



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2024 – 02:28 PM EST

PDB ID : 9CZU  
Title : HPK1 kinase domain T165E,S171E phosphomimetic mutant in complex with compound 9  
Authors : Johnson, E.; Mc Tigue, M.  
Deposited on : 2024-08-05  
Resolution : 1.85 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](mailto: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>.

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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) : 2.40

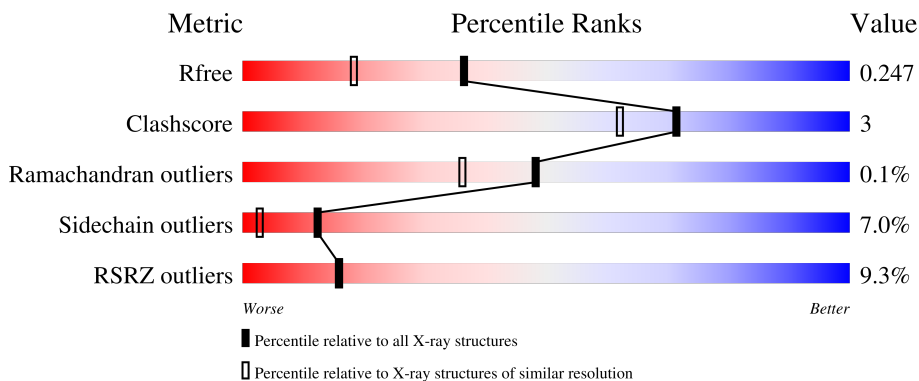
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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  $\geq 3$ , 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	309	 7% 79% 12% • 6%
1	B	309	 7% 80% 10% • 9%
1	C	309	 11% 82% 10% • 7%
1	D	309	 8% 80% 9% • 9%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9919 atoms, of which 92 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 kinase kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2292	1476	395	410	11	0	1	0
1	B	281	2220	1432	384	393	11	0	1	0
1	C	287	2270	1463	393	403	11	0	1	0
1	D	282	2237	1445	388	393	11	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

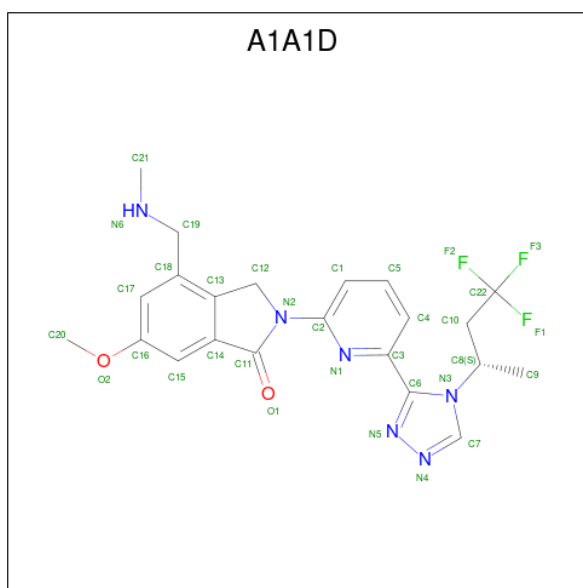
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q92918
A	0	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	engineered mutation	UNP Q92918
A	171	GLU	SER	engineered mutation	UNP Q92918
B	-1	GLY	-	expression tag	UNP Q92918
B	0	SER	-	expression tag	UNP Q92918
B	165	GLU	THR	engineered mutation	UNP Q92918
B	171	GLU	SER	engineered mutation	UNP Q92918
C	-1	GLY	-	expression tag	UNP Q92918
C	0	SER	-	expression tag	UNP Q92918
C	165	GLU	THR	engineered mutation	UNP Q92918
C	171	GLU	SER	engineered mutation	UNP Q92918
D	-1	GLY	-	expression tag	UNP Q92918
D	0	SER	-	expression tag	UNP Q92918
D	165	GLU	THR	engineered mutation	UNP Q92918
D	171	GLU	SER	engineered mutation	UNP Q92918

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	O	S				
			5	4	1		0	0	

- Molecule 3 is 6-methoxy-4-[(methylamino)methyl]-2-(6-{4-[(2S)-4,4,4-trifluorobutan-2-yl]-4H-1,2,4-triazol-3-yl}pyridin-2-yl)-2,3-dihydro-1H-isoindol-1-one (three-letter code: A1A1D) (formula: C<sub>22</sub>H<sub>23</sub>F<sub>3</sub>N<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	F	H	N	O		
			56	22	3	23	6	2	23	0
3	B	1	Total	C	F	H	N	O		
			56	22	3	23	6	2	23	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		
3	D	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		

