



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2025 – 12:07 PM EDT

PDB ID : 9CSK
Title : Crystal structure of CDK4 cyclin D1 in complex with atirmociclib
Authors : Johnson, E.
Deposited on : 2024-07-24
Resolution : 2.25 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

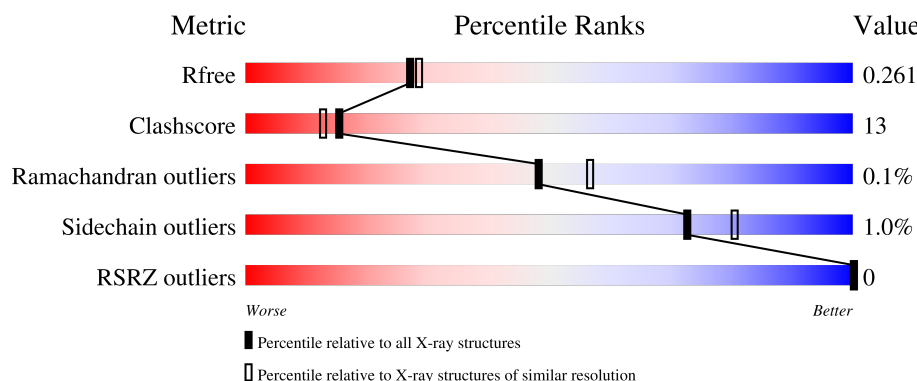
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	257	 77% 13% 9%
1	C	257	 82% 12% 5%
2	B	314	 64% 25% 11%
2	D	314	 66% 24% 10%

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	Res	Chirality	Geometry	Clashes	Electron density
3	A1AZ4	B	9001	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8626 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 G1/S-specific cyclin-D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1855	1184	312	339	20			
1	C	243	Total	C	N	O	S	0	1	0
			1933	1235	325	353	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP P24385
C	15	MET	-	initiating methionine	UNP P24385

- Molecule 2 is a protein called Cyclin-dependent kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2201	1409	386	396	10			
2	D	283	Total	C	N	O	S	0	0	0
			2245	1438	394	403	10			

There are 38 discrepancies between the modelled and reference sequences:

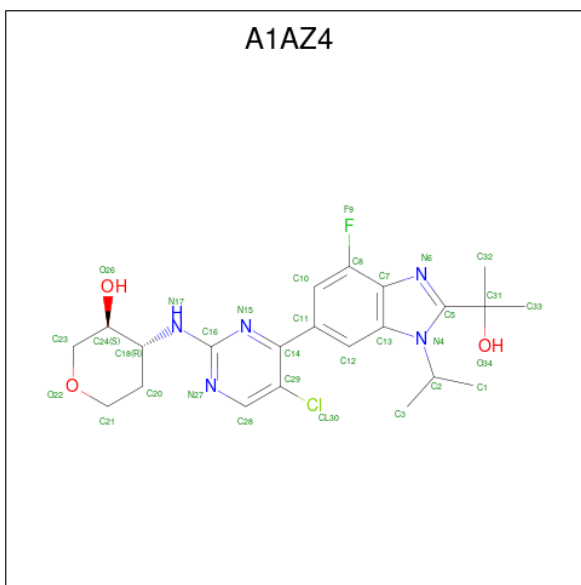
Chain	Residue	Modelled	Actual	Comment	Reference
B	43	GLU	GLY	engineered mutation	UNP P11802
B	44	GLU	GLY	engineered mutation	UNP P11802
B	?	-	GLY	deletion	UNP P11802
B	?	-	GLY	deletion	UNP P11802
B	?	-	GLY	deletion	UNP P11802
B	304	LEU	-	expression tag	UNP P11802
B	305	GLU	-	expression tag	UNP P11802
B	306	ASN	-	expression tag	UNP P11802
B	307	LEU	-	expression tag	UNP P11802
B	308	TYR	-	expression tag	UNP P11802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	309	PHE	-	expression tag	UNP P11802
B	310	GLN	-	expression tag	UNP P11802
B	311	GLY	-	expression tag	UNP P11802
B	312	HIS	-	expression tag	UNP P11802
B	313	HIS	-	expression tag	UNP P11802
B	314	HIS	-	expression tag	UNP P11802
B	315	HIS	-	expression tag	UNP P11802
B	316	HIS	-	expression tag	UNP P11802
B	317	HIS	-	expression tag	UNP P11802
D	43	GLU	GLY	engineered mutation	UNP P11802
D	44	GLU	GLY	engineered mutation	UNP P11802
D	?	-	GLY	deletion	UNP P11802
D	?	-	GLY	deletion	UNP P11802
D	?	-	GLY	deletion	UNP P11802
D	304	LEU	-	expression tag	UNP P11802
D	305	GLU	-	expression tag	UNP P11802
D	306	ASN	-	expression tag	UNP P11802
D	307	LEU	-	expression tag	UNP P11802
D	308	TYR	-	expression tag	UNP P11802
D	309	PHE	-	expression tag	UNP P11802
D	310	GLN	-	expression tag	UNP P11802
D	311	GLY	-	expression tag	UNP P11802
D	312	HIS	-	expression tag	UNP P11802
D	313	HIS	-	expression tag	UNP P11802
D	314	HIS	-	expression tag	UNP P11802
D	315	HIS	-	expression tag	UNP P11802
D	316	HIS	-	expression tag	UNP P11802
D	317	HIS	-	expression tag	UNP P11802

