



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:40 PM UTC

PDB ID : 5UJB / pdb_00005ujb
Title : Structure of a Mcl-1 Inhibitor Binding to Site 3 of Human Serum Albumin
Authors : Zhao, B.
Deposited on : 2017-01-17
Resolution : 2.70 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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

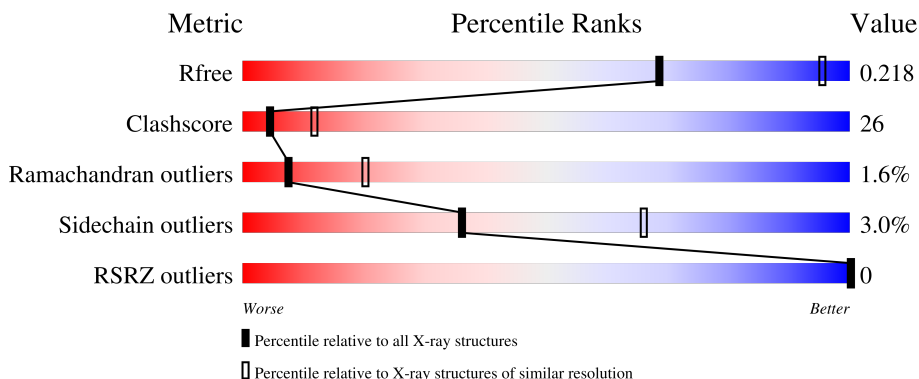
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	609	 54% 36% 7%
1	B	609	 51% 40% 7%

2 Entry composition i

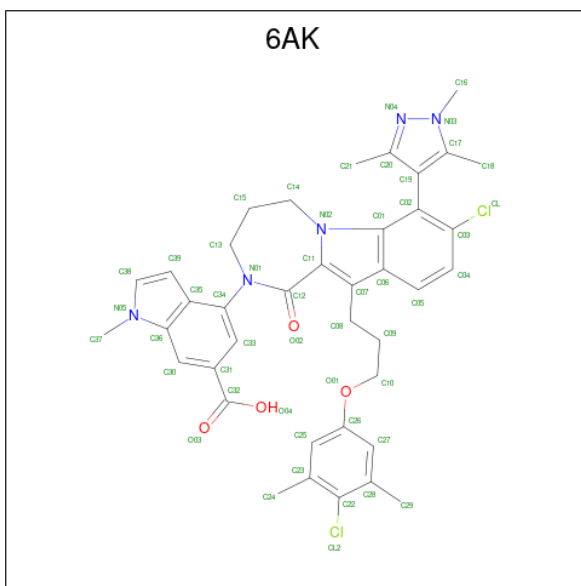
There are 3 unique types of molecules in this entry. The entry contains 8812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	Total 4364	C 2760	N 736	O 828	S 40	0	0	0
1	B	565	Total 4338	C 2749	N 722	O 826	S 41	0	0	0

- Molecule 2 is 4-{8-chloro-11-[3-(4-chloro-3,5-dimethylphenoxy)propyl]-1-oxo-7-(1,3,5-trimethyl-1H-pyrazol-4-yl)-4,5-dihydro-1H-[1,4]diazepino[1,2-a]indol-2(3H)-yl}-1-methyl-1H-indole-6-carboxylic acid (CCD ID: 6AK) (formula: C₃₉H₃₉Cl₂N₅O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	Total 50	C 39	Cl 2	N 5	O 4	0	0
2	B	1	Total 50	C 39	Cl 2	N 5	O 4	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



