

wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 08:43 pm GMT

PDB ID : 7BO7

Title : CRYSTAL STRUCTURE OF THE HUMAN PRMT5:MEP50 COMPLEX

with JNJB44355437

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Deposited on : 2021-01-24

Resolution : 2.83 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

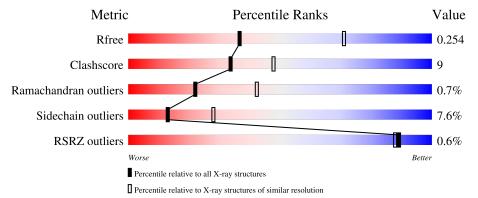
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.83 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain							
1	AAA	645	78%		17% • •					
2	BBB	348	67%	18%	• 13%					

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
ſ	3	U6K	AAA	701	X	-	_	_



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14566 atoms, of which 7155 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 arginine N-methyltransferase 5.

Mol	Chain	Residues			Atom	S			ZeroOcc	AltConf	Trace
1	AAA	625	Total 9908	C 3210	H 4888	N 857	O 929	S 24	160	5	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-7	MET	-	initiating methionine	UNP O14744
AAA	-6	ASP	-	expression tag	UNP O14744
AAA	-5	TYR	-	expression tag	UNP O14744
AAA	-4	LYS	-	expression tag	UNP O14744
AAA	-3	ASP	-	expression tag	UNP O14744
AAA	-2	ASP	-	expression tag	UNP O14744
AAA	-1	ASP	-	expression tag	UNP O14744
AAA	0	ASP	-	expression tag	UNP O14744
AAA	1	LYS	-	expression tag	UNP O14744

• Molecule 2 is a protein called Methylosome protein 50.

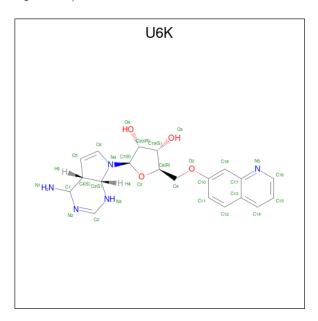
Mol	Chain	Residues			Atom	ıs			ZeroOcc	AltConf	Trace
2	BBB	303	Total 4478	C 1433	H 2202	N 389	O 442	S 12	97	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
BBB	-5	MET	-	initiating methionine	UNP Q9BQA1
BBB	-4	HIS	-	expression tag	UNP Q9BQA1
BBB	-3	HIS	-	expression tag	UNP Q9BQA1
BBB	-2	HIS	-	expression tag	UNP Q9BQA1
BBB	-1	HIS	-	expression tag	UNP Q9BQA1
BBB	0	HIS	-	expression tag	UNP Q9BQA1
BBB	1	HIS	-	expression tag	UNP Q9BQA1

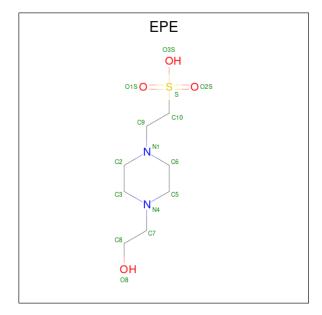


• Molecule 3 is $(2 \{R\},3 \{R\},4 \{S\},5 \{R\})-2-[(4 \{a\} \{S\},7 \{a\} \{S\})-4-azanyl-1,4,4 \{a\},7 \{a\}-tetrahydropyrrolo[2,3-d]pyrimidin-7-yl]-5-(quinolin-7-yloxymethyl)oxolane-3, 4-diol (three-letter code: U6K) (formula: <math>C_{20}H_{23}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	ΛΛΛ	1	Total	С	Н	N	О	1	0
3	AAA	1	48	20	19	5	4	1	0

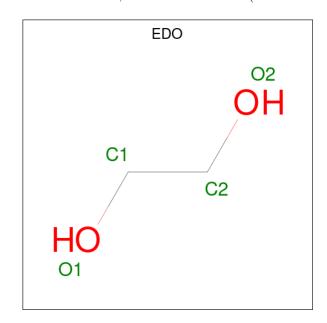
• Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).





Mol	Chain	Residues		A	ton	ıs			ZeroOcc	AltConf
4	Λ Λ Λ	1	Total	С	Н	N	О	S	9	0
4	AAA	1	33	8	18	2	4	1	2	0

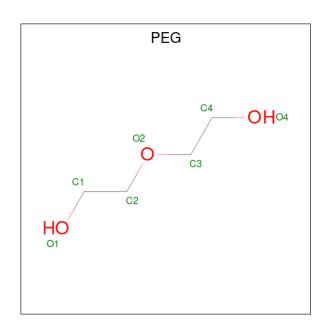
 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0

 $\bullet \ \ Molecule \ 6 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$





Mol	Chain	Residues	A	Atoms				AltConf
6	Λ Λ Λ	1	Total	С	Н	О	1	0
	АЛЛ	1	17	4	10	3	1	

• Molecule 7 is water.

