Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2025 – 02:06 PM EDT

PDB ID	:	9CUE / pdb_00009cue
Title	:	Human STING H232R variant bound to ABZI
Authors	:	Sack, J.S.; Critton, D.A.
Deposited on	:	2024-07-26
Resolution	:	1.95 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

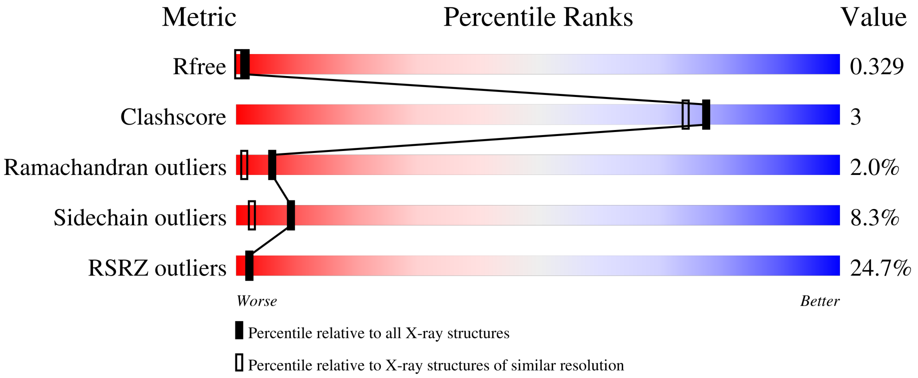
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

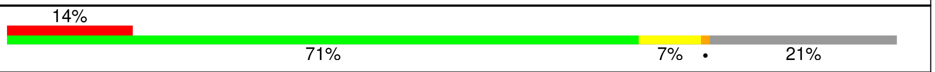
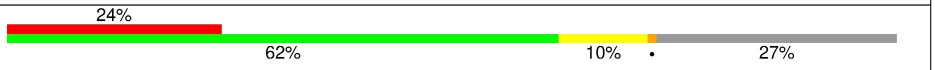
The reported resolution of this entry is 1.95 Å.

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	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	A	210	
1	B	210	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4855 atoms, of which 2332 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 Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	166	2432	807	1174	211	235	5	1174	0	0
1	B	154	2260	748	1096	196	215	5	1096	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	initiating methionine	UNP Q86WV6
A	133	GLY	-	expression tag	UNP Q86WV6
A	134	SER	-	expression tag	UNP Q86WV6
A	135	SER	-	expression tag	UNP Q86WV6
A	136	HIS	-	expression tag	UNP Q86WV6
A	137	HIS	-	expression tag	UNP Q86WV6
A	138	HIS	-	expression tag	UNP Q86WV6
A	139	HIS	-	expression tag	UNP Q86WV6
A	140	HIS	-	expression tag	UNP Q86WV6
A	141	HIS	-	expression tag	UNP Q86WV6
A	142	SER	-	expression tag	UNP Q86WV6
A	143	SER	-	expression tag	UNP Q86WV6
A	144	GLY	-	expression tag	UNP Q86WV6
A	145	GLU	-	expression tag	UNP Q86WV6
A	146	THR	-	expression tag	UNP Q86WV6
A	147	VAL	-	expression tag	UNP Q86WV6
A	148	ARG	-	expression tag	UNP Q86WV6
A	149	PHE	-	expression tag	UNP Q86WV6
A	150	GLN	-	expression tag	UNP Q86WV6
A	151	GLY	-	expression tag	UNP Q86WV6
A	152	HIS	-	expression tag	UNP Q86WV6
A	153	MET	-	expression tag	UNP Q86WV6
A	154	SER	-	expression tag	UNP Q86WV6
A	232	ARG	HIS	variant	UNP Q86WV6
B	132	MET	-	initiating methionine	UNP Q86WV6

