Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:47 pm BST

PDB ID	:	2BAL
Title	:	p38alpha MAP kinase bound to pyrazoloamine
Authors	:	Gerhardt, S.; Pauptit, R.A.; Read, J.; Tucker, J.; Norman, R.A.; Breed, J.
Deposited on	:	2005-10-14
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

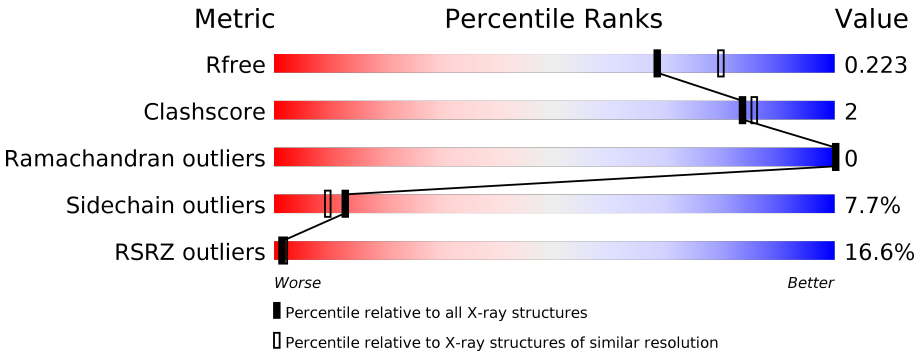
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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
1	A	365	15% 81% 10% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2843 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.

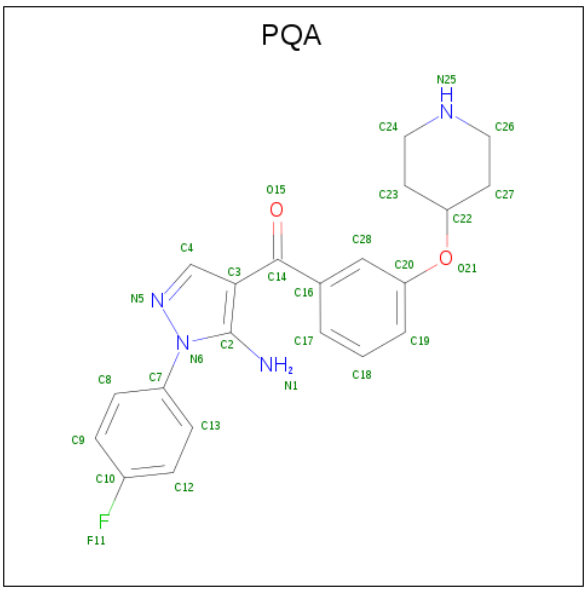
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2726	1750	465	498	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP Q16539
A	-3	HIS	-	EXPRESSION TAG	UNP Q16539
A	-2	HIS	-	EXPRESSION TAG	UNP Q16539
A	-1	HIS	-	EXPRESSION TAG	UNP Q16539
A	0	HIS	-	EXPRESSION TAG	UNP Q16539
A	1	HIS	-	EXPRESSION TAG	UNP Q16539
A	162	CSS	CYS	MODIFIED RESIDUE	UNP Q16539

- Molecule 2 is [5-AMINO-1-(4-FLUOROPHENYL)-1H-PYRAZOL-4-YL][3-(PIPERIDIN-4-YLOXY)PHENYL]METHANONE (three-letter code: PQA) (formula: $C_{21}H_{21}FN_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	21	1	4	2		