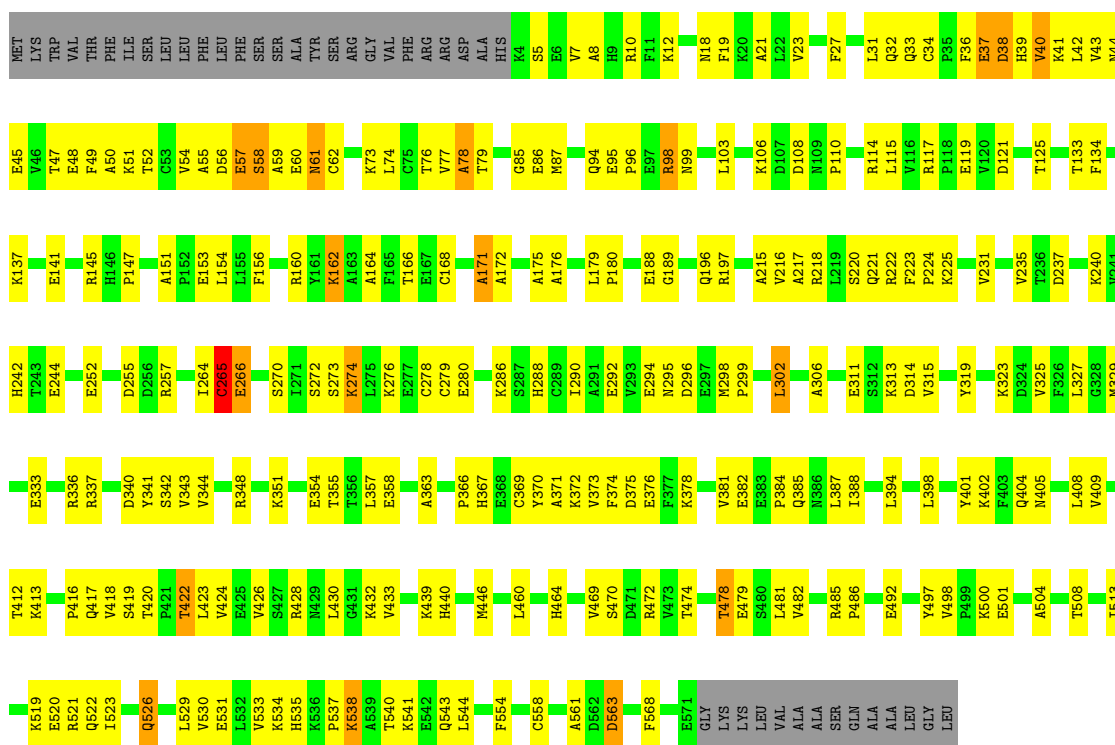
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

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.

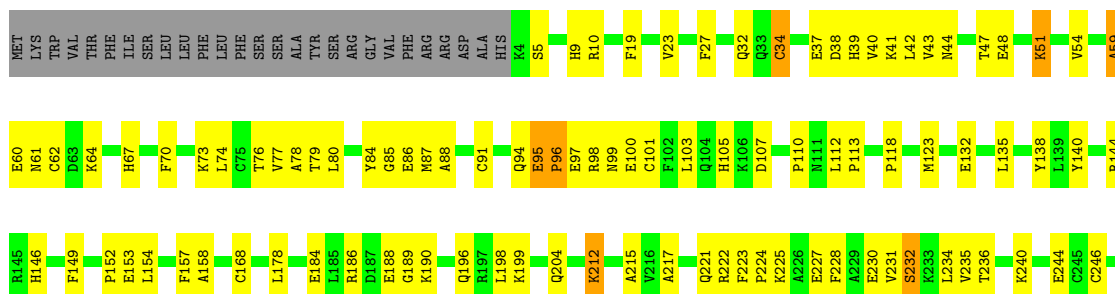
- Molecule 1: Serum albumin

Chain A: 



- Molecule 1: Serum albumin

Chain B: 



GLN	F607	R410	Y334	D249
ALA	A511	Y411	A335	L250
ALA	D612	T412	R336	L251
LEU	I513	K413	R337	E252
GLY	C514	K414	D340	R257
LEU	T515	W415	Y341	
	L516	P416	S342	L260
	E520	Q417	V343	A261
	R521	V418	V344	K262
	A522	T420	L345	Y263
	K525	P421	L346	I264
	Q526	T422	I347	C265
	T527	V426	R348	E266
	A528	S427	L349	N267
	V530	R428	A350	Q268
	E531	G431	K351	S272
	L532	G434	T355	S273
	V533	S435	T356	K274
	K534	K436	L357	L275
	H535	K437	E358	K276
	K538	C438	K359	E280
	A539	K439	C360	K281
	T540	H440	P366	F282
	K541	P441	H367	L283
	E542	E442	Y370	L284
	Q543	K444	D375	E285
	L544	M445	E376	K286
	R545	M446	F377	D286
	V547	C448	K378	
	M548	A449	P379	P299
	D549	E450	L380	A300
	D550	D451	V381	D301
	F554	Y452	P384	L302
	A561	L453	Q385	P303
	D562	S454	N386	A306
	K564	V455	L387	
	E565	N458	I388	F309
	T566	Q459	K389	V310
	C567	L460	Q390	E311
	F568	C461	N391	K317
ALA	ALA	V462	C392	N318
GLU	GLU	L463	E393	Y319
GLU	GLU	L461	L394	A320
GLY	GLY	L481	L398	E321
LYS	LYS	R484	G399	V325
LYS	LYS	R485	E400	F326
LEU	LEU	P486	Q404	L327
VAL	VAL	F488	N405	G328
ALA	ALA	K500	L408	M329
ALA	ALA		L331	F330
SER	SER		V409	Y332
				E333