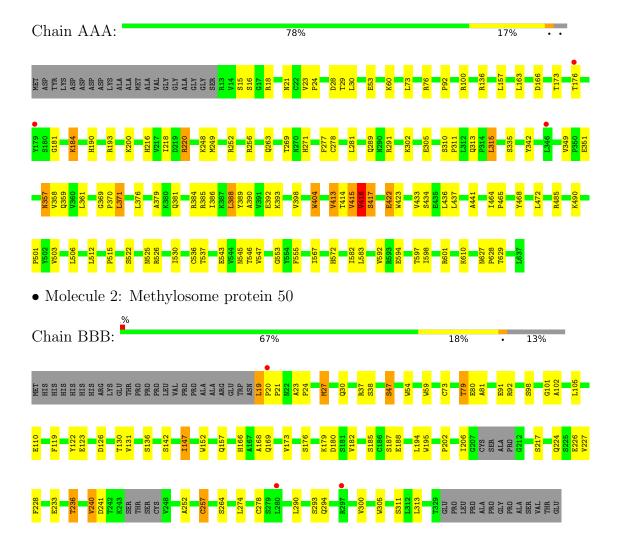
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
7	AAA	40	Total O 40 40	0	0
7	BBB	12	Total O 12 12	0	0



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: Protein arginine N-methyltransferase 5





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	101.19Å 137.25Å 179.37Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.37 - 2.83	Depositor
Resolution (A)	60.29 - 2.83	EDS
% Data completeness	99.6 (60.37-2.83)	Depositor
(in resolution range)	99.6 (60.29-2.83)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.205 , 0.250	Depositor
R, R_{free}	0.210 , 0.254	DCC
R_{free} test set	1310 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 42.7	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14566	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: U6K, EDO, EPE, PEG

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		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.66	0/5161	0.87	0/7038	
2	BBB	0.74	0/2330	0.86	0/3185	
All	All	0.69	0/7491	0.86	0/10223	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	5020	4888	4832	77	0
2	BBB	2276	2202	2175	47	0
3	AAA	29	19	0	1	0
4	AAA	15	18	18	2	0
5	AAA	12	18	18	0	0
6	AAA	7	10	10	2	0
7	AAA	40	0	0	0	0
7	BBB	12	0	0	0	0
All	All	7411	7155	7053	123	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 9.



The worst 5 of 123 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:AAA:415[B]:VAL:HG12	1:AAA:423:TRP:HE1	1.28	0.97
2:BBB:227:VAL:HG22	2:BBB:241:ASP:HB3	1.43	0.97
1:AAA:220:ARG:HG3	1:AAA:220:ARG:HH11	1.44	0.83
1:AAA:414[B]:THR:OG1	1:AAA:416[B]:VAL:HG13	1.78	0.83
2:BBB:102:ALA:HB2	2:BBB:122:TYR:CD1	2.23	0.73

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	P	erce	ntiles
1	AAA	628/645 (97%)	584 (93%)	36 (6%)	8 (1%)		12	26
2	BBB	297/348 (85%)	268 (90%)	27 (9%)	2 (1%)		22	42
All	All	925/993~(93%)	852 (92%)	63 (7%)	10 (1%)		22	30

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	417[A]	SER
1	AAA	417[B]	SER
2	BBB	147	ILE
2	BBB	21	PRO
1	AAA	413[A]	VAL

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	544/570 (95%)	502 (92%)	42 (8%)	13 27		
2	BBB	250/296~(84%)	231 (92%)	19 (8%)	13 28		
All	All	794/866 (92%)	733 (92%)	61 (8%)	13 27		

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	404	TRP
2	BBB	257	CYS
1	AAA	522	SER
2	BBB	240	VAL
2	BBB	294	GLN

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)

6 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	Tuno	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	AAA	703	-	3,3,3	0.07	0	2,2,2	0.30	0
5	EDO	AAA	704	-	3,3,3	0.12	0	2,2,2	0.33	0
6	PEG	AAA	706	-	6,6,6	0.24	0	5,5,5	0.22	0
4	EPE	AAA	702	-	15,15,15	0.74	1 (6%)	18,20,20	0.70	0
5	EDO	AAA	705	-	3,3,3	0.09	0	2,2,2	0.09	0
3	U6K	AAA	701	-	27,33,33	2.77	4 (14%)	34,48,48	1.62	1 (2%)

