Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 11:14 pm BST

PDB ID	:	7ZUK
Title	:	PENICILLIN-BINDING PROTEIN 1B (PBP-1B) in complex with lactone 7Az - Streptococcus pneumoniae R6
Authors	:	Flanders, P.L.; Contreras-Martel, C.; Martins, A.; Brown, N.W.; Shirley, J.D.; Nauta, K.M.; Dessen, A.; Carlson, E.E.; Ambrose, E.A.
Deposited on	:	2022-05-12
Resolution	:	1.63 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:

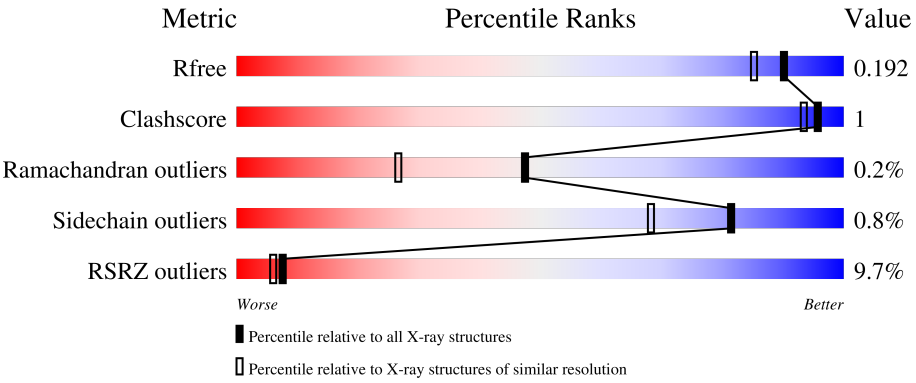
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	821	5% 52% · 45%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4093 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.

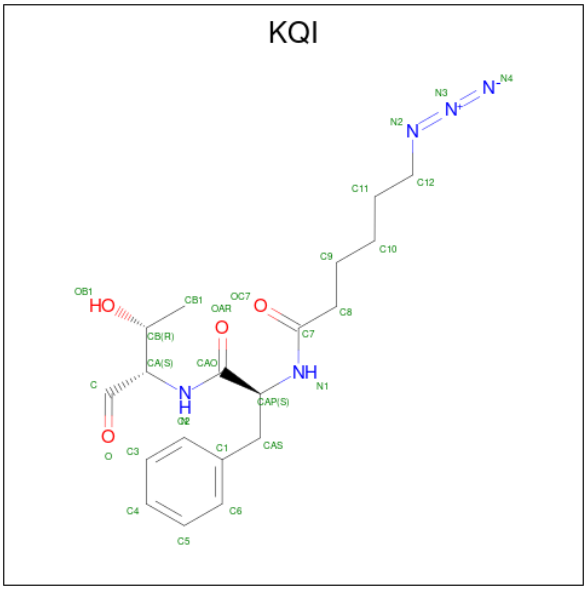
- Molecule 1 is a protein called Penicillin-binding protein 1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	454	Total	C	N	O	S	0	7	0
			3543	2220	603	705	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	656	GLY	ASN	engineered mutation	UNP Q7CRA4
AAA	686	GLN	ARG	engineered mutation	UNP Q7CRA4
AAA	687	GLN	ARG	engineered mutation	UNP Q7CRA4

- Molecule 2 is 6-azido-N-[(2S)-1-oxidanylidene-1-[[(2S,3R)-3-oxidanyl-1-oxidanylidene-butan-2-yl]amino]-3-phenyl-propan-2-yl]hexanamide (three-letter code: KQI) (formula: $C_{19}H_{27}N_5O_4$) (labeled as "Ligand of Interest" by depositor).