- Molecule 3 is Atirmociclib (three-letter code: A1AZ4) (formula: $C_{22}H_{27}ClFN_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			32	22	1	1	5	3		
3	D	1	Total	C	Cl	F	N	O	0	0
			32	22	1	1	5	3		

- Molecule 4 is water.

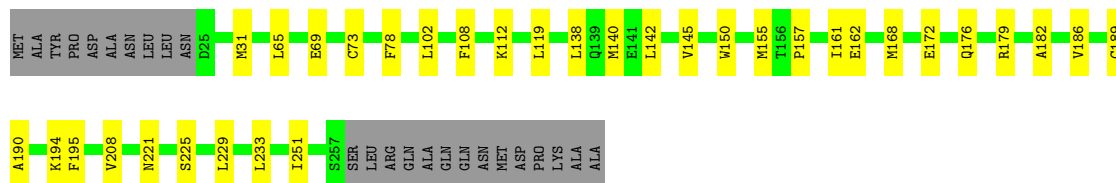
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	59	Total	O	0	0
			59	59		
4	C	95	Total	O	0	0
			95	95		
4	D	83	Total	O	0	0
			83	83		

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.

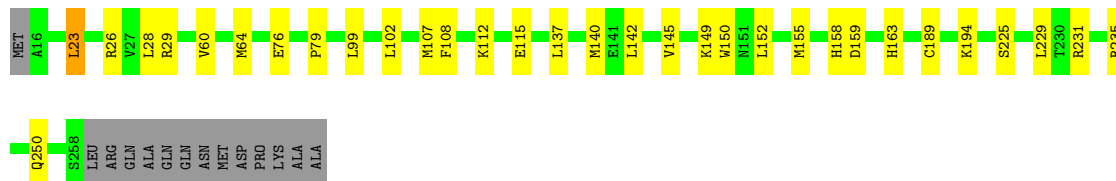
- Molecule 1: G1/S-specific cyclin-D1

Chain A:



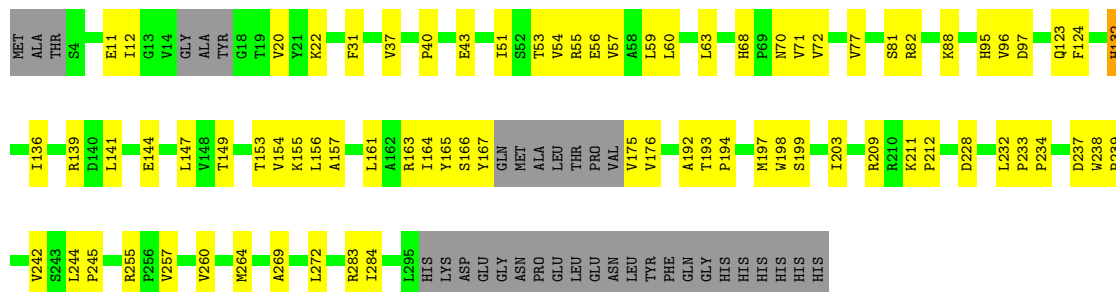
- Molecule 1: G1/S-specific cyclin-D1

Chain C:



- Molecule 2: Cyclin-dependent kinase 4

Chain B:



