

wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2022 – 12:13 pm GMT

PDB ID Title		6H5O Crystal structure of PBP2a from MRSA in complex with piperacillin at active site.
Deposited on	:	Batuecas, M.T.; Martinez-Caballero, S.; Hermoso, J.A. 2018-07-25 2.82 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 following versions of software and data (see references (1)) were used in the production of this report:

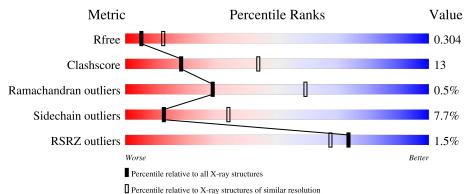
MolProbity		4 02b 467
•		
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	642	^{2%} 67%	23%	• 7%			
1	В	642	% 68%	28%	•••			



6H5O

2 Entry composition (i)

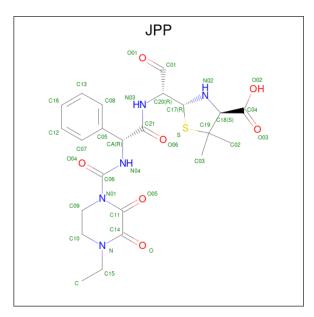
There are 4 unique types of molecules in this entry. The entry contains 10093 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin binding protein 2 prime.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1 A 598	508	Total	С	Ν	0	S	0	0	0
		590	4791	3018	808	950	15	0		
1	В	636	Total	С	Ν	0	S	0	0	0
	ГВ	030	5109	3222	862	1009	16			0

• Molecule 2 is Piperacillin (Open Form) (three-letter code: JPP) (formula: $C_{23}H_{29}N_5O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
2	Δ	1	Total	С	Ν	0	S	0	0	
		1	36	23	5	7	1	0		
2	2 B	Р	1	Total	С	Ν	0	S	0	0
		1	36	23	5	7	1		0	

• Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	8	Total Cd 8 8	0	0
3	В	1	Total Cd 1 1	0	0

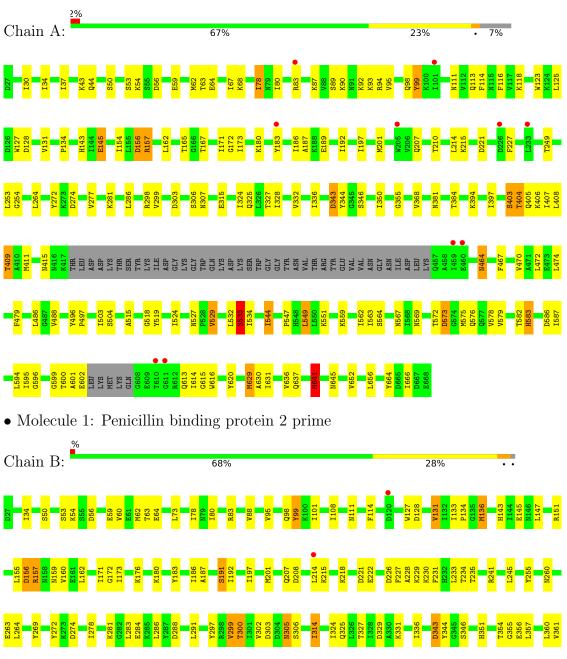
• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	57	Total O 57 57	0	0
4	В	55	$\begin{array}{cc} \text{Total} & \text{O} \\ 55 & 55 \end{array}$	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: Penicillin binding protein 2 prime



S403 T404 Q405 K406 L408 L408 T409 V448 V449 N450 1464 1465 1465 1466 T572 D573 S476 N567 1568 N569 **I534** E480 M483 V488 Y496 P497 G5 18 149 N659 E668 <mark>M628</mark> M629 A630 I631 <mark>D635</mark> V636 Q637 A642 A646 K647 M605 LYS GLN GLN GLU THR GLU GLY 1014 G615 W616 F617 S643 Y644 Y620 1012 1613



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	80.71Å 105.01Å 185.62Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 - 2.82	Depositor
Resolution (A)	46.41 - 2.82	EDS
% Data completeness	99.7 (46.45 - 2.82)	Depositor
(in resolution range)	99.7 (46.41 - 2.82)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
D D.	0.241 , 0.311	Depositor
R, R_{free}	0.238 , 0.304	DCC
R_{free} test set	1856 reflections $(4.80%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	94.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10093	wwPDB-VP
Average B, all atoms $(Å^2)$	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.43% 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: CD, JPP

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.36	1/4868~(0.0%)	0.62	1/6543~(0.0%)	
1	В	0.37	1/5194~(0.0%)	0.63	1/6983~(0.0%)	
All	All	0.37	2/10062~(0.0%)	0.62	2/13526~(0.0%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	403	SER	CB-OG	6.56	1.50	1.42
1	В	403	SER	CB-OG	6.51	1.50	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	645	ASN	CB-CA-C	7.15	124.71	110.40
1	А	403	SER	CA-CB-OG	5.68	126.53	111.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	157	ARG	Sidechain



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	4791	0	4786	126	0
1	В	5109	0	5108	137	0
2	А	36	0	27	1	0
2	В	36	0	27	4	0
3	А	8	0	0	0	0
3	В	1	0	0	0	0
4	А	57	0	0	3	0
4	В	55	0	0	1	0
All	All	10093	0	9948	264	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.