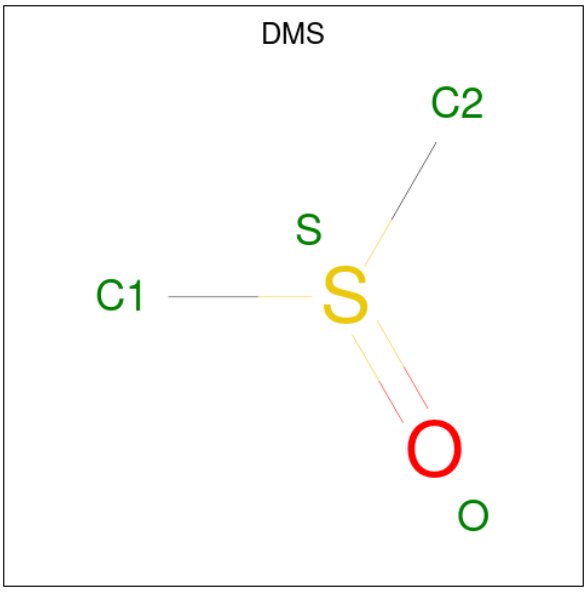


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			28	19	5	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	23	Total Cl 23 23	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is water.

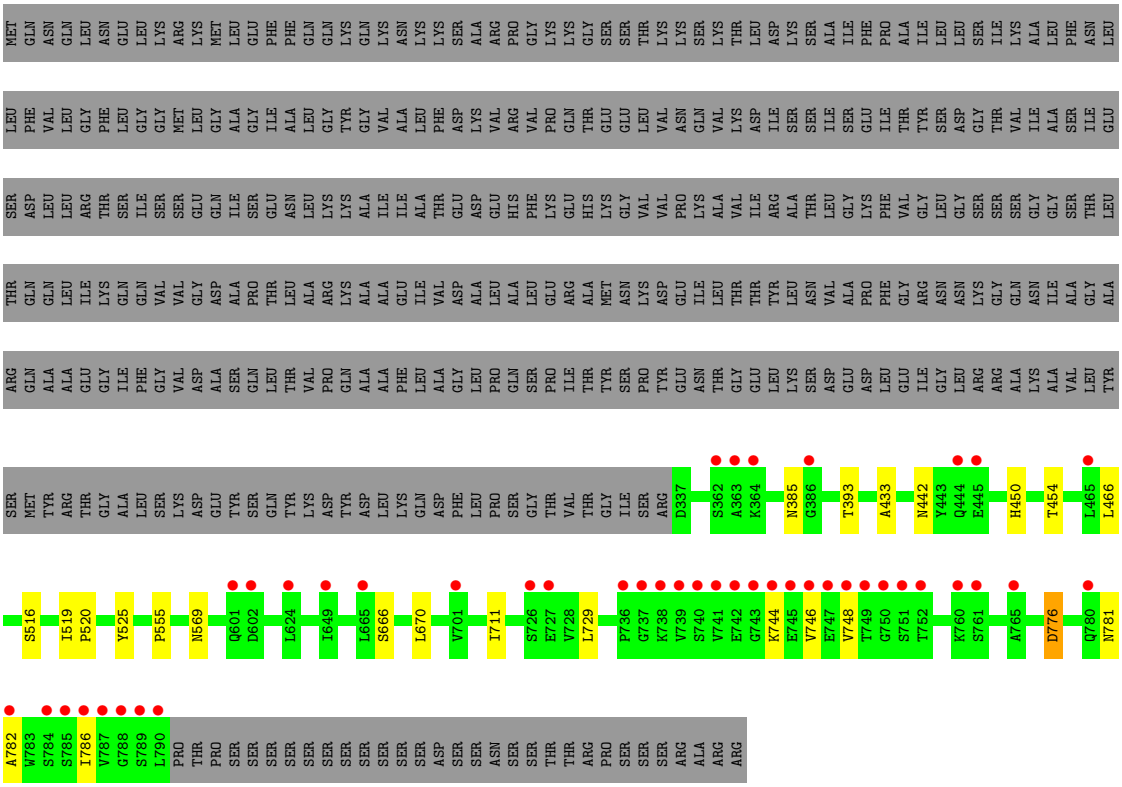
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	495	Total O 495 495	0	0

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 1b

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.61Å 148.94Å 99.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.16 – 1.63 44.16 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.16-1.63) 97.0 (44.16-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.168 , 0.187 0.176 , 0.192	Depositor DCC
R_{free} test set	2169 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4093	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, DMS, KQI

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	0.64	1/3637 (0.0%)	0.67	1/4935 (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	AAA	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	776	ASP	C-O	6.11	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	781	ASN	O-C-N	5.41	131.35	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	385	ASN	Peptide
1	AAA	666	SER	Peptide
1	AAA	776	ASP	Mainchain

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	3543	0	3435	8	0
2	AAA	28	0	0	0	0
3	AAA	23	0	0	0	0
4	AAA	4	0	6	0	0
5	AAA	495	0	0	0	0
All	All	4093	0	3441	8	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 1.