- Molecule 2: Cyclin-dependent kinase 4

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.51Å 64.29Å 186.21Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	38.93 – 2.25 38.93 – 2.25	Depositor EDS
% Data completeness (in resolution range)	77.9 (38.93-2.25) 78.0 (38.93-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.8 (24-FEB-2021)	Depositor
R, R_{free}	0.224 , 0.270 0.228 , 0.261	Depositor DCC
R_{free} test set	2479 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.097 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8626	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1AZ4

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	0.51	0/1888	0.58	0/2550
1	C	0.57	1/1971 (0.1%)	0.59	0/2664
2	B	0.54	0/2256	0.64	0/3068
2	D	0.58	0/2302	0.67	2/3130 (0.1%)
All	All	0.55	1/8417 (0.0%)	0.62	2/11412 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	GLU	CD-OE1	-5.33	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	217	ASN	CB-CA-C	-7.82	94.75	110.40
2	D	145	ASN	CB-CA-C	5.66	121.71	110.40

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	1855	0	1909	35	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1933	0	1989	31	0
2	B	2201	0	2192	89	1
2	D	2245	0	2252	76	0
3	B	32	0	0	10	0
3	D	32	0	0	3	0
4	A	91	0	0	0	0
4	B	59	0	0	1	0
4	C	95	0	0	1	0
4	D	83	0	0	0	0
All	All	8626	0	8342	221	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 13.

The worst 5 of 221 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:142:LEU:CD1	2:B:82:ARG:HD3	1.58	1.30
2:D:107:ALA:HB2	2:D:112:LEU:HD11	1.18	1.18
1:A:142:LEU:HD11	2:B:82:ARG:HD3	1.11	1.09
2:D:107:ALA:HB2	2:D:112:LEU:CD1	1.92	0.99
2:B:22:LYS:HE3	2:B:31:PHE:CD2	1.98	0.98

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)
1:A:221:ASN:ND2	2:B:166:SER:OG[2_555]	2.02	0.18

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	231/257 (90%)	229 (99%)	2 (1%)	0	100	100
1	C	242/257 (94%)	239 (99%)	3 (1%)	0	100	100
2	B	273/314 (87%)	267 (98%)	6 (2%)	0	100	100
2	D	279/314 (89%)	271 (97%)	7 (2%)	1 (0%)	30	32
All	All	1025/1142 (90%)	1006 (98%)	18 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	175	VAL

5.3.2 Protein sidechains ⓘ

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	210/229 (92%)	210 (100%)	0	100	100
1	C	218/229 (95%)	215 (99%)	3 (1%)	62	72
2	B	239/272 (88%)	237 (99%)	2 (1%)	79	86
2	D	245/272 (90%)	241 (98%)	4 (2%)	58	69
All	All	912/1002 (91%)	903 (99%)	9 (1%)	73	80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	184	GLU
2	D	288	ARG
1	C	76	GLU
1	C	137	LEU
2	D	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	213	GLN
2	D	98	GLN
2	D	222	GLN
2	D	123	GLN
2	B	123	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](#)

2 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	A1AZ4	B	9001	-	31,35,35	1.49	6 (19%)	37,53,53	2.43	11 (29%)
3	A1AZ4	D	9001	-	31,35,35	1.58	5 (16%)	37,53,53	2.72	12 (32%)

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
3	A1AZ4	B	9001	-	-	0/14/29/29	0/4/4/4
3	A1AZ4	D	9001	-	-	1/14/29/29	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	9001	A1AZ4	C16-N17	4.80	1.40	1.34
3	B	9001	A1AZ4	C16-N17	4.38	1.39	1.34
3	D	9001	A1AZ4	C11-C14	-3.53	1.45	1.49
3	B	9001	A1AZ4	C11-C14	-3.33	1.45	1.49
3	D	9001	A1AZ4	C2-N4	-3.07	1.43	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	9001	A1AZ4	C28-C29-C14	-7.88	116.35	120.43
3	D	9001	A1AZ4	C16-N17-C18	-7.49	112.67	124.32
3	D	9001	A1AZ4	F9-C8-C7	6.84	120.21	117.37
3	B	9001	A1AZ4	F9-C8-C7	6.72	120.16	117.37
3	B	9001	A1AZ4	C28-C29-C14	-5.94	117.35	120.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	9001	A1AZ4	C3-C2-N4-C13