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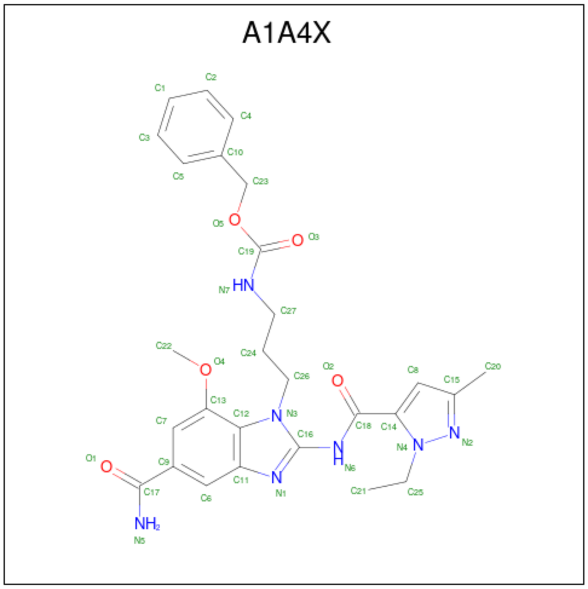
Chain	Residue	Modelled	Actual	Comment	Reference
B	133	GLY	-	expression tag	UNP Q86WV6
B	134	SER	-	expression tag	UNP Q86WV6
B	135	SER	-	expression tag	UNP Q86WV6
B	136	HIS	-	expression tag	UNP Q86WV6
B	137	HIS	-	expression tag	UNP Q86WV6
B	138	HIS	-	expression tag	UNP Q86WV6
B	139	HIS	-	expression tag	UNP Q86WV6
B	140	HIS	-	expression tag	UNP Q86WV6
B	141	HIS	-	expression tag	UNP Q86WV6
B	142	SER	-	expression tag	UNP Q86WV6
B	143	SER	-	expression tag	UNP Q86WV6
B	144	GLY	-	expression tag	UNP Q86WV6
B	145	GLU	-	expression tag	UNP Q86WV6
B	146	THR	-	expression tag	UNP Q86WV6
B	147	VAL	-	expression tag	UNP Q86WV6
B	148	ARG	-	expression tag	UNP Q86WV6
B	149	PHE	-	expression tag	UNP Q86WV6
B	150	GLN	-	expression tag	UNP Q86WV6
B	151	GLY	-	expression tag	UNP Q86WV6
B	152	HIS	-	expression tag	UNP Q86WV6
B	153	MET	-	expression tag	UNP Q86WV6
B	154	SER	-	expression tag	UNP Q86WV6
B	232	ARG	HIS	variant	UNP Q86WV6

- Molecule 2 is benzyl (3-{5-carbamoyl-2-[(1-ethyl-3-methyl-1H-pyrazole-5-carbonyl)amino]-7-methoxy-1H-1,3-benzimidazol-1-yl}propyl)carbamate (CCD ID: A1A4X) (formula: $C_{27}H_{31}N_7O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	B	1	140	54	62	14	10	62	1

- Molecule 3 is water.

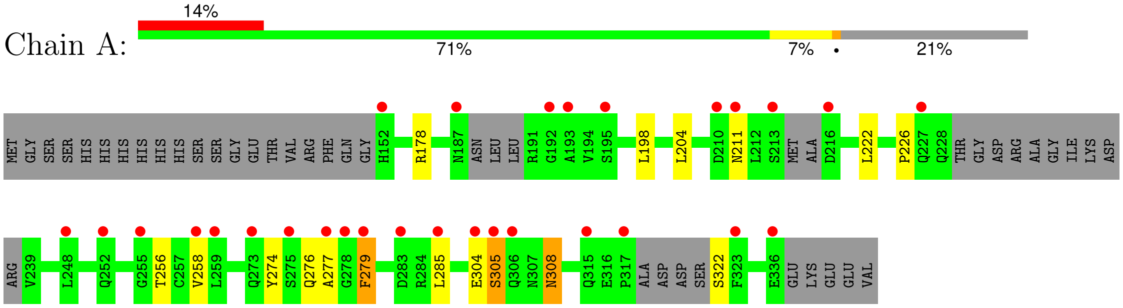
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	12	12	12	0	0
3	B	11	11	11	0	0

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.