All (8) 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:450:HIS:HA	1:AAA:454:THR:OG1	2.14	0.47
1:AAA:744:LYS:O	1:AAA:746:VAL:HG23	2.18	0.44
1:AAA:525:TYR:HB2	1:AAA:555:PRO:HG3	2.00	0.43
1:AAA:782:ALA:O	1:AAA:786:ILE:HG13	2.20	0.42
1:AAA:670:LEU:HD11	1:AAA:711:ILE:HG13	2.01	0.41
1:AAA:393:THR:HB	1:AAA:433:ALA:HB1	2.02	0.41
1:AAA:729:LEU:HD13	1:AAA:748:VAL:HG12	2.03	0.41
1:AAA:519:ILE:N	1:AAA:520:PRO:CD	2.85	0.40

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	459/821 (56%)	448 (98%)	10 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	442	ASN

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	379/679 (56%)	376 (99%)	3 (1%)	81 68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	466	LEU
1	AAA	516	SER
1	AAA	569	ASN

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)

Of 25 ligands modelled in this entry, 23 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KQI	AAA	901	1	26,28,28	0.53	1 (3%)	31,34,34	0.47	0
4	DMS	AAA	925	-	3,3,3	0.29	0	3,3,3	0.11	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
2	KQI	AAA	901	1	-	3/28/30/30	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	901	KQI	N3-N2	2.50	1.29	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	901	KQI	C7-C8-C9-C10
2	AAA	901	KQI	C11-C10-C9-C8
2	AAA	901	KQI	C9-C10-C11-C12

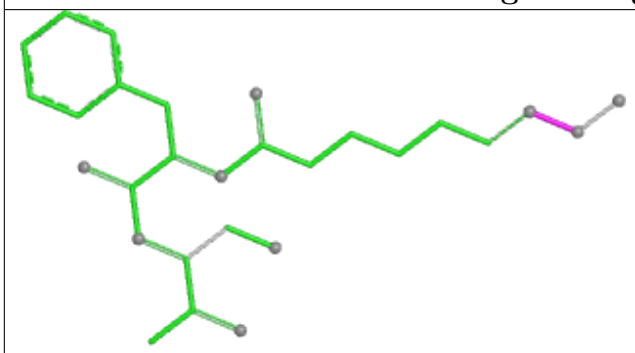
There are no ring outliers.

No monomer is involved in short contacts.

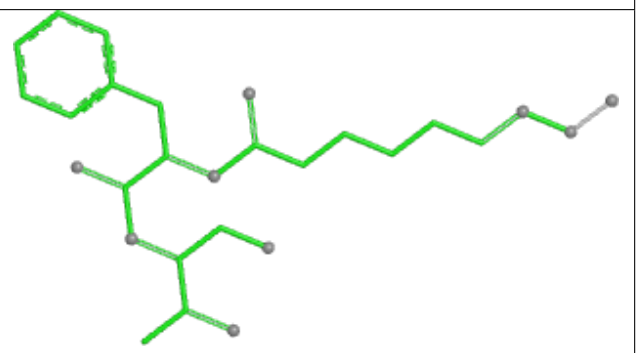
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