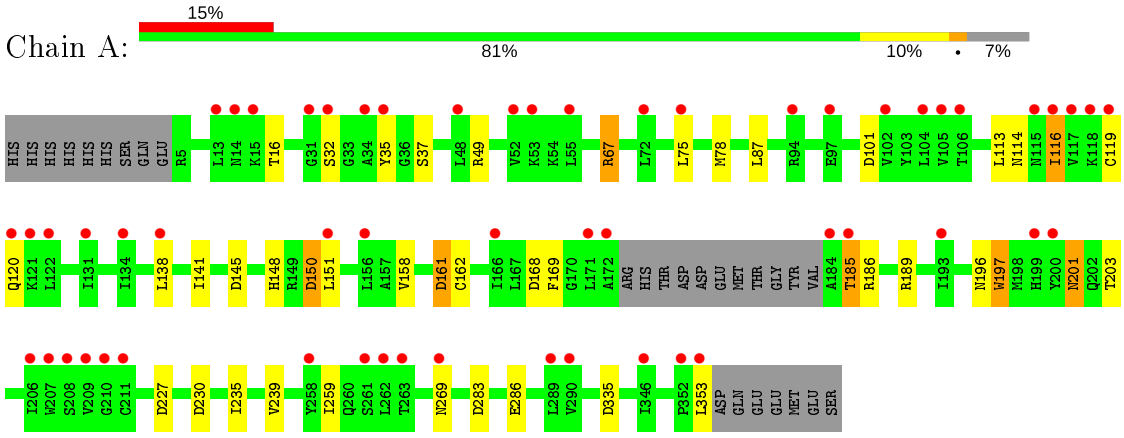
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Mitogen-activated protein kinase 14



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.19Å 75.16Å 77.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.54 – 2.10 24.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.1 (24.54-2.10) 89.1 (24.51-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.265 0.234 , 0.223	Depositor DCC
R_{free} test set	1067 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2843	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% 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: PQA, CSS

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	A	0.44	0/2781	0.73	8/3774 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	283	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	150	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	227	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	101	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	145	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	335	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	168	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	2726	0	2731	13	0
2	A	28	0	21	0	0
3	A	89	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2843	0	2752	13	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 2.

All (13) 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:148:HIS:CD2	1:A:169:PHE:HA	2.17	0.80
1:A:148:HIS:CD2	1:A:169:PHE:CA	2.85	0.60
1:A:35:TYR:CE1	1:A:67:ARG:HG3	2.41	0.55
1:A:78:MET:HG3	1:A:169:PHE:CZ	2.43	0.54
1:A:116:ILE:HG21	1:A:158:VAL:CG2	2.39	0.53
1:A:148:HIS:HD2	1:A:169:PHE:HB3	1.75	0.50
1:A:150:ASP:OD1	1:A:185:THR:OG1	2.27	0.50
1:A:138:LEU:HD23	1:A:141:ILE:HD11	1.94	0.50
1:A:201:ASN:ND2	1:A:203:THR:OG1	2.44	0.48
1:A:161:ASP:O	1:A:162:CSS:HB3	2.14	0.48
1:A:235:ILE:O	1:A:239:VAL:HG22	2.18	0.43
1:A:197:TRP:CZ3	1:A:259:ILE:HD11	2.54	0.41
1:A:116:ILE:HG21	1:A:158:VAL:HG21	2.04	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	A	333/365 (91%)	324 (97%)	9 (3%)	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	A	298/324 (92%)	275 (92%)	23 (8%)	13 9

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	32	SER
1	A	37	SER
1	A	49	ARG
1	A	67	ARG
1	A	75	LEU
1	A	87	LEU
1	A	113	LEU
1	A	114	ASN
1	A	116	ILE
1	A	119	CYS
1	A	120	GLN
1	A	151	LEU
1	A	161	ASP
1	A	185	THR
1	A	186	ARG
1	A	189	ARG
1	A	196	ASN
1	A	197	TRP
1	A	201	ASN
1	A	269	ASN
1	A	286	GLU
1	A	353	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	114	ASN

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	201	ASN
1	A	272	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSS	A	162	1	4,6,7	0.66	0	1,6,8	0.31	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
1	CSS	A	162	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	162	CSS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PQA	A	401	-	29,31,31	0.99	2 (6%)	32,43,43	1.35	5 (15%)

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	PQA	A	401	-	-	2/12/24/24	1/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PQA	C2-N6	2.51	1.39	1.37
2	A	401	PQA	C3-C14	-2.30	1.45	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	PQA	C8-C7-N6	3.68	126.48	119.50
2	A	401	PQA	C13-C7-N6	-3.00	113.80	119.50
2	A	401	PQA	C4-C3-C14	2.66	132.24	127.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	PQA	C20-O21-C22	-2.49	114.14	119.13
2	A	401	PQA	C8-C9-C10	2.17	120.60	118.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PQA	C19-C20-O21-C22
2	A	401	PQA	C28-C20-O21-C22