The worst 5 of 264 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:411:MET:HG2	1:A:563:ILE:HD11	1.39	1.01
1:A:30:ILE:HD11	1:A:116:PHE:CZ	1.99	0.97
1:A:407:ILE:O	1:A:411:MET:HG3	1.69	0.92
1:B:464:ASN:ND2	2:B:701:JPP:O06	2.04	0.90
1:B:407:ILE:O	1:B:411:MET:HG3	1.76	0.86

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	Analysed Favoured Allowed		Outliers	Percentiles
1	А	592/642~(92%)	553~(93%)	36~(6%)	3~(0%)	29 59
1	В	632/642~(98%)	586~(93%)	43 (7%)	3~(0%)	29 59
All	All	1224/1284~(95%)	1139 (93%)	79~(6%)	6 (0%)	29 59

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	641	MET
1	В	404	THR
1	А	404	THR
1	А	533	SER
1	В	533	SER

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	533/572~(93%)	494 (93%)	39~(7%)	14 37
1	В	568/572~(99%)	522~(92%)	46 (8%)	11 32
All	All	1101/1144 (96%)	1016~(92%)	85~(8%)	13 34

5 of 85 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	272	TYR
1	В	409	THR
1	В	283	LEU
1	В	314	ILE
1	В	483	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such side chains are listed below:

Mol	Chain	Res	Type
1	В	396	GLN

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Mol	Chain	Res	Type
1	В	555	ASN
1	В	548	HIS
1	В	567	ASN
1	А	576	GLN

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)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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	Type Chain R		e Chain Res	Link	В	Bond lengths			Bond angles		
	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2		
2	JPP	В	701	1	31,38,38	4.40	11 (35%)	39,55,55	2.73	14 (35%)		
2	JPP	А	701	1	31,38,38	4.38	12 (38%)	39,55,55	2.54	13 (33%)		

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	JPP	В	701	1	-	3/22/64/64	0/3/3/3
2	JPP	А	701	1	-	5/22/64/64	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	701	JPP	O04-C06	11.04	1.43	1.23
2	А	701	JPP	O04-C06	10.99	1.43	1.23
2	В	701	JPP	O06-C21	10.27	1.43	1.23
2	А	701	JPP	O06-C21	10.09	1.43	1.23
2	А	701	JPP	O-C14	9.70	1.43	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	701	JPP	N04-C06-N01	6.84	124.00	114.04
2	А	701	JPP	N04-C06-N01	6.27	123.16	114.04
2	В	701	JPP	C20-N03-C21	-5.71	116.88	123.12
2	А	701	JPP	C20-N03-C21	-5.27	117.36	123.12
2	В	701	JPP	C10-C09-N01	5.23	118.64	108.78

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	JPP	C-C15-N-C10
2	А	701	JPP	C-C15-N-C14
2	В	701	JPP	C-C15-N-C10
2	В	701	JPP	O06-C21-CA-N04
2	В	701	JPP	C-C15-N-C14

There are no ring outliers.

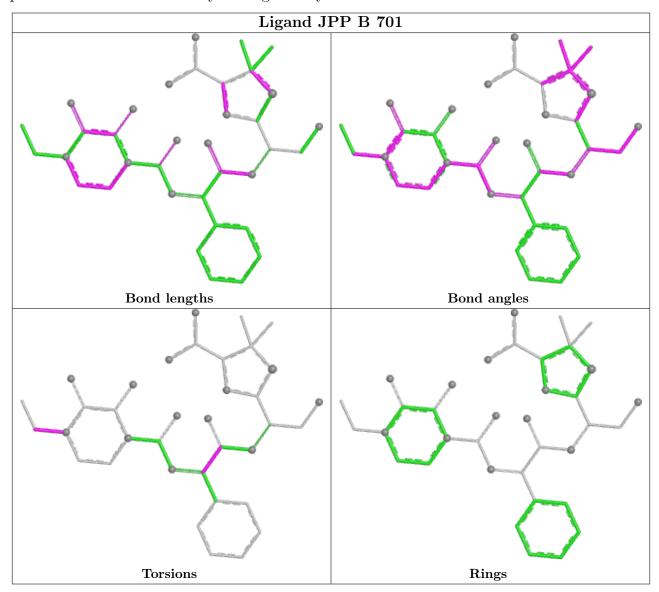
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	701	JPP	4	0
2	А	701	JPP	1	0