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 182.34Å 58.92Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	28.76 – 2.70 28.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.9 (28.76-2.70) 92.4 (28.76-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.174 , 0.215 0.185 , 0.218	Depositor DCC
R_{free} test set	2003 reflections (6.55%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.299 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8812	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: 6AK, PO4

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	0.53	1/4448 (0.0%)	0.89	0/6024
1	B	0.53	0/4425	0.90	2/6001 (0.0%)
All	All	0.53	1/8873 (0.0%)	0.89	2/12025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	ASP	CA-C	-5.21	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	LEU	CA-C-N	-5.72	114.07	119.85
1	B	302	LEU	C-N-CA	-5.72	114.07	119.85

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	A	4364	0	4111	226	0
1	B	4338	0	4082	221	0
2	A	50	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	50	0	0	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
All	All	8812	0	8193	445	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 26.

The worst 5 of 445 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:59:ALA:HB3	1:A:62:CYS:SG	1.46	1.55
1:A:302:LEU:HD12	1:A:337:ARG:NH1	1.27	1.48
1:A:302:LEU:CD1	1:A:337:ARG:HH12	1.38	1.35
1:A:59:ALA:CB	1:A:62:CYS:SG	2.20	1.28
1:A:265:CYS:SG	1:A:279:CYS:SG	1.45	1.23

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	566/609 (93%)	506 (89%)	50 (9%)	10 (2%)	6	18
1	B	563/609 (92%)	505 (90%)	50 (9%)	8 (1%)	9	23
All	All	1129/1218 (93%)	1011 (90%)	100 (9%)	18 (2%)	7	20

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	SER

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Mol	Chain	Res	Type
1	A	78	ALA
1	B	60	GLU
1	B	439	LYS
1	A	57	GLU

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	441/533 (83%)	420 (95%)	21 (5%)	23	50
1	B	448/533 (84%)	442 (99%)	6 (1%)	61	83
All	All	889/1066 (83%)	862 (97%)	27 (3%)	36	66

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LEU
1	A	481	LEU
1	B	440	HIS
1	A	478	THR
1	A	482	VAL

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

Mol	Chain	Res	Type
1	B	61	ASN
1	B	130	ASN
1	B	104	GLN
1	B	268	GLN
1	A	385	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	A	801	-	4,4,4	1.17	0	6,6,6	2.67	3 (50%)
2	6AK	B	802	-	55,56,56	1.18	7 (12%)	70,85,85	2.14	20 (28%)
3	PO4	B	801	-	4,4,4	1.12	0	6,6,6	1.61	1 (16%)
2	6AK	A	800	-	55,56,56	1.23	5 (9%)	70,85,85	2.39	26 (37%)

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	6AK	B	802	-	-	5/19/33/33	0/6/7/7
2	6AK	A	800	-	-	7/19/33/33	0/6/7/7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	6AK	C08-C07	-3.15	1.46	1.51
2	B	802	6AK	C05-C04	2.60	1.43	1.38
2	A	800	6AK	C35-C34	2.54	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	6AK	C19-C20	2.52	1.46	1.42
2	B	802	6AK	C30-C31	2.50	1.43	1.39

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	6AK	C09-C08-C07	-9.26	98.71	113.30
2	B	802	6AK	C13-C15-C14	-5.70	100.64	113.99
2	B	802	6AK	C16-N03-C17	-5.19	123.35	128.09
2	B	802	6AK	C09-C08-C07	-5.15	105.19	113.30
3	A	801	PO4	O4-P-O2	-5.14	91.91	107.91