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
5	EDO	AAA	703	-	-	0/1/1/1	-
5	EDO	AAA	704	_	-	0/1/1/1	_
6	PEG	AAA	706	-	-	1/4/4/4	-
4	EPE	AAA	702	-	-	4/9/19/19	0/1/1/1
5	EDO	AAA	705	-	-	1/1/1/1	-
3	U6K	AAA	701	-	3/3/11/12	2/9/48/48	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
3	AAA	701	U6K	C3-N3	-8.83	1.35	1.46
3	AAA	701	U6K	C4-C3	-8.75	1.41	1.56
3	AAA	701	U6K	C3-N4	-4.96	1.38	1.47
3	AAA	701	U6K	C4-C5	-4.71	1.43	1.51
4	AAA	702	EPE	O3S-S	2.63	1.56	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	AAA	701	U6K	C4-C3-N3	8.33	125.19	113.04

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AAA	701	U6K	С3

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Mol	Chain	Res	Type	Atom
3	AAA	701	U6K	C4
3	AAA	701	U6K	C1

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	701	U6K	O1-C8-C9-O2
3	AAA	701	U6K	C19-C8-C9-O2
4	AAA	702	EPE	C8-C7-N4-C5
6	AAA	706	PEG	O2-C3-C4-O4
5	AAA	705	EDO	O1-C1-C2-O2

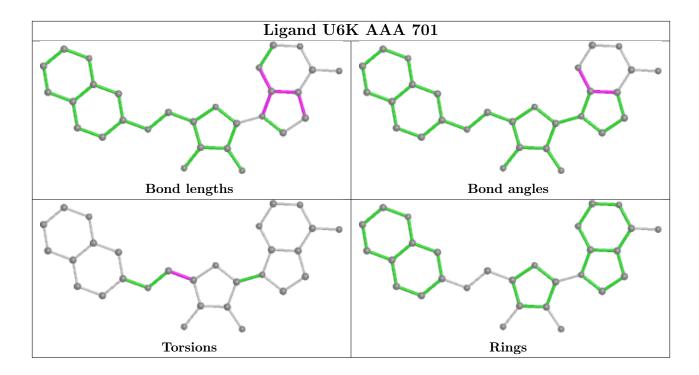
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	706	PEG	2	0
4	AAA	702	EPE	2	0
3	AAA	701	U6K	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	AAA	625/645~(96%)	0.02	3 (0%) 91 89	39, 62, 99, 140	0
2	BBB	303/348 (87%)	0.05	3 (0%) 82 79	53, 76, 100, 143	0
All	All	928/993 (93%)	0.03	6 (0%) 89 88	39, 67, 99, 143	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	179	TYR	3.5
2	BBB	280	LEU	3.0
1	AAA	176	THR	2.4
2	BBB	20	PRO	2.3
1	AAA	346	LEU	2.3

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.

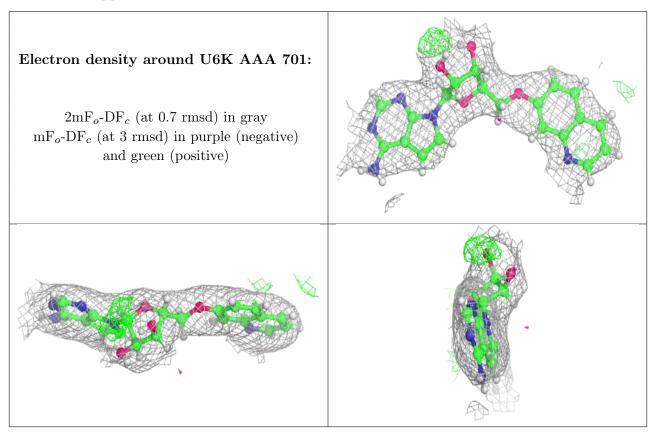
6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
6	PEG	AAA	706	7/7	0.62	0.20	30,94,103,105	1
4	EPE	AAA	702	15/15	0.83	0.29	30,123,138,142	2
5	EDO	AAA	704	4/4	0.93	0.15	30,57,57,58	1
5	EDO	AAA	705	4/4	0.96	0.12	30,51,52,53	1
5	EDO	AAA	703	4/4	0.97	0.23	30,64,66,66	1
3	U6K	AAA	701	29/29	0.97	0.17	30,51,56,61	1

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.