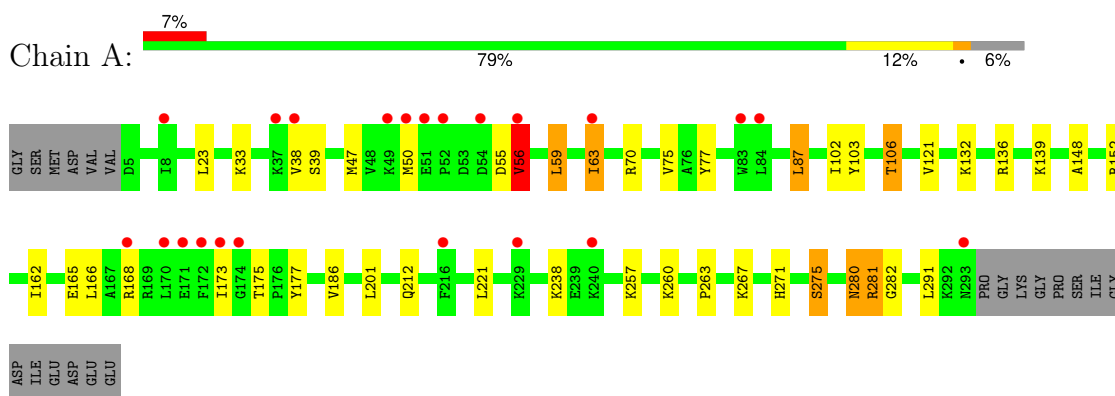
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	179	Total	O	0	0
			179	179		
4	C	148	Total	O	0	0
			148	148		
4	D	145	Total	O	0	0
			145	145		

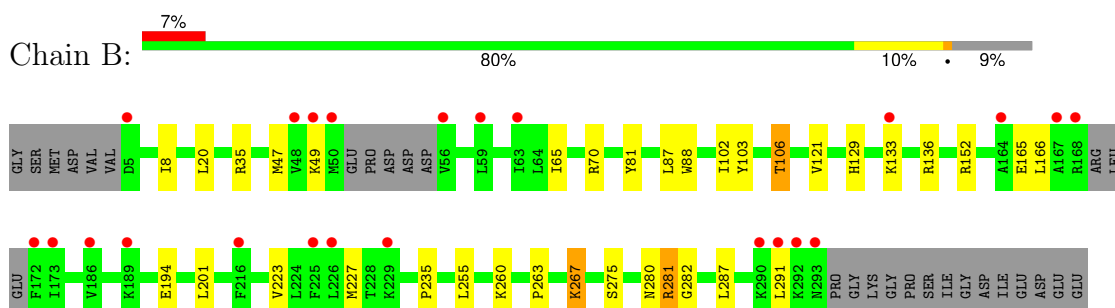
### 3 Residue-property plots

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.

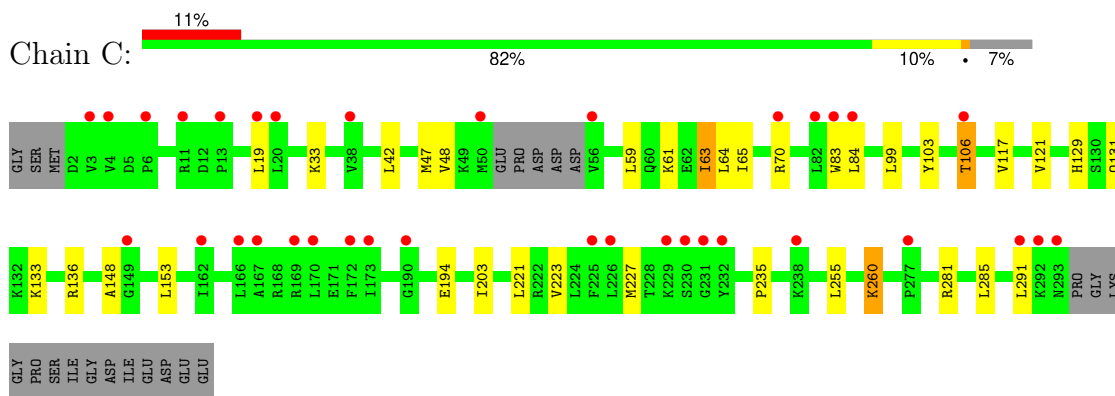
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



