

Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2022 – 02:08 PM EDT

PDB ID	:	8CSG
Title	:	Human PRMT5:MEP50 structure with Fragment 1 and MTA Bound
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Deposited on		
Resolution	:	2.48 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 (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:

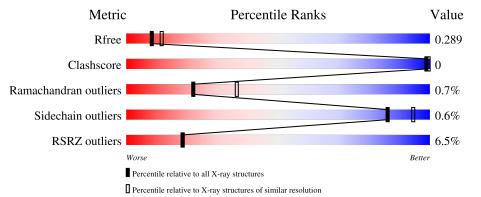
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	А	645	94%	• •					
2	В	350	9%	15%					

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	chirality Geometry		Electron density
5	PEG	А	705	-	-	-	Х
5	PEG	А	706	-	-	-	Х



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2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7571 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 arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	625	Total 5066	C 3241	N 869	0 931	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	72	1	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	MET	-	initiating methionine	UNP 014744
А	-6	ASP	-	expression tag	UNP 014744
А	-5	TYR	-	expression tag	UNP 014744
А	-4	LYS	-	expression tag	UNP 014744
А	-3	ASP	-	expression tag	UNP 014744
А	-2	ASP	-	expression tag	UNP 014744
А	-1	ASP	-	expression tag	UNP 014744
А	0	ASP	-	expression tag	UNP 014744
А	1	LYS	-	expression tag	UNP 014744

• Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	296	Total 2252	C 1415	N 385	O 440	S 12	18	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-7	MET	-	initiating methionine	UNP Q9BQA1
В	-6	HIS	-	expression tag	UNP Q9BQA1
В	-5	HIS	-	expression tag	UNP Q9BQA1
В	-4	HIS	-	expression tag	UNP Q9BQA1
В	-3	HIS	-	expression tag	UNP Q9BQA1
В	-2	HIS	-	expression tag	UNP Q9BQA1
В	-1	HIS	-	expression tag	UNP Q9BQA1

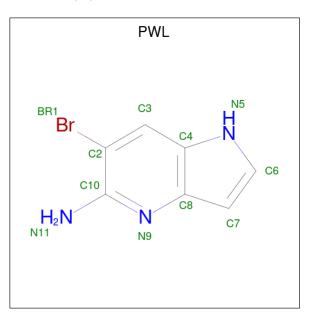
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Chain	Residue	Modelled	Actual	Comment	Reference
В	0	HIS	-	expression tag	UNP Q9BQA1
В	1	HIS	-	expression tag	UNP Q9BQA1

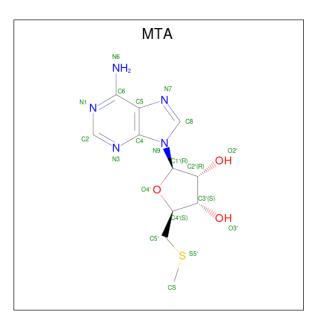
• Molecule 3 is 6-bromo-1H-pyrrolo[3,2-b]pyridin-5-amine (three-letter code: PWL) (formula: $C_7H_6BrN_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	tom	ıs		ZeroOcc	AltConf
3	А	1	Total 11	Br 1	$\begin{array}{c} \mathrm{C} \\ 7 \end{array}$	N 3	0	0

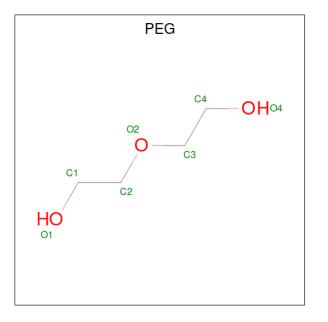
• Molecule 4 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: C₁₁H₁₅N₅O₃S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	А	1	Total 20	C 11	N 5	O 3	S 1	0	0

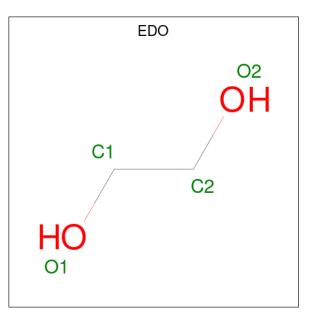
• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0



• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 7 is water.