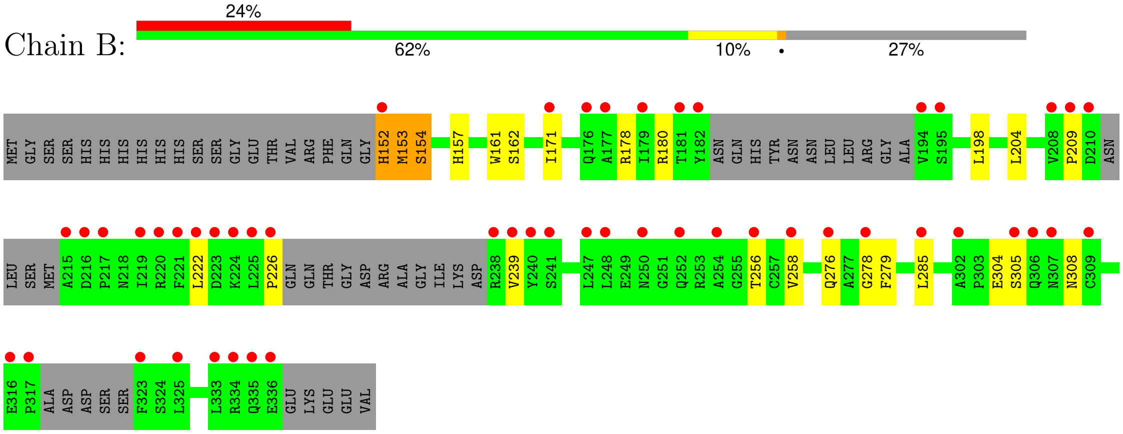
- Molecule 1: Stimulator of interferon genes protein

Chain A:



- Molecule 1: Stimulator of interferon genes protein

Chain B:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	93.10Å 130.17Å 35.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.40 – 1.95 16.40 – 1.95	Depositor EDS
% Data completeness (in resolution range)	65.3 (16.40-1.95) 65.5 (16.40-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.11.8 (20-OCT-2021)	Depositor
R, R_{free}	0.307 , 0.334 0.299 , 0.329	Depositor DCC
R_{free} test set	12276 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4855	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1A4X

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	0.78	0/1282	1.07	4/1745 (0.2%)
1	B	0.82	0/1186	1.05	7/1614 (0.4%)
All	All	0.80	0/2468	1.06	11/3359 (0.3%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	ASN	CA-CB-CG	6.75	119.35	112.60
1	A	274	TYR	CA-C-N	5.77	128.29	120.38
1	A	274	TYR	C-N-CA	5.77	128.29	120.38
1	B	154	SER	CA-C-N	5.41	127.58	120.60
1	B	154	SER	C-N-CA	5.41	127.58	120.60
1	B	279	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	279	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	278	GLY	CA-C-N	5.20	129.99	122.44
1	B	278	GLY	C-N-CA	5.20	129.99	122.44
1	B	304	GLU	CA-C-N	5.13	131.33	121.54
1	B	304	GLU	C-N-CA	5.13	131.33	121.54

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	1258	1174	1174	4	0
1	B	1164	1096	1096	10	0
2	B	78	62	0	2	0
3	A	12	0	0	0	0
3	B	11	0	0	1	0
All	All	2523	2332	2270	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 3.