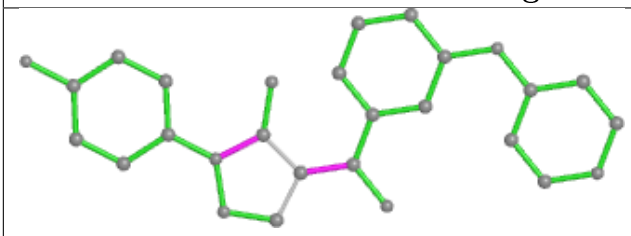
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PQA	C22-C23-C24-C26-C27-N25

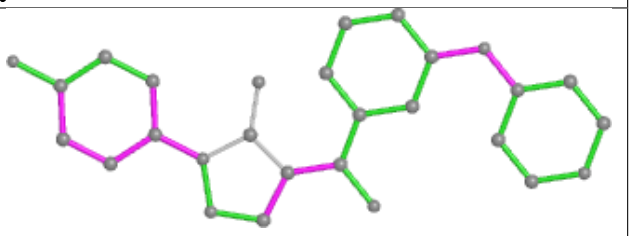
No monomer is involved in short contacts.

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.

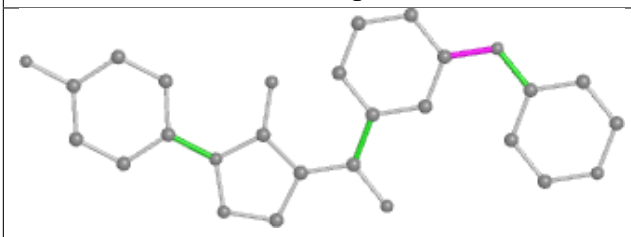
Ligand PQA A 401



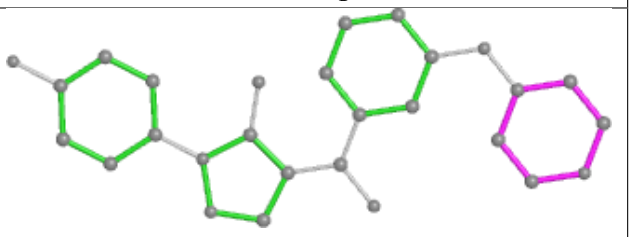
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	337/365 (92%)	1.00	56 (16%) 1 2	18, 26, 44, 56	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	CYS	8.4
1	A	120	GLN	6.4
1	A	14	ASN	5.7
1	A	118	LYS	5.3
1	A	104	LEU	5.3
1	A	48	LEU	5.2
1	A	353	LEU	4.9
1	A	121	LYS	4.9
1	A	184	ALA	4.8
1	A	185	THR	4.7
1	A	134	ILE	4.6
1	A	131	ILE	4.3
1	A	209	VAL	4.1
1	A	263	THR	3.9
1	A	94	ARG	3.9
1	A	166	ILE	3.9
1	A	211	CYS	3.7
1	A	352	PRO	3.7
1	A	34	ALA	3.7
1	A	171	LEU	3.6
1	A	52	VAL	3.5
1	A	117	VAL	3.4
1	A	207	TRP	3.3
1	A	200	TYR	3.2
1	A	289	LEU	3.2
1	A	172	ALA	3.1
1	A	138	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	206	ILE	2.9
1	A	15	LYS	2.8
1	A	102	VAL	2.8
1	A	210	GLY	2.8
1	A	55	LEU	2.8
1	A	105	VAL	2.7
1	A	35	TYR	2.7
1	A	13	LEU	2.7
1	A	193	ILE	2.7
1	A	116	ILE	2.5
1	A	97	GLU	2.4
1	A	75	LEU	2.4
1	A	151	LEU	2.4
1	A	262	LEU	2.3
1	A	208	SER	2.3
1	A	290	VAL	2.3
1	A	269	ASN	2.3
1	A	258	TYR	2.3
1	A	32	SER	2.3
1	A	261	SER	2.2
1	A	72	LEU	2.2
1	A	115	ASN	2.2
1	A	156	LEU	2.2
1	A	122	LEU	2.1
1	A	31	GLY	2.1
1	A	106	THR	2.1
1	A	346	ILE	2.1
1	A	53	LYS	2.1
1	A	199	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSS	A	162	7/8	0.91	0.13	24,25,25,27	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