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

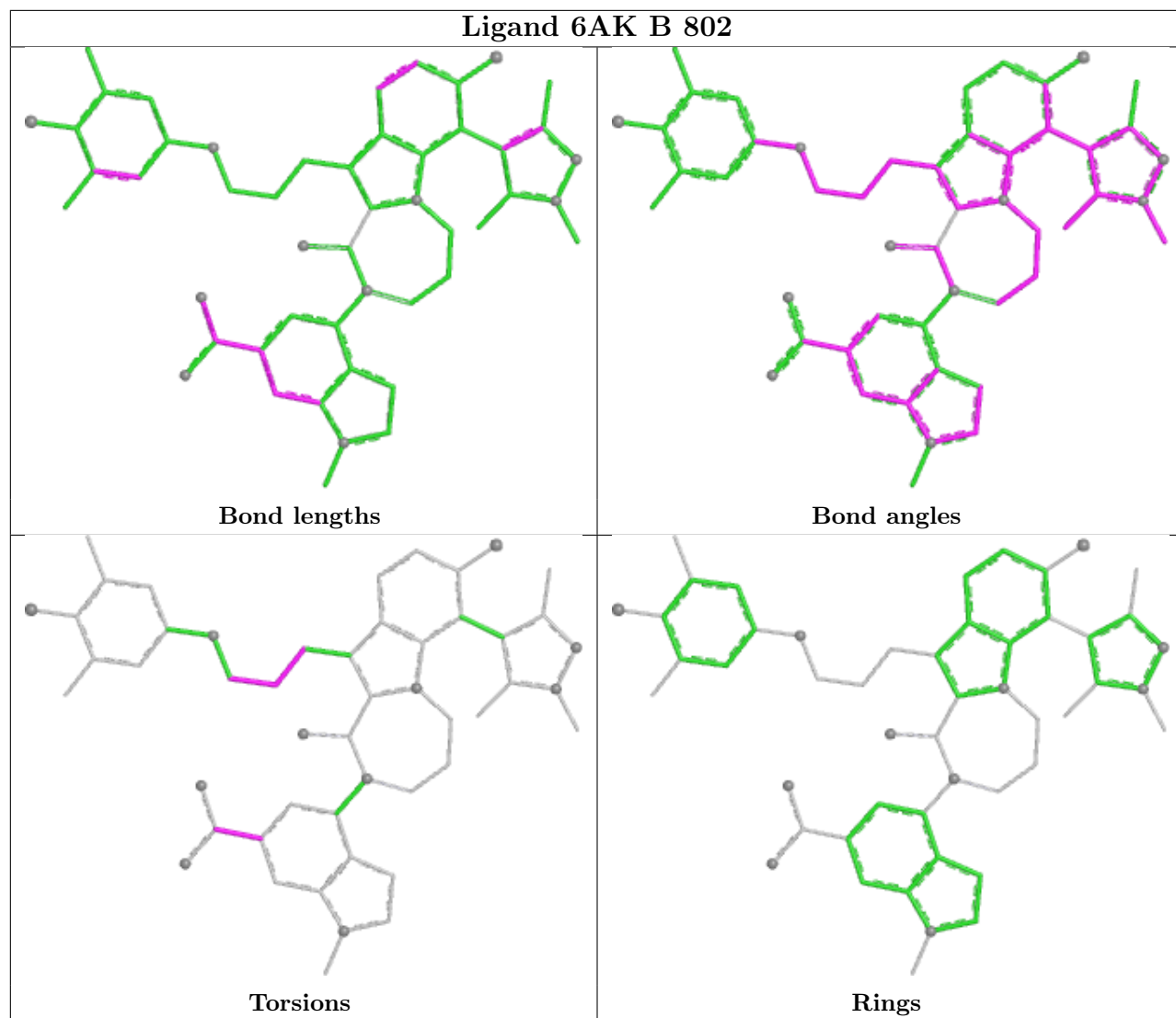
Mol	Chain	Res	Type	Atoms
2	A	800	6AK	C07-C08-C09-C10
2	B	802	6AK	C07-C08-C09-C10
2	B	802	6AK	C08-C09-C10-O01
2	A	800	6AK	C08-C09-C10-O01
2	A	800	6AK	C33-C31-C32-O04