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:178:ARG:HD2	1:A:226:PRO:O	1.97	0.64
1:B:178:ARG:HD2	1:B:226:PRO:O	1.97	0.64
1:A:304:GLU:O	1:A:305:SER:HB3	2.07	0.54
1:A:277:ALA:HA	1:B:152:HIS:CD2	2.43	0.54
1:B:152:HIS:HB3	1:B:157:HIS:CG	2.46	0.50
1:B:171:ILE:CB	1:B:239:VAL:CB	2.88	0.50
2:B:401[B]:A1A4X:C23	3:B:504:HOH:O	2.58	0.50
1:B:152:HIS:ND1	1:B:157:HIS:CD2	2.80	0.48
1:B:152:HIS:CD2	1:B:161:TRP:HE1	2.31	0.48
1:B:152:HIS:O	1:B:153:MET:CB	2.65	0.45
1:B:162:SER:OG	2:B:401[B]:A1A4X:N2	2.51	0.44
1:A:277:ALA:O	1:B:152:HIS:HA	2.18	0.43
1:B:152:HIS:HB3	1:B:157:HIS:CB	2.50	0.42

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	156/210 (74%)	145 (93%)	8 (5%)	3 (2%)	6	1
1	B	144/210 (69%)	133 (92%)	8 (6%)	3 (2%)	5	1
All	All	300/420 (71%)	278 (93%)	16 (5%)	6 (2%)	6	1

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	305	SER
1	B	153	MET
1	B	209	PRO
1	A	279	PHE
1	B	305	SER

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	125/183 (68%)	116 (93%)	9 (7%)	12	4
1	B	116/183 (63%)	105 (90%)	11 (10%)	7	1
All	All	241/366 (66%)	221 (92%)	20 (8%)	9	2

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LEU
1	A	204	LEU
1	A	222	LEU
1	A	256	THR
1	A	258	VAL
1	A	276	GLN
1	A	285	LEU
1	A	308	ASN
1	A	322	SER
1	B	152	HIS

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Mol	Chain	Res	Type
1	B	154	SER
1	B	180	ARG
1	B	198	LEU
1	B	204	LEU
1	B	222	LEU
1	B	256	THR
1	B	258	VAL
1	B	276	GLN
1	B	285	LEU
1	B	308	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	327	GLN
1	B	327	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\|Z\| > 2$
2	A1A4X	B	401[B]	-	36,42,42	0.55	0	44,58,58	0.54	0
2	A1A4X	B	401[A]	-	36,42,42	0.54	0	44,58,58	0.52	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	A1A4X	B	401[B]	-	-	7/23/28/28	0/4/4/4
2	A1A4X	B	401[A]	-	-	8/23/28/28	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401[A]	A1A4X	C12-C13-O4-C22
2	B	401[B]	A1A4X	C27-C24-C26-N3
2	B	401[B]	A1A4X	C24-C27-N7-C19
2	B	401[A]	A1A4X	C7-C13-O4-C22
2	B	401[B]	A1A4X	C26-C24-C27-N7
2	B	401[A]	A1A4X	C27-C24-C26-N3
2	B	401[A]	A1A4X	O1-C17-C9-C6
2	B	401[A]	A1A4X	N5-C17-C9-C6
2	B	401[A]	A1A4X	O1-C17-C9-C7
2	B	401[A]	A1A4X	N5-C17-C9-C7
2	B	401[A]	A1A4X	C26-C24-C27-N7
2	B	401[B]	A1A4X	N5-C17-C9-C6
2	B	401[B]	A1A4X	N5-C17-C9-C7
2	B	401[B]	A1A4X	O1-C17-C9-C6
2	B	401[B]	A1A4X	O1-C17-C9-C7