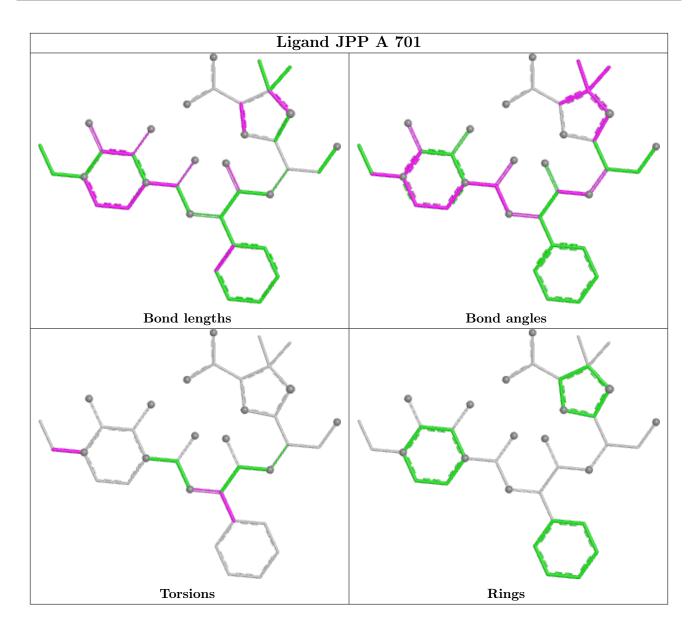
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	$OWAB(A^2)$	Q<0.9
1	А	598/642~(93%)	0.02	10 (1%) 70 63	79, 119, 169, 247	0
1	В	636/642~(99%)	-0.01	8 (1%) 77 72	75, 124, 175, 211	2 (0%)
All	All	1234/1284~(96%)	0.00	18 (1%) 73 67	75, 122, 172, 247	2 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	441	TYR	4.8
1	В	635	ASP	4.3
1	А	205	TRP	3.1
1	А	459	ILE	3.0
1	А	233	LEU	2.9

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.

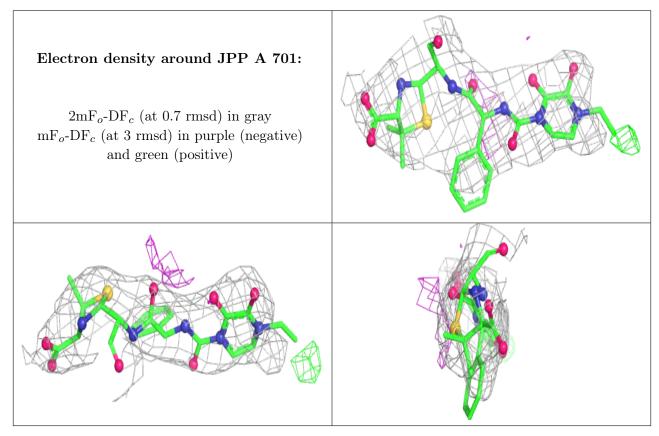
6.4 Ligands (i)

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.

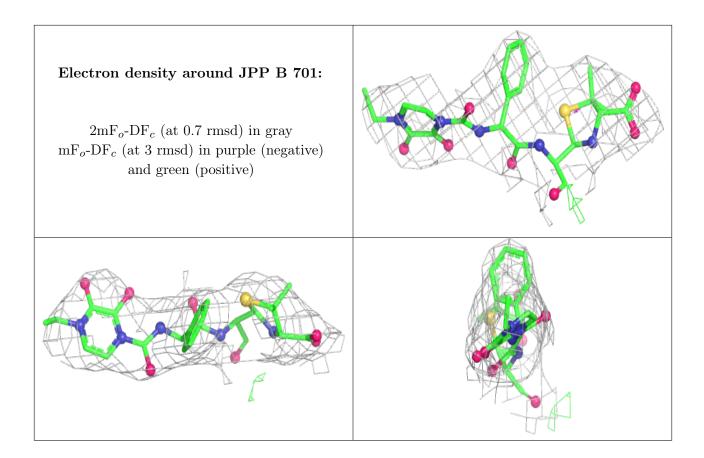


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
2	JPP	А	701	36/36	0.89	0.24	$115,\!137,\!153,\!156$	0
3	CD	А	707	1/1	0.91	0.12	176,176,176,176	0
2	JPP	В	701	36/36	0.94	0.13	87,109,143,144	0
3	CD	А	705	1/1	0.99	0.14	$153,\!153,\!153,\!153$	0
3	CD	А	706	1/1	0.99	0.09	202,202,202,202	0
3	CD	А	703	1/1	0.99	0.10	128,128,128,128	0
3	CD	А	709	1/1	0.99	0.16	92,92,92,92	1
3	CD	А	702	1/1	1.00	0.14	102,102,102,102	0
3	CD	А	708	1/1	1.00	0.16	94,94,94,94	0
3	CD	А	704	1/1	1.00	0.18	99,99,99,99	0
3	CD	В	702	1/1	1.00	0.15	122,122,122,122	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.