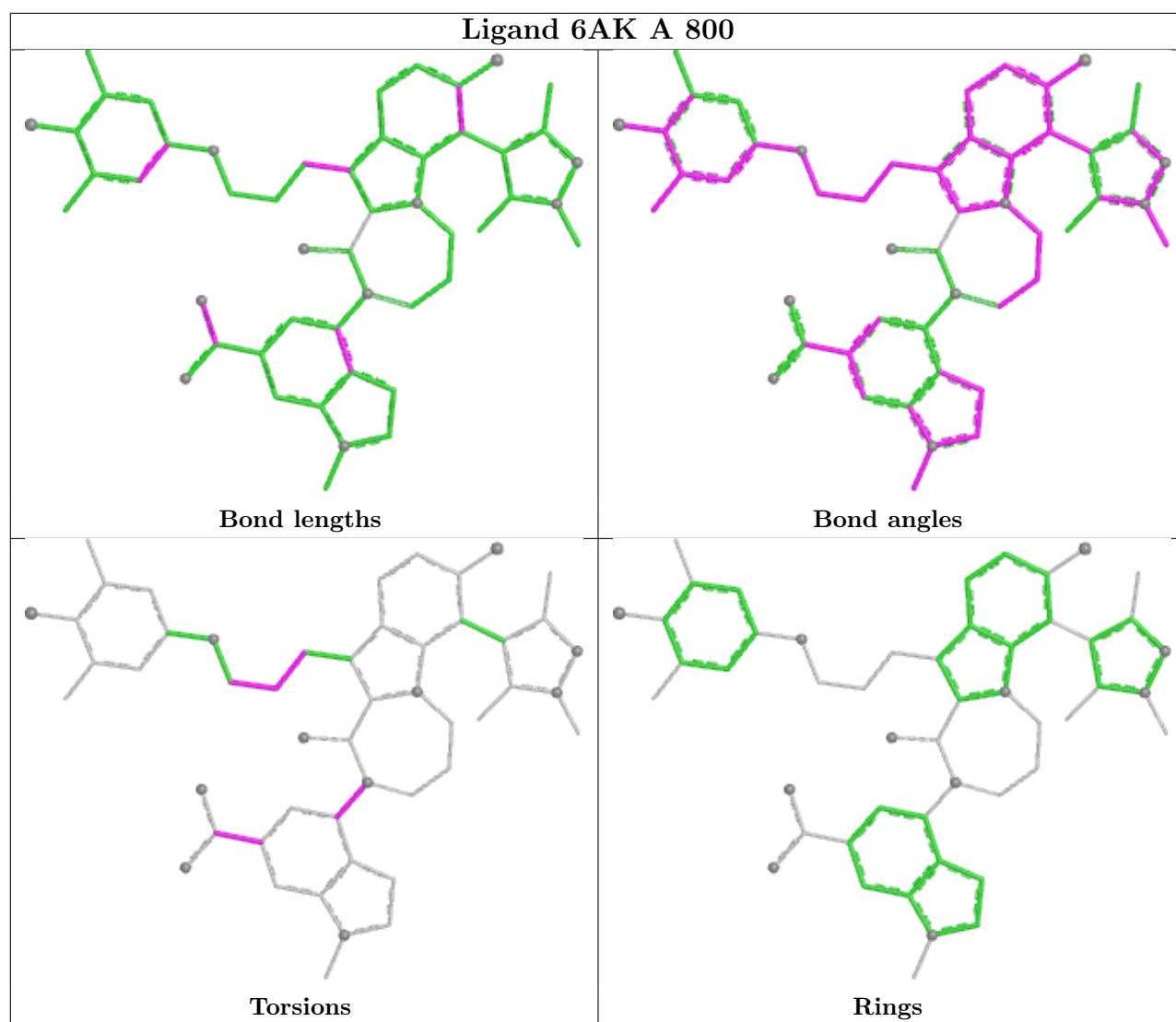
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PO4	1	0
2	B	802	6AK	4	0
2	A	800	6AK	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 than 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	A	568/609 (93%)	-0.93	0 100 100	36, 64, 110, 134	0
1	B	565/609 (92%)	-0.87	0 100 100	42, 70, 110, 139	0
All	All	1133/1218 (93%)	-0.90	0 100 100	36, 67, 110, 139	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