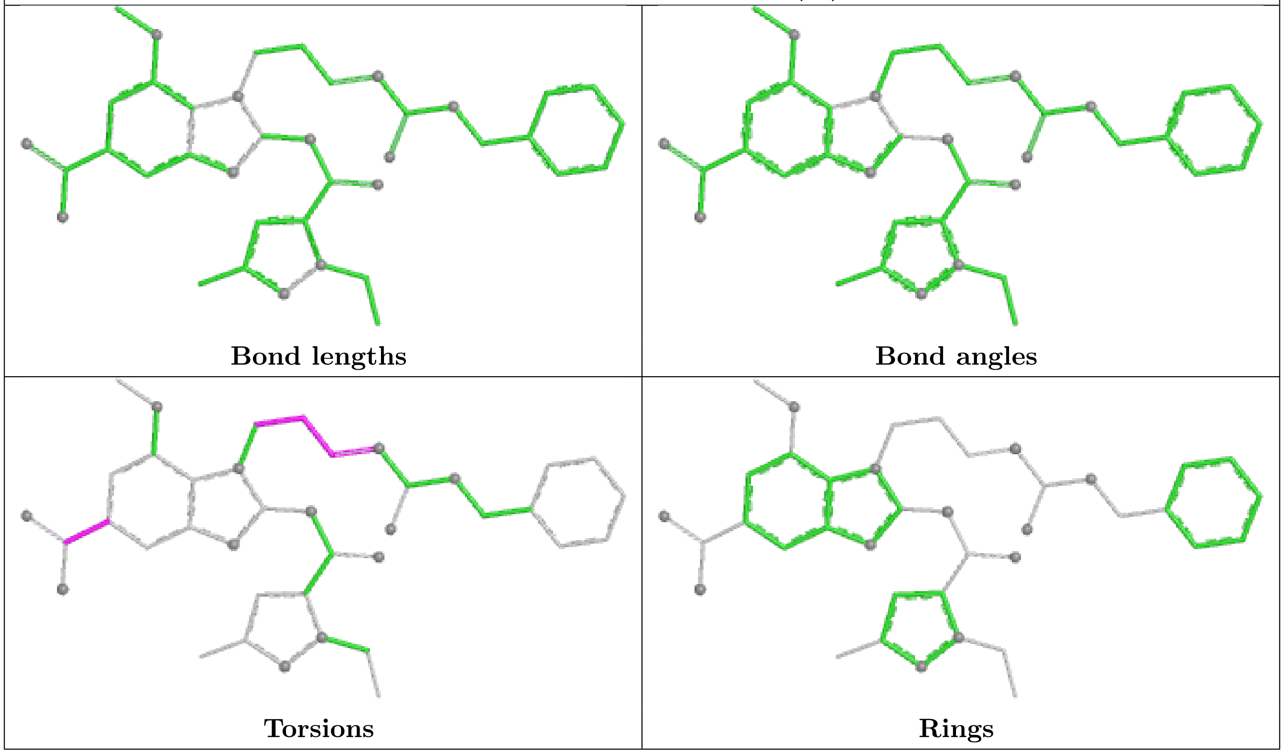
There are no ring outliers.

1 monomer is involved in 2 short contacts:

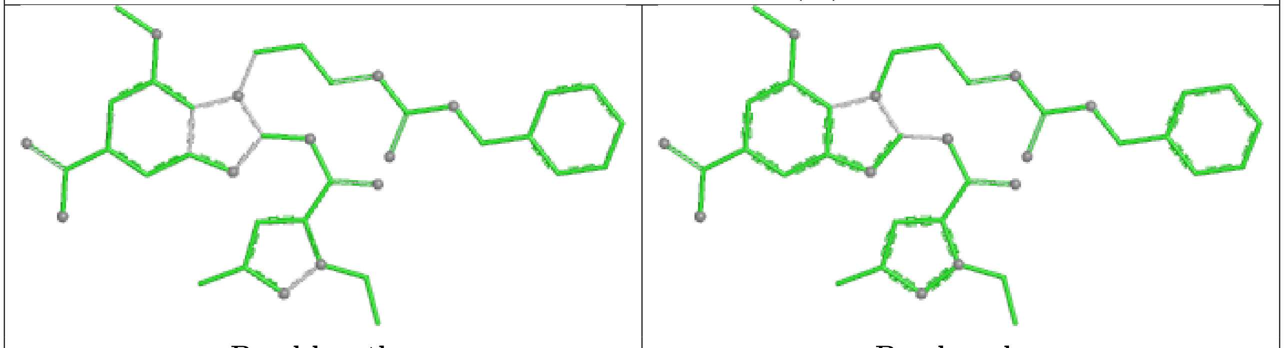
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401[B]	A1A4X	2	0

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.