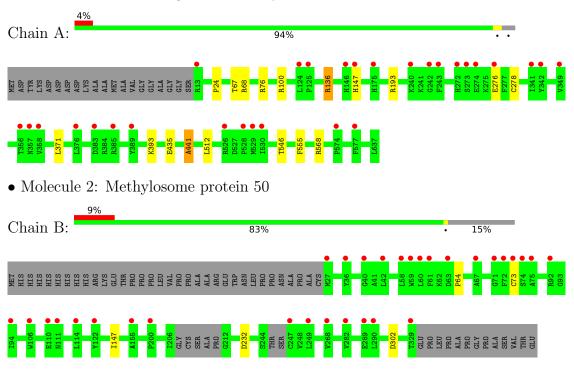
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	158	Total O 158 158	0	0
7	В	33	Total O 35 35	0	2



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	100.66Å 137.18Å 177.89Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.63 - 2.48	Depositor
Resolution (A)	45.67 - 2.48	EDS
% Data completeness	95.7(108.63-2.48)	Depositor
(in resolution range)	95.7 (45.67 - 2.48)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.69 (at 2.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D.	0.263 , 0.292	Depositor
R, R_{free}	0.265 , 0.289	DCC
R_{free} test set	1031 reflections (2.45%)	wwPDB-VP
Wilson B-factor $(Å^2)$	43.5	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 29.5	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	0.92	EDS
Total number of atoms	7571	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: PEG, PWL, EDO, MTA

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.60	0/5211	0.82	4/7088~(0.1%)	
2	В	0.57	0/2303	0.81	2/3141~(0.1%)	
All	All	0.59	0/7514	0.81	6/10229~(0.1%)	

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	76	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	А	136	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	А	568	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	В	302	ASP	CB-CG-OD1	5.14	122.93	118.30
2	В	232	ASP	CB-CG-OD1	5.10	122.89	118.30
1	А	100	ARG	NE-CZ-NH1	5.04	122.82	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	А	5066	0	4961	5	0
2	В	2252	0	2173	0	0
3	А	11	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	20	0	15	0	0
5	А	21	0	30	0	0
6	А	8	0	12	0	0
7	А	158	0	0	0	0
7	В	35	0	0	0	0
All	All	7571	0	7191	5	0

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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 0.

All (5) 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:435:GLU:HG2	3:A:701:PWL:BR1	2.56	0.60
1:A:371:LEU:HD11	1:A:435:GLU:HB2	1.96	0.48
1:A:67:THR:OG1	1:A:68:ARG:N	2.52	0.43
1:A:512:LEU:HD13	1:A:546:THR:HG21	2.01	0.42
1:A:441:ALA:HB2	1:A:555:PHE:HB2	2.01	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	А	624/645~(97%)	599~(96%)	20~(3%)	5(1%)	19 33
2	В	290/350~(83%)	272 (94%)	17~(6%)	1 (0%)	41 59
All	All	914/995~(92%)	871 (95%)	37~(4%)	6 (1%)	22 36

All (6) Ramachandran outliers are listed below:



Mol	Chain	\mathbf{Res}	Type
1	А	147	HIS
2	В	147	ILE
1	А	276	GLU
1	А	278	CYS
1	А	441	ALA
1	А	24	PRO

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	А	559/570~(98%)	556 (100%)	3~(0%)	88 95
2	В	253/298~(85%)	251 (99%)	2(1%)	81 92
All	All	812/868~(94%)	807~(99%)	5 (1%)	86 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	136	ARG
1	А	193	ARG
1	А	393	LYS
2	В	64	PRO
2	В	73	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	272	HIS

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	Turne	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	PEG	А	703	-	$6,\!6,\!6$	0.48	0	$5,\!5,\!5$	0.40	0
5	PEG	А	706	-	$6,\!6,\!6$	0.44	0	$5,\!5,\!5$	0.38	0
6	EDO	А	704	-	3,3,3	0.54	0	2,2,2	0.24	0
6	EDO	А	707	-	3,3,3	0.56	0	2,2,2	0.20	0
3	PWL	А	701	-	11,12,12	1.23	1 (9%)	9,17,17	1.47	1 (11%)
5	PEG	А	705	-	$6,\!6,\!6$	0.46	0	$5,\!5,\!5$	0.26	0
4	MTA	А	702	-	19,22,22	1.62	4 (21%)	19,32,32	3.01	8 (42%)

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	PEG	А	703	-	-	2/4/4/4	-
5	PEG	А	706	-	-	1/4/4/4	-
6	EDO	А	704	-	-	0/1/1/1	-
6	EDO	А	707	-	-	1/1/1/1	-
3	PWL	А	701	-	-	-	0/2/2/2
5	PEG	А	705	-	-	2/4/4/4	-
4	MTA	А	702	-	-	0/3/23/23	0/3/3/3