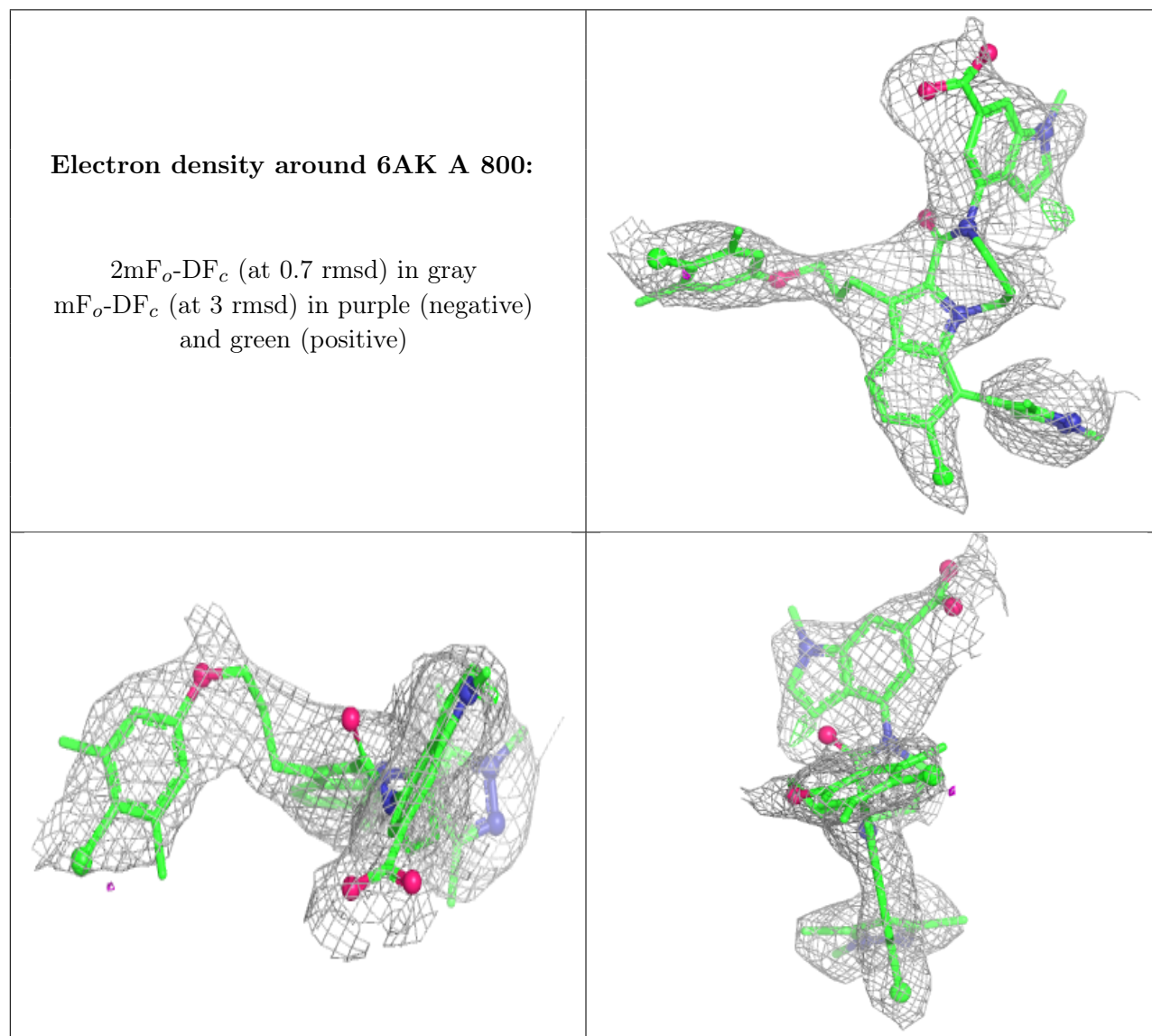
6.4 Ligands [i](#)