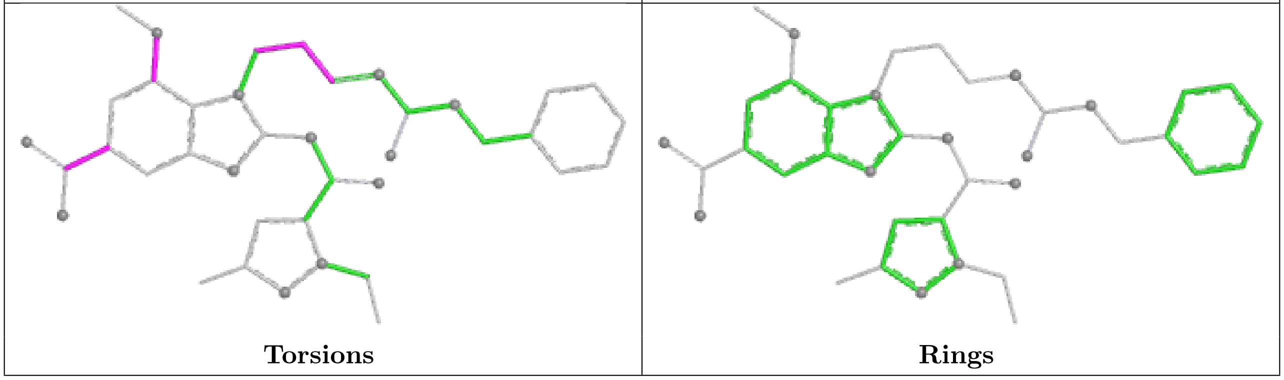
Ligand A1A4X B 401 (B)



Ligand A1A4X B 401 (A)



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	166/210 (79%)	1.10	29 (17%)	5	5	9, 18, 32, 41	0
1	B	154/210 (73%)	1.65	50 (32%)	1	1	8, 21, 39, 50	0
All	All	320/420 (76%)	1.36	79 (24%)	2	2	8, 19, 37, 50	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	TYR	7.7
1	B	238	ARG	5.8
1	B	152	HIS	5.8
1	B	226	PRO	5.1
1	B	335	GLN	4.7
1	B	225	LEU	4.6
1	B	181	THR	4.3
1	B	222	LEU	4.2
1	B	333	LEU	4.0
1	A	187	ASN	4.0
1	A	211	ASN	3.9
1	B	210	ASP	3.9
1	B	305	SER	3.9
1	B	240	TYR	3.9
1	A	279	PHE	3.9
1	B	252	GLN	3.9
1	B	306	GLN	3.8
1	A	317	PRO	3.7
1	A	277	ALA	3.6
1	B	248	LEU	3.5
1	B	325	LEU	3.5
1	A	323	PHE	3.5
1	B	256	THR	3.5
1	A	192	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	213	SER	3.4
1	B	219	ILE	3.3
1	B	194	VAL	3.3
1	A	304	GLU	3.3
1	B	323	PHE	3.3
1	B	179	ILE	3.2
1	B	223	ASP	3.2
1	A	285	LEU	3.1
1	B	208	VAL	3.0
1	B	307	ASN	2.9
1	B	221	PHE	2.8
1	B	278	GLY	2.8
1	B	334	ARG	2.7
1	B	336	GLU	2.7
1	A	255	GLY	2.7
1	A	273	GLN	2.7
1	B	241	SER	2.6
1	B	176	GLN	2.6
1	B	254	ALA	2.6
1	A	210	ASP	2.6
1	B	224	LYS	2.6
1	B	220	ARG	2.6
1	B	258	VAL	2.5
1	A	252	GLN	2.5
1	B	285	LEU	2.5
1	B	239	VAL	2.5
1	B	309	CYS	2.5
1	A	275	SER	2.5
1	B	247	LEU	2.5
1	A	336	GLU	2.5
1	B	317	PRO	2.4
1	A	306	GLN	2.4
1	A	193	ALA	2.4
1	B	195	SER	2.4
1	B	276	GLN	2.4
1	B	209	PRO	2.3
1	B	216	ASP	2.3
1	B	302	ALA	2.3
1	B	217	PRO	2.3
1	B	177	ALA	2.2
1	A	278	GLY	2.2
1	A	258	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	2.2
1	A	305	SER	2.2
1	A	315	GLN	2.2
1	B	215	ALA	2.1
1	A	195	SER	2.1
1	A	227	GLN	2.1
1	A	152	HIS	2.1
1	A	216	ASP	2.1
1	B	171	ILE	2.1
1	B	250	ASN	2.1
1	A	248	LEU	2.1
1	A	259	LEU	2.1
1	B	316	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