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	702	MTA	C5'-S5'	-3.90	1.75	1.80
4	А	702	MTA	C2'-C1'	-3.57	1.48	1.53
3	А	701	PWL	C10-N11	2.63	1.40	1.34
4	А	702	MTA	C5-C4	2.33	1.47	1.40
4	А	702	MTA	C2-N3	2.22	1.35	1.32

All (5) bond length outliers are listed below:

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	702	MTA	O4'-C4'-C3'	-7.74	89.79	105.11
4	А	702	MTA	C2'-C3'-C4'	6.43	115.13	102.64
4	А	702	MTA	O4'-C1'-C2'	-4.27	100.69	106.93
4	А	702	MTA	N3-C2-N1	-4.00	122.43	128.68
4	А	702	MTA	C3'-C2'-C1'	-2.55	97.14	100.98
4	А	702	MTA	O4'-C4'-C5'	2.52	115.31	108.83
4	А	702	MTA	C1'-N9-C4	-2.36	122.49	126.64
3	А	701	PWL	BR1-C2-C10	2.31	122.46	120.15
4	А	702	MTA	C2-N1-C6	2.17	122.47	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	705	PEG	O1-C1-C2-O2
5	А	703	PEG	O2-C3-C4-O4
5	А	706	PEG	O2-C3-C4-O4
6	А	707	EDO	O1-C1-C2-O2
5	А	703	PEG	O1-C1-C2-O2
5	А	705	PEG	O2-C3-C4-O4

There are no ring outliers.

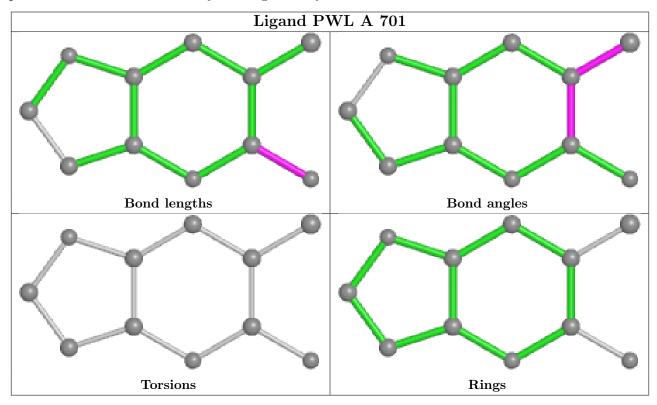
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	701	PWL	1	0

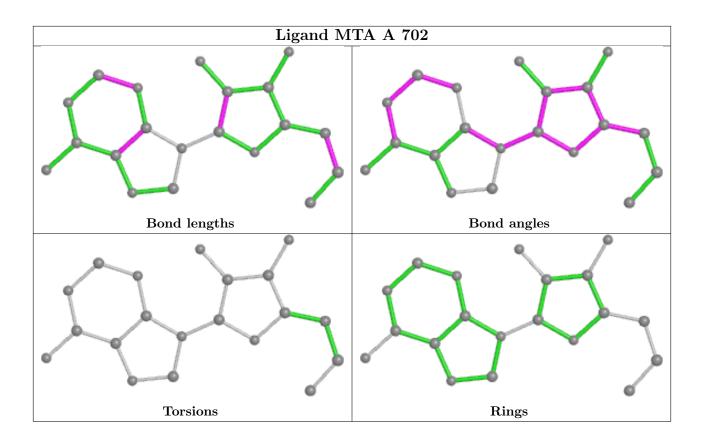
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	625/645~(96%)	0.45	29 (4%) 32 34	14, 25, 53, 105	25 (4%)
2	В	296/350~(84%)	0.76	31 (10%) 6 5	18, 28, 41, 81	8 (2%)
All	All	921/995~(92%)	0.55	60 (6%) 18 18	14, 26, 48, 105	33 (3%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	247	CYS	6.9
1	А	528	PRO	5.5
1	А	274	GLU	4.4
1	А	242	GLY	4.2
2	В	72	PHE	3.8
2	В	114	LEU	3.8
2	В	290	LEU	3.8
1	А	530	ILE	3.7
2	В	71	GLY	3.7
1	А	349	VAL	3.6
1	А	273	SER	3.5
2	В	61	PHE	3.5
1	А	147	HIS	3.3
2	В	59	TRP	3.3
1	А	357	ASN	3.2
2	В	249	LEU	3.2
1	А	376	LEU	3.1
2	В	268	VAL	3.1
1	А	243	PHE	3.1
1	А	529	MET	3.1
1	А	526	ARG	3.1
2	В	75	ALA	3.0
2	В	111	ASN	2.9
1	А	358	VAL	2.8