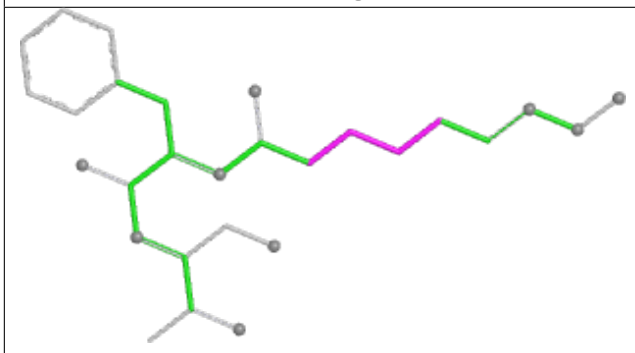
Ligand KQI AAA 901



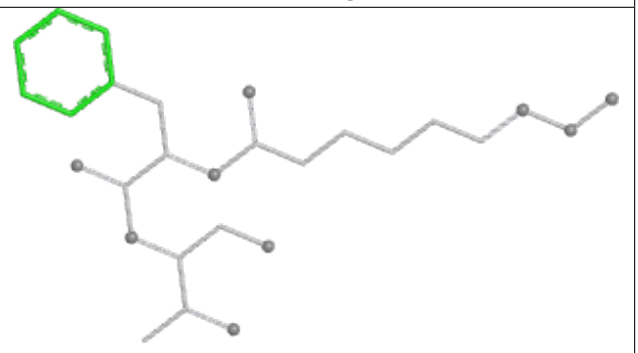
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AAA	454/821 (55%)	0.50	44 (9%) 7 6	33, 44, 78, 112	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	790	LEU	6.4
1	AAA	746	VAL	5.9
1	AAA	787	VAL	5.7
1	AAA	743	GLY	5.6
1	AAA	789	SER	5.0
1	AAA	788	GLY	5.0
1	AAA	742	GLU	4.9
1	AAA	363	ALA	4.4
1	AAA	748	VAL	4.4
1	AAA	744	LYS	4.1
1	AAA	740	SER	3.7
1	AAA	752	THR	3.7
1	AAA	765	ALA	3.7
1	AAA	749	THR	3.7
1	AAA	747	GLU	3.5
1	AAA	738	LYS	3.5
1	AAA	741	VAL	3.4
1	AAA	739	VAL	3.3
1	AAA	736	PRO	3.3
1	AAA	745	GLU	3.3
1	AAA	737	GLY	3.2
1	AAA	364	LYS	3.2
1	AAA	784	SER	3.0
1	AAA	465	LEU	3.0
1	AAA	624	LEU	3.0
1	AAA	780	GLN	2.9
1	AAA	785	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	444	GLN	2.8
1	AAA	649	ILE	2.7
1	AAA	602	ASP	2.6
1	AAA	760	LYS	2.6
1	AAA	701	VAL	2.6
1	AAA	362	SER	2.6
1	AAA	445	GLU	2.5
1	AAA	751	SER	2.3
1	AAA	761	SER	2.2
1	AAA	386	GLY	2.2
1	AAA	665	LEU	2.2
1	AAA	601	GLN	2.1
1	AAA	726	SER	2.1
1	AAA	750	GLY	2.1
1	AAA	786	ILE	2.1
1	AAA	727	GLU	2.1
1	AAA	782	ALA	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	B-factors(Å^2)	Q<0.9
3	CL	AAA	918	1/1	0.82	0.17	77,77,77,77	0
3	CL	AAA	906	1/1	0.86	0.22	74,74,74,74	0
3	CL	AAA	909	1/1	0.88	0.16	68,68,68,68	0
3	CL	AAA	907	1/1	0.88	0.23	74,74,74,74	0
3	CL	AAA	902	1/1	0.90	0.08	55,55,55,55	0
3	CL	AAA	922	1/1	0.91	0.14	67,67,67,67	0