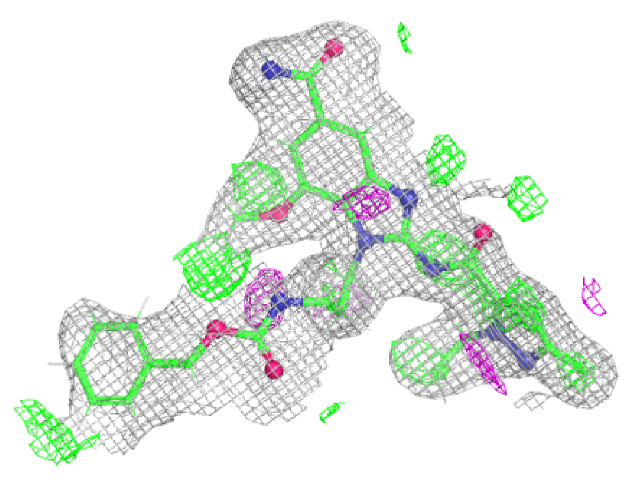
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

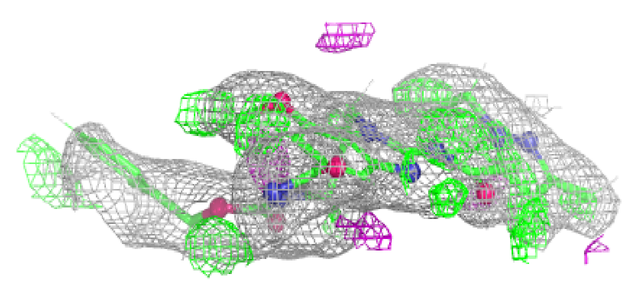
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1A4X	B	401[A]	39/39	0.81	0.15	0,12,27,28	70
2	A1A4X	B	401[B]	39/39	0.81	0.15	0,16,31,31	70

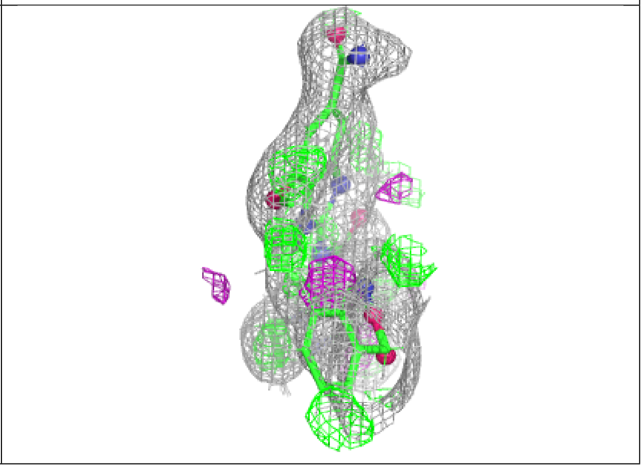
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

