

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 09:02 PM BST

PDB ID	:	5N84
Title	:	TTK kinase domain in complex with Mps-BAY2b
Authors	:	Uitdehaag, J.; Willemsen-Seegers, N.; de Man, J.; Buijsman, R.C.; Zaman,
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Deposited on		
Resolution	:	2.30 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 following versions of software and data (see references (1)) were used in the production of this report:

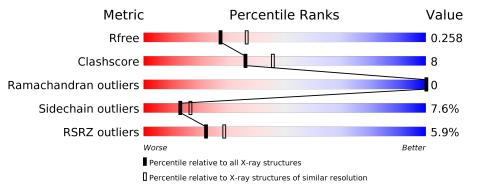
Ū.	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster -report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R_{free}	130704	5042(2.30-2.30)
Clashscore	141614	5643(2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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			
			5%			
1	А	313	66%	14%	•	18%

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	\mathbf{Res}	Chirality	Geometry	Clashes	Electron density
4	PG0	А	907	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2192 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 Dual specificity protein kinase TTK.

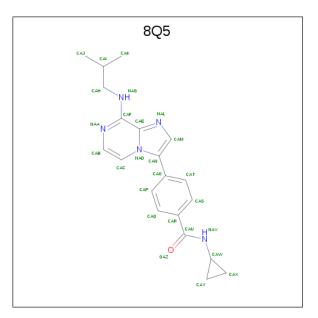
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	256	Total	C	N	0	S	0	0	0
			2093	1346	350	385	12			

Chain	Residue	Modelled	Actual	Comment	Reference
А	496	MET	-	initiating methionine	UNP P33981
A	497	HIS	-	expression tag	UNP P33981
A	498	HIS	-	expression tag	UNP P33981
A	499	HIS	-	expression tag	UNP P33981
A	500	HIS	-	expression tag	UNP P33981
A	501	HIS	-	expression tag	UNP P33981
A	502	HIS	-	expression tag	UNP P33981
A	503	SER	-	expression tag	UNP P33981
A	504	SER	-	expression tag	UNP P33981
A	505	GLY	-	expression tag	UNP P33981
A	506	VAL	-	expression tag	UNP P33981
A	507	ASP	-	expression tag	UNP P33981
A	508	LEU	-	expression tag	UNP P33981
A	509	GLY	-	expression tag	UNP P33981
A	510	THR	-	expression tag	UNP P33981
A	511	GLU	-	expression tag	UNP P33981
A	512	ASN	-	expression tag	UNP P33981
A	513	LEU	-	expression tag	UNP P33981
A	514	TYR	-	expression tag	UNP P33981
А	515	PHE	-	expression tag	UNP P33981
А	516	GLN	-	expression tag	UNP P33981
А	517	SER	-	expression tag	UNP P33981
А	518	MET	-	expression tag	UNP P33981
А	797	LEU	PRO	$\operatorname{conflict}$	UNP P33981

There are 24 discrepancies between the modelled and reference sequences:

• Molecule 2 is {N}-cyclopropyl-4-[8-(2-methylpropylamino)imidazo[1,2-a]pyrazin-3-yl]benza mide (three-letter code: 8Q5) (formula: $C_{20}H_{23}N_5O$).



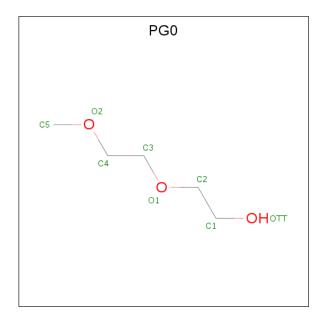


Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
2	Δ	1	Total	С	Ν	Ο	0	Ο
2	11	T	26	20	5	1	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	5	Total Na 5 5	0	0

• Molecule 4 is 2-(2-METHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	А	1	Total 8	$\begin{array}{c} \mathrm{C} \\ 5 \end{array}$	O 3	0	0

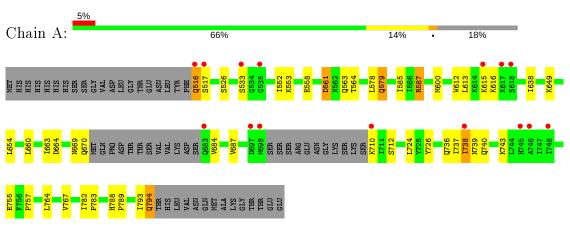
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	60	Total O 60 60	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: Dual specificity protein kinase TTK



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness (in resolution range)	$\begin{array}{c} 99.7 \ (41.73\text{-}2.30) \\ 99.7 \ (41.73\text{-}2.30) \end{array}$	Depositor EDS
R _{merge}	0.05	Depositor
$\frac{\mathbf{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available) 1.61 (at 2.29Å)	Depositor Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor DCC
R_{free} test set	1076 reflections (5.14%)	wwPDB-VP
Wilson B-factor $(Å^2)$	58.8	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	$0.33\ ,\ 52.3$	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2192	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.19% 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: NA, 8Q5, PG0

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).