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Mol	nued fron Chain	Res	Type	RSRZ
1	А	175	HIS	2.8
1	А	13	ARG	2.7
1	А	272	HIS	2.7
1	А	383	ASP	2.7
2	В	60	LEU	2.6
1	А	577	PHE	2.6
1	А	341	ILE	2.6
2	В	106	TRP	2.5
2	В	155	ALA	2.5
1	А	276	GLU	2.4
1	А	385	ARG	2.3
1	А	240	LYS	2.3
2	В	73	CYS	2.3
1	А	342	TYR	2.3
2	В	74	SER	2.3
2	В	200	PRO	2.3
2	В	58	LEU	2.3
2	В	329	THR	2.3
2	В	110	GLU	2.2
2	В	92	ARG	2.2
2	В	27	MET	2.2
1	А	125	PRO	2.2
2	В	63	ASP	2.2
2	В	282	VAL	2.2
2	В	94	ILE	2.2
2	В	36	TYR	2.1
1	А	124	LEU	2.1
1	А	356	THR	2.1
1	А	146	HIS	2.1
2	В	40	GLY	2.1
2	В	42	LEU	2.1
1	А	389	TYR	2.1
2	В	67	ALA	2.0
2	В	122	TYR	2.0
2	В	289	GLU	2.0
1	А	574	PRO	2.0

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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.

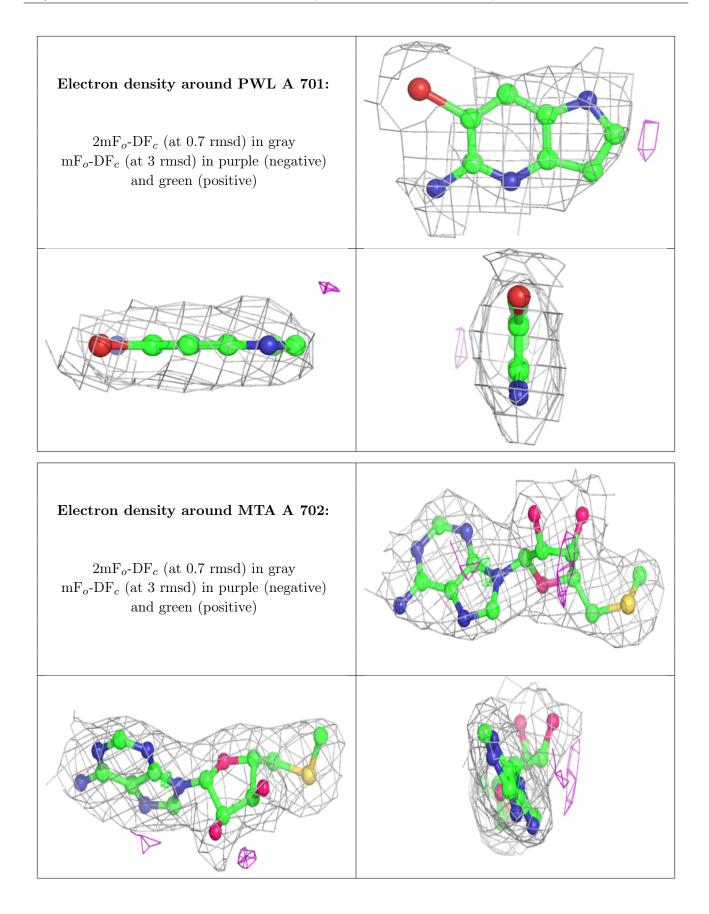
6.4 Ligands (i)

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	B -factors($Å^2$)	Q<0.9
5	PEG	А	703	7/7	0.60	0.35	80,82,85,86	7
5	PEG	А	706	7/7	0.75	0.47	32,37,49,50	7
5	PEG	А	705	7/7	0.79	0.48	29,40,43,46	7
6	EDO	А	704	4/4	0.79	0.27	56,57,60,64	0
6	EDO	А	707	4/4	0.90	0.35	54,54,61,61	0
3	PWL	А	701	11/11	0.93	0.19	39,45,55,88	0
4	MTA	А	702	20/20	0.96	0.23	24,32,41,45	0

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







6.5 Other polymers (i)

There are no such residues in this entry.