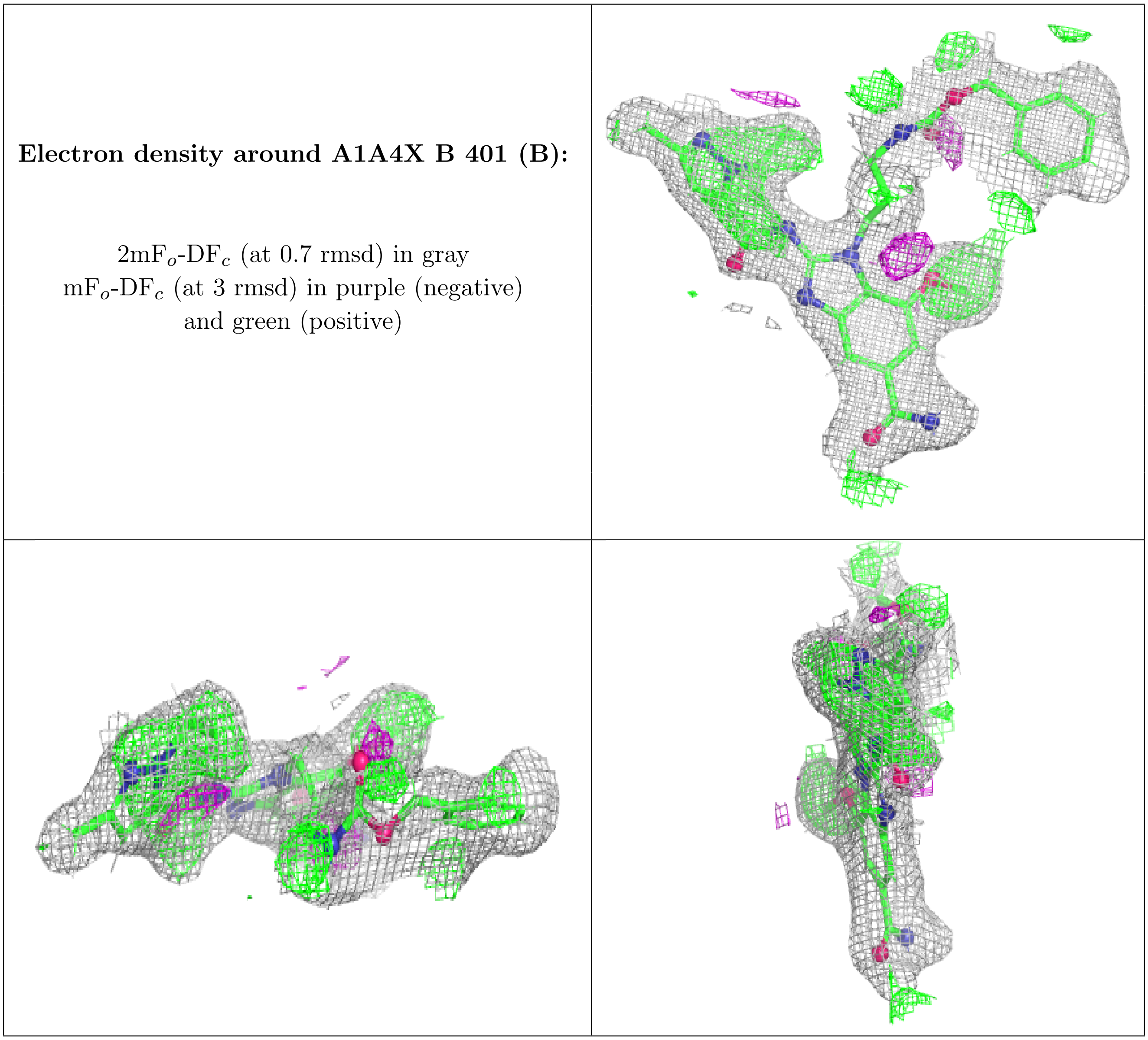
Electron density around A1A4X B 401 (A):

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









Electron density around A1A4X B 401 (B):

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 ⓘ

There are no such residues in this entry.