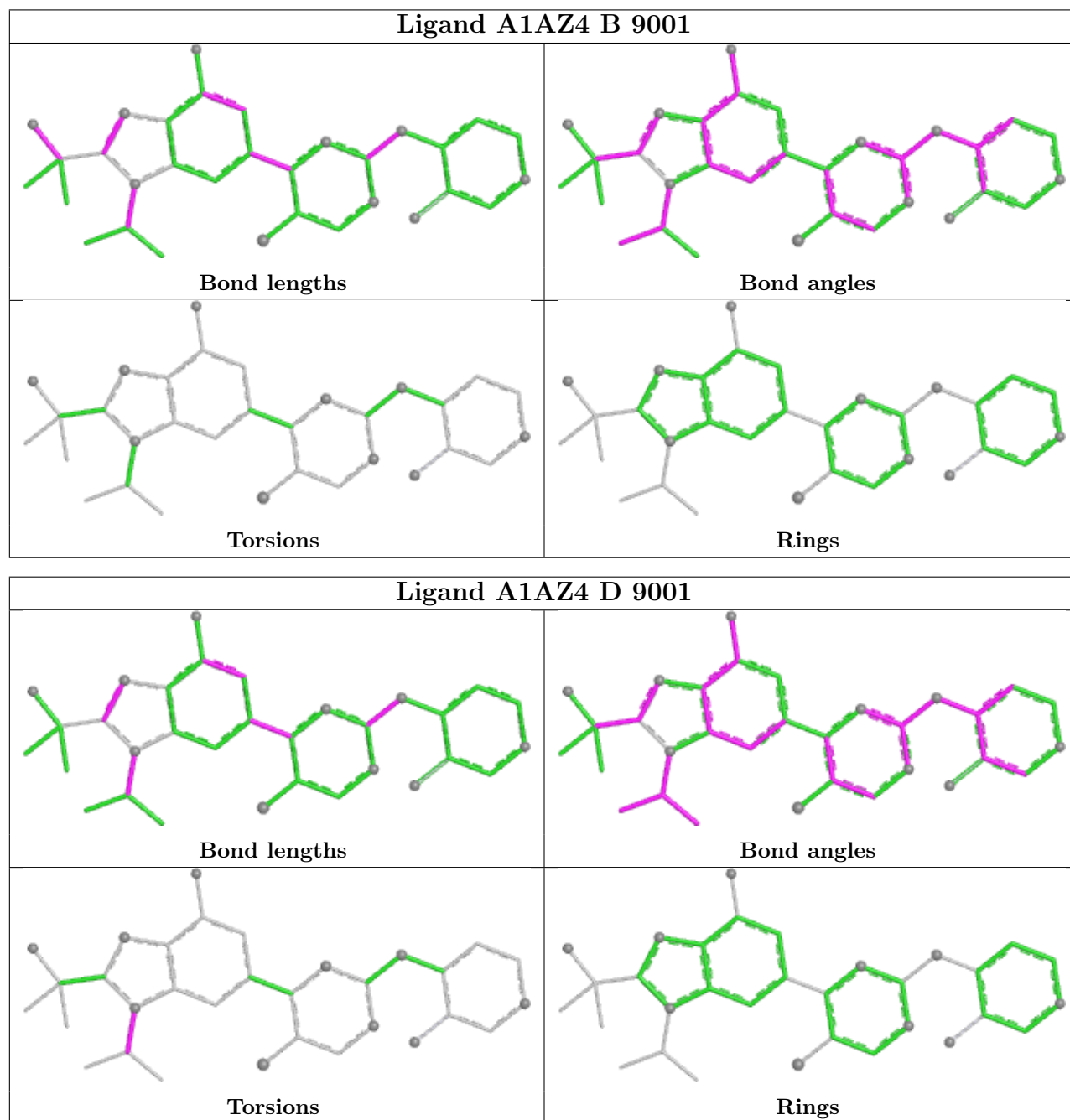
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	9001	A1AZ4	10	0
3	D	9001	A1AZ4	3	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 ⓘ

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 [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	233/257 (90%)	-1.51	0 100 100	34, 47, 70, 92	0
1	C	243/257 (94%)	-1.49	0 100 100	27, 43, 71, 93	1 (0%)
2	B	279/314 (88%)	-1.16	0 100 100	30, 74, 120, 128	0
2	D	283/314 (90%)	-1.34	0 100 100	30, 60, 86, 97	0
All	All	1038/1142 (90%)	-1.36	0 100 100	27, 56, 92, 128	1 (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 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, 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.