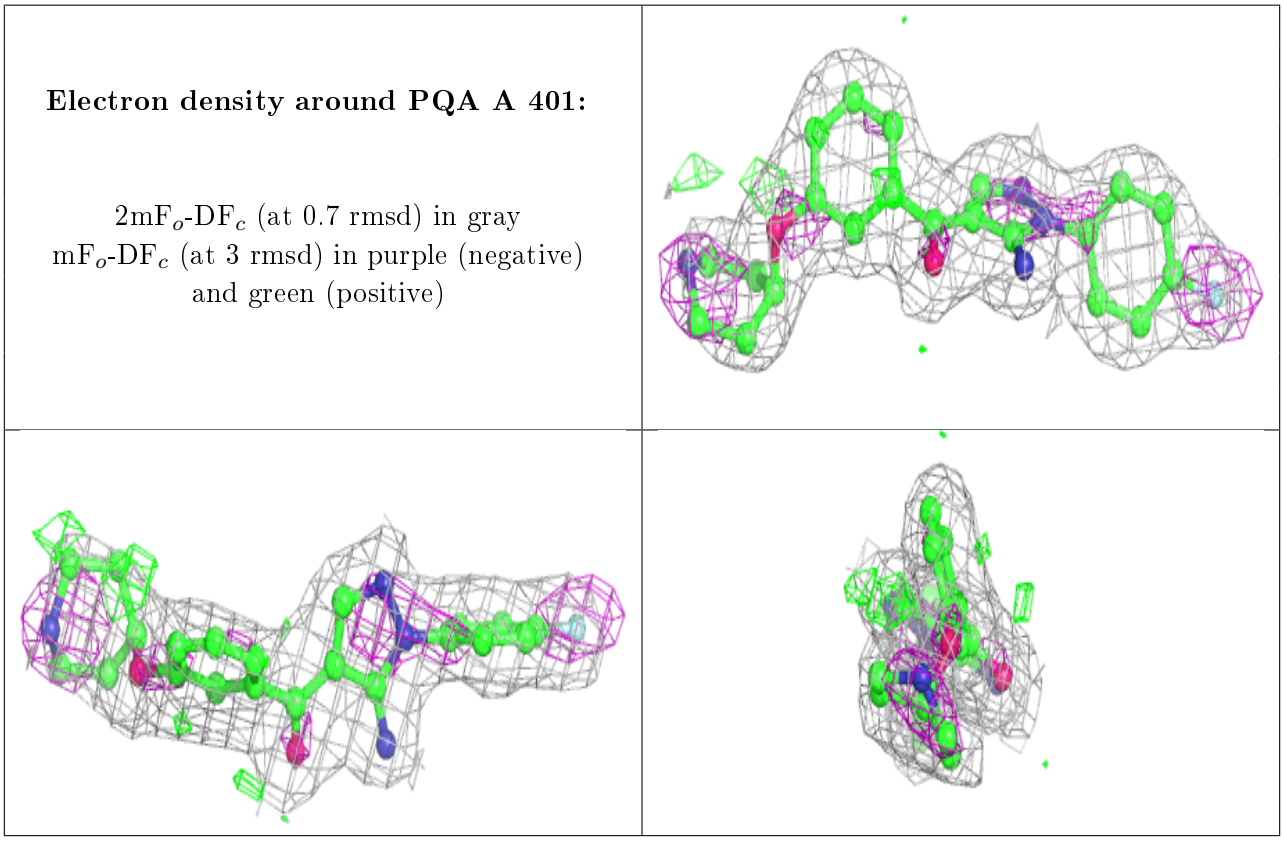
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	PQA	A	401	28/28	0.85	0.17	20,26,37,37	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 PQA A 401:

$2mF_o$-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.