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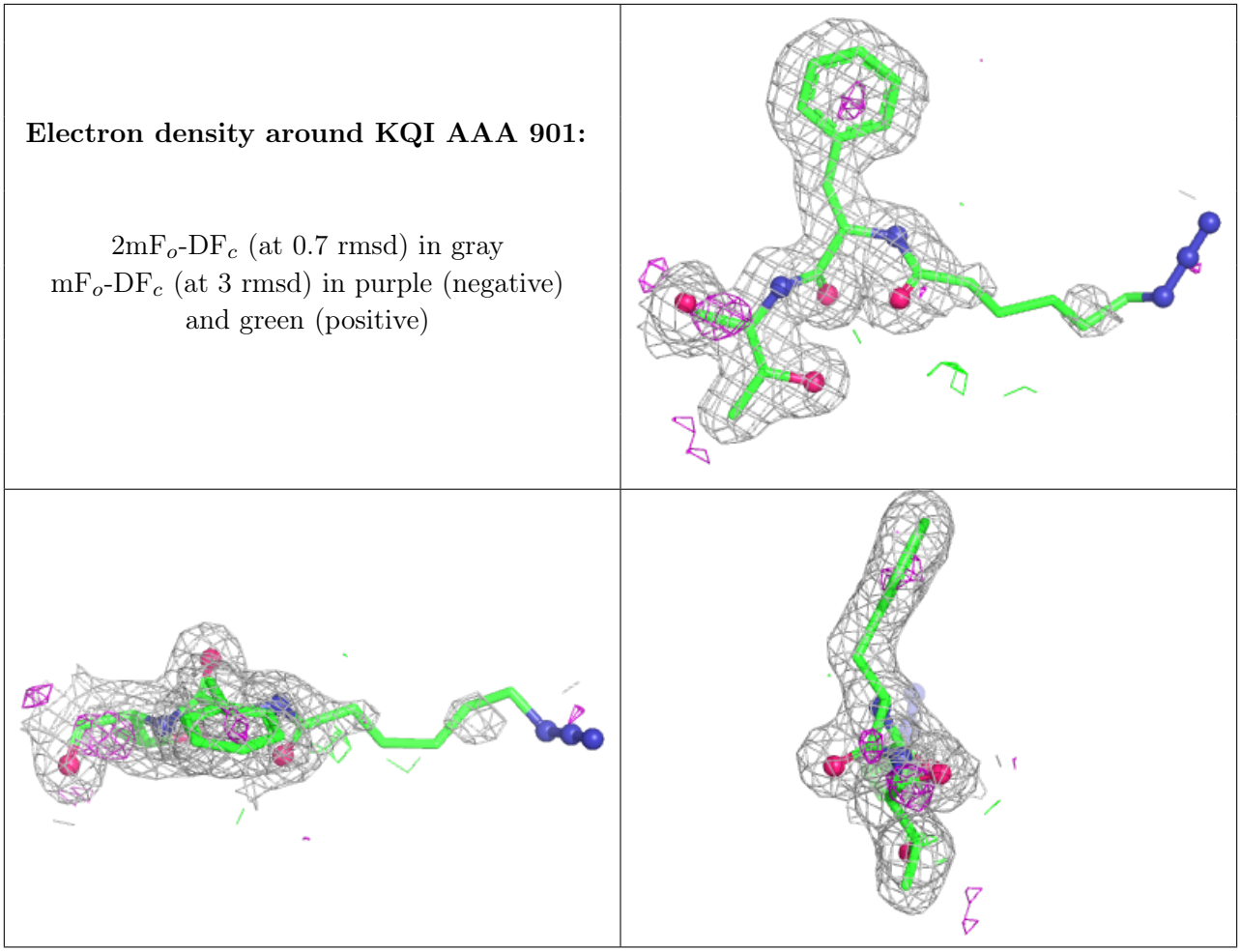
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	AAA	921	1/1	0.92	0.08	60,60,60,60	0
3	CL	AAA	924	1/1	0.93	0.18	72,72,72,72	0
3	CL	AAA	908	1/1	0.94	0.14	66,66,66,66	0
2	KQI	AAA	901	28/28	0.94	0.13	35,48,124,135	0
3	CL	AAA	923	1/1	0.94	0.06	68,68,68,68	0
3	CL	AAA	905	1/1	0.94	0.06	55,55,55,55	0
3	CL	AAA	919	1/1	0.95	0.05	67,67,67,67	0
3	CL	AAA	920	1/1	0.95	0.11	60,60,60,60	0
3	CL	AAA	904	1/1	0.96	0.07	56,56,56,56	0
4	DMS	AAA	925	4/4	0.96	0.12	58,59,65,65	0
3	CL	AAA	903	1/1	0.98	0.09	47,47,47,47	0
3	CL	AAA	910	1/1	0.98	0.10	59,59,59,59	0
3	CL	AAA	911	1/1	0.98	0.09	45,45,45,45	0
3	CL	AAA	912	1/1	0.98	0.06	47,47,47,47	0
3	CL	AAA	913	1/1	0.98	0.06	48,48,48,48	0
3	CL	AAA	914	1/1	0.98	0.05	52,52,52,52	0
3	CL	AAA	916	1/1	0.98	0.16	39,39,39,39	1
3	CL	AAA	917	1/1	0.98	0.04	56,56,56,56	0
3	CL	AAA	915	1/1	0.99	0.04	57,57,57,57	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 KQI AAA 901:

$2mF_o$-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.