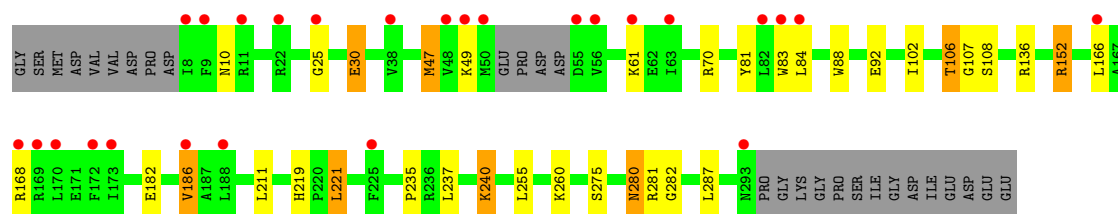
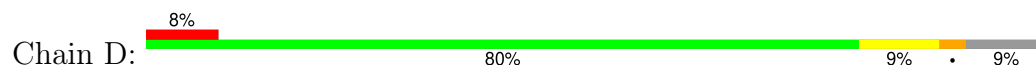
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.19Å 84.26Å 87.32Å 67.33° 73.51° 76.15°	Depositor
Resolution (Å)	78.71 – 1.85 78.71 – 1.85	Depositor EDS
% Data completeness (in resolution range)	54.1 (78.71-1.85) 54.4 (78.71-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.84Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.195 , 0.248 0.196 , 0.247	Depositor DCC
$R_{free}$ test set	6321 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1A1D, SO4

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	0/2345	0.67	0/3170
1	B	0.54	0/2269	0.68	0/3064
1	C	0.52	0/2320	0.66	0/3135
1	D	0.50	0/2287	0.66	0/3087
All	All	0.52	0/9221	0.67	0/12456

There are no bond length outliers.

There are no bond angle outliers.

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	2292	0	2345	16	0
1	B	2220	0	2286	14	0
1	C	2270	0	2339	15	0
1	D	2237	0	2308	15	0
2	A	5	0	0	0	0
3	A	33	23	0	0	0
3	B	33	23	0	0	0
3	C	33	23	0	0	0
3	D	33	23	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	199	0	0	1	0
4	B	179	0	0	1	0
4	C	148	0	0	1	0
4	D	145	0	0	0	0
All	All	9827	92	9278	58	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 (58) 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:B:280:ASN:HD22	1:B:282:GLY:H	1.36	0.73
1:D:106:THR:HG21	1:D:287:LEU:HD11	1.76	0.67
1:D:280:ASN:HD22	1:D:282:GLY:H	1.44	0.65
1:A:280:ASN:HD22	1:A:282:GLY:H	1.46	0.63
1:D:83:TRP:CD1	1:D:84:LEU:HG	2.34	0.62
1:A:103:TYR:HA	1:A:106:THR:HG22	1.83	0.61
1:B:263:PRO:HB3	1:B:267:LYS:HD2	1.83	0.61
1:B:223:VAL:O	1:B:227:MET:HG3	2.04	0.56
1:B:65:ILE:HG12	1:B:133:LYS:HD2	1.88	0.55
1:A:23:LEU:HD21	1:A:33:LYS:HB2	1.89	0.55
1:D:106:THR:HG22	1:D:107:GLY:O	2.07	0.55
1:C:65:ILE:HG12	1:C:133:LYS:HD2	1.90	0.54
1:A:148:ALA:HB1	1:A:281:ARG:HH21	1.73	0.54
1:A:175:THR:HG21	4:A:664:HOH:O	2.07	0.53
1:A:55:ASP:O	1:A:56:VAL:HB	2.10	0.51
1:B:281:ARG:HG2	4:B:593:HOH:O	2.11	0.51
1:C:83:TRP:CD1	1:C:84:LEU:HG	2.46	0.51
1:A:271:HIS:O	1:A:275:SER:HB2	2.11	0.50
1:C:148:ALA:HB1	1:C:281:ARG:HH21	1.75	0.50
1:A:59:LEU:HG	1:A:87:LEU:HD22	1.94	0.50
1:A:263:PRO:HB3	1:A:267:LYS:HD3	1.94	0.49
1:B:103:TYR:HA	1:B:106:THR:HG22	1.94	0.48
1:C:103:TYR:HA	1:C:106:THR:HG22	1.95	0.48
1:B:106:THR:HG21	1:B:287:LEU:HD11	1.97	0.47
1:C:260:LYS:HE2	1:C:260:LYS:H	1.79	0.47
1:A:63:ILE:HD13	1:A:77:TYR:OH	2.14	0.47
1:B:129:HIS:CD2	1:B:194:GLU:HB2	2.50	0.46
1:D:92:GLU:OE2	1:D:152:ARG:HD2	2.15	0.46
1:D:237:LEU:O	1:D:240:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:HG3	1:D:88:TