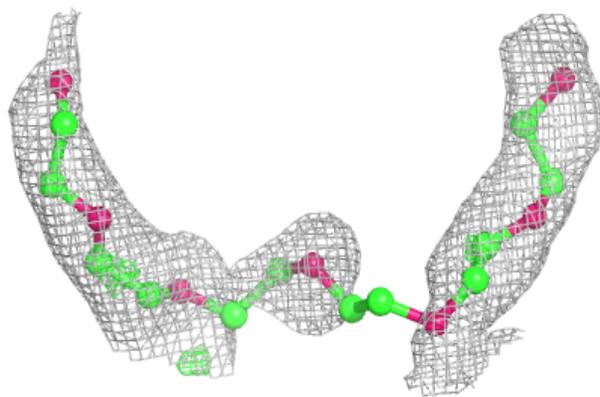
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	P6G	BBB	103	19/19	0.76	0.20	49,64,71,71	0
3	P6G	BBB	102	19/19	0.90	0.16	47,60,84,87	0
2	SO4	AAA	601	5/5	0.93	0.15	74,81,105,105	0
3	P6G	CCC	601	19/19	0.95	0.10	23,34,55,59	0
2	SO4	DDD	601	5/5	0.96	0.16	58,67,82,86	0
4	PO4	BBB	104	5/5	0.96	0.19	32,40,47,55	0
2	SO4	BBB	101	5/5	0.97	0.17	51,54,70,71	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.

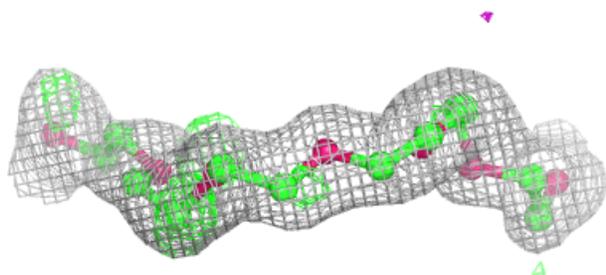
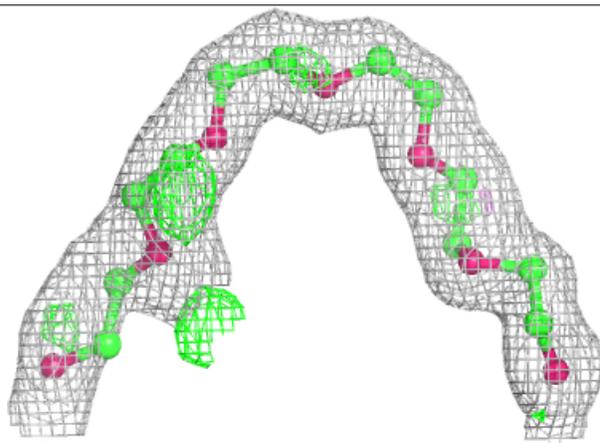


Electron density around P6G BBB 102:

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

**Electron density around P6G CCC 601:**

$2mF_o-DF_c$ (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.