Mal	Chain	Bond	lengths	Bond angles		
Mol		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.84	0/2138	0.89	0/2886	

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	А	2093	0	2114	30	0
2	А	26	0	0	4	0
3	А	5	0	0	0	0
4	А	8	0	12	8	0
5	А	60	0	0	2	1
All	All	2192	0	2126	34	1

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 8.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:A:901:8Q5:CAX	4:A:907:PG0:C5	2.14	1.25
2:A:901:8Q5:CAX	4:A:907:PG0:H51	1.78	1.09
1:A:579:GLN:O	1:A:587:ARG:NH1	1.97	0.98
1:A:738:ILE:H	1:A:738:ILE:HD12	1.42	0.84
2:A:901:8Q5:CAX	4:A:907:PG0:H52	2.07	0.84
1:A:654:LEU:HB2	1:A:663:ILE:HD11	1.61	0.82
1:A:585:ILE:O	1:A:587:ARG:NH2	2.22	0.72
1:A:553:LYS:NZ	4:A:907:PG0:H53	2.14	0.63
1:A:782:ILE:HB	1:A:783:PRO:HD3	1.82	0.61
1:A:654:LEU:HB2	1:A:663:ILE:CD1	2.33	0.57
1:A:793:ILE:O	1:A:794:GLN:HB2	2.05	0.56
1:A:789:PRO:HB3	1:A:793:ILE:HD12	1.86	0.56
1:A:737:ILE:O	1:A:743:LYS:HE3	2.08	0.53
1:A:516:GLN:N	5:A:1002:HOH:O	2.40	0.53
2:A:901:8Q5:CAX	4:A:907:PG0:H53	2.27	0.52
1:A:649:LYS:HE3	1:A:684:VAL:HG12	1.92	0.51
1:A:615:LYS:O	1:A:615:LYS:HG3	2.11	0.50
1:A:553:LYS:HZ1	4:A:907:PG0:H53	1.78	0.48
1:A:553:LYS:HZ3	4:A:907:PG0:H53	1.78	0.48
1:A:553:LYS:HE2	4:A:907:PG0:H41	1.97	0.46
1:A:612:TRP:O	1:A:616:LYS:HB2	2.15	0.46
1:A:755:GLU:HG2	1:A:757:PRO:HD3	1.98	0.45
1:A:578:LEU:HD12	1:A:638:ILE:HG22	1.98	0.44
1:A:552:ILE:HA	1:A:600:MET:O	2.17	0.44
1:A:724:LEU:HD21	1:A:764:LEU:CD1	2.48	0.43
1:A:612:TRP:CE3	1:A:613:LEU:HD23	2.55	0.42
1:A:687:VAL:HG12	1:A:687:VAL:O	2.19	0.42
1:A:561:ASP:OD1	1:A:564:THR:OG1	2.36	0.41
1:A:660:LEU:HA	1:A:660:LEU:HD23	1.91	0.41
1:A:561:ASP:N	1:A:561:ASP:OD1	2.46	0.41
1:A:767:VAL:HG23	1:A:788:HIS:CE1	2.56	0.41
1:A:737:ILE:HG22	1:A:739:ASN:O	2.21	0.40
1:A:587:ARG:HG3	5:A:1042:HOH:O	2.21	0.40
1:A:564:THR:HA	1:A:669:ASN:ND2	2.36	0.40

All (1) 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)
5:A:1047:HOH:O	5:A:1047:HOH:O[2_665]	2.14	0.06



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	250/313~(80%)	244~(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	А	236/288 ($82%$)	218~(92%)	18 (8%)	13 16	

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	516	GLN
1	А	517	SER
1	А	526	SER
1	А	533	SER
1	А	558	GLU
1	А	561	ASP
1	А	563	GLN
1	А	579	GLN
1	А	587	ARG
1	А	664	ASP
1	А	670	GLN
1	А	710	LYS
1	А	712	SER

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Mol	Chain	Res	Type
1	А	726	TYR
1	А	736	GLN
1	А	738	ILE
1	А	740	GLN
1	А	794	GLN

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

Mol	Chain	Res	Type	
1	А	739	ASN	

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 7 ligands modelled in this entry, 5 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).