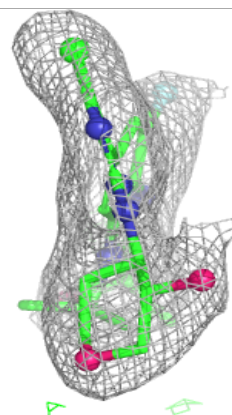
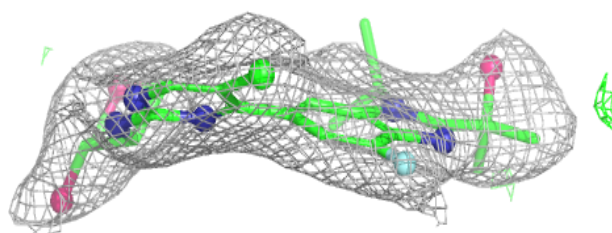
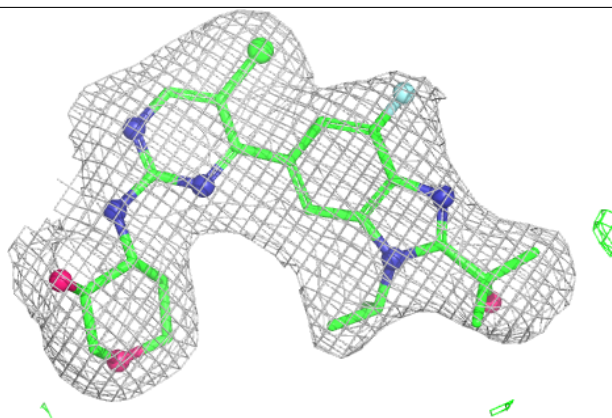
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1AZ4	B	9001	32/32	0.98	0.06	65,68,68,69	0
3	A1AZ4	D	9001	32/32	0.99	0.04	44,46,51,51	0

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.

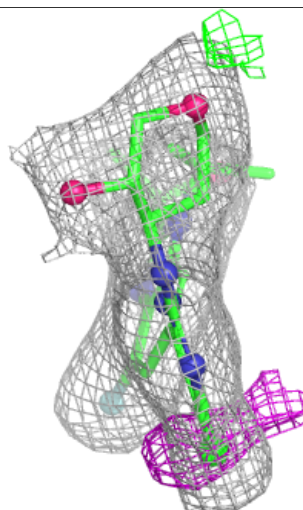
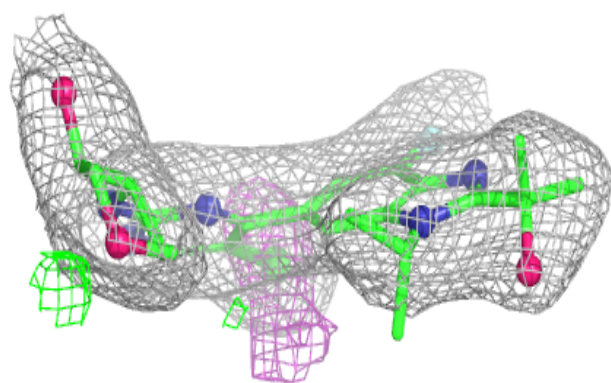
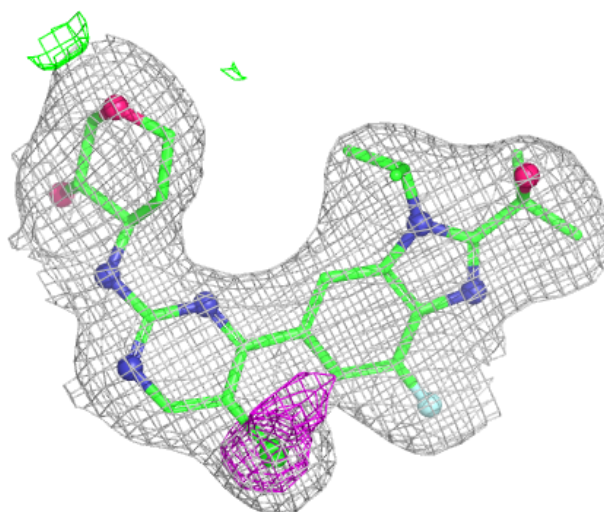
Electron density around A1AZ4 B 9001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1AZ4 D 9001:

$2mF_o-DF_c$ (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.