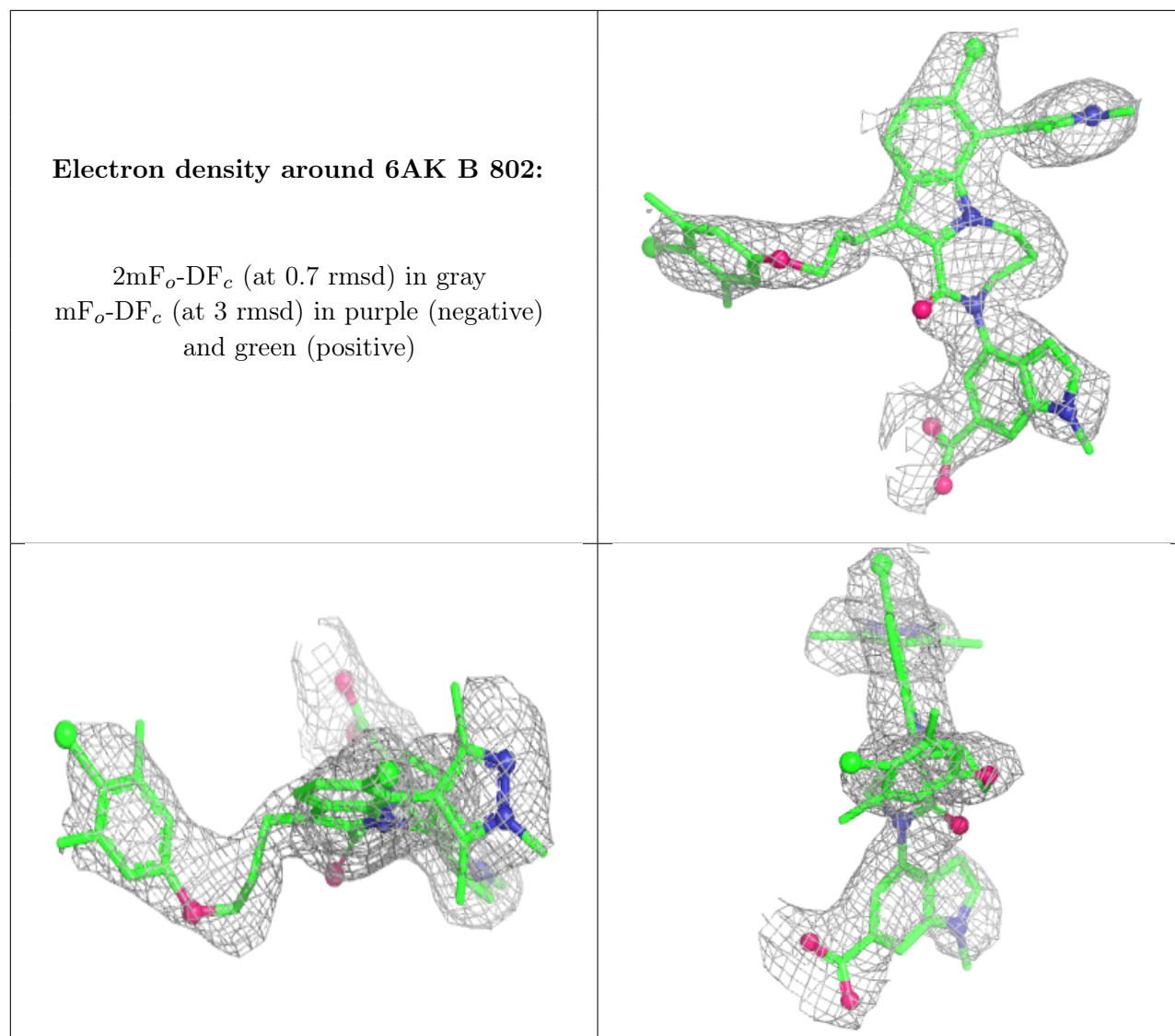
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	PO4	A	801	5/5	0.96	0.04	37,47,60,77	0
3	PO4	B	801	5/5	0.97	0.04	30,42,55,56	0
2	6AK	A	800	50/50	0.98	0.07	26,61,87,91	50
2	6AK	B	802	50/50	0.98	0.06	23,51,61,88	50

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.