Mal	Mol Type Chain Res Lin		Link	Bo	Bond lengths			Bond angles		
	туре	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PG0	А	907	-	7,7,7	0.48	0	$6,\!6,\!6$	0.75	0
2	8Q5	А	901	-	25,29,29	1.24	2 (8%)	$30,\!41,\!41$	1.70	<mark>6 (20%)</mark>



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
4	PG0	А	907	-	-	4/5/5/5	-
2	8Q5	А	901	-	-	0/17/19/19	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	А	901	8Q5	CAX-CAW	2.80	1.54	1.48
2	А	901	8Q5	CAY-CAW	2.48	1.54	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	901	8Q5	CAY-CAW-NAV	-5.20	111.15	118.61
2	А	901	8Q5	CAR-CAU-NAV	3.52	123.81	117.06
2	А	901	8Q5	OAZ-CAU-CAR	-3.35	114.96	120.94
2	А	901	8Q5	CAX-CAW-NAV	2.85	122.70	118.61
2	А	901	8Q5	CAP-CAO-CAN	-2.42	116.97	121.00
2	А	901	8Q5	NAG-CAF-NAA	2.17	122.10	118.54

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}	Atoms
4	А	907	PG0	OTT-C1-C2-O1
4	А	907	PG0	O1-C3-C4-O2
4	А	907	PG0	C3-C4-O2-C5
4	А	907	PG0	C4-C3-O1-C2

There are no ring outliers.

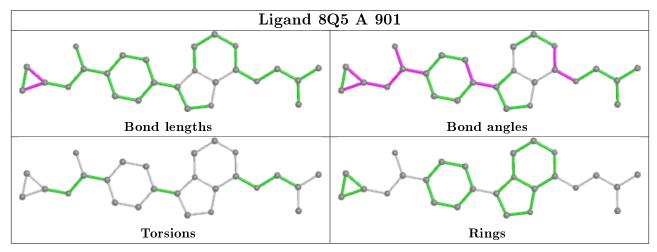
2 monomers are involved in 8 short contacts:

Μ	ol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
4	1	А	907	PG0	8	0
2	2	А	901	8Q5	4	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, 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	А	256/313~(81%)	0.36	15 (5%) 22 28	40, 64, 107, 140	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	617	LYS	4.2
1	А	535	GLY	4.1
1	А	738	ILE	3.5
1	А	710	LYS	3.3
1	А	746	ALA	3.3
1	А	698	MET	3.2
1	А	516	GLN	3.0
1	А	517	SER	3.0
1	А	748	ILE	2.8
1	А	615	LYS	2.7
1	А	618	SER	2.6
1	А	745	HIS	2.6
1	А	697	ASP	2.5
1	А	683	GLN	2.2
1	А	533	SER	2.0

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.

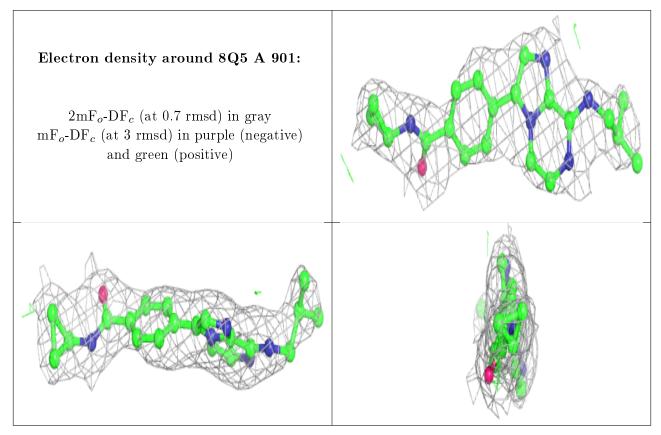


6.4 Ligands (i)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
3	NA	А	906	1/1	0.91	0.53	$79,\!79,\!79,\!79$	0
3	NA	А	905	1/1	0.92	0.38	89,89,89,89	0
2	8Q5	А	901	26/26	0.92	0.17	$52,\!85,\!93,\!100$	0
4	PG0	А	907	8/8	0.93	0.14	$54,\!63,\!66,\!71$	0
3	NA	А	903	1/1	0.93	0.18	$58,\!58,\!58,\!58$	0
3	NA	А	904	1/1	0.93	0.23	72,72,72,72	0
3	NA	А	902	1/1	0.94	0.61	64,64,64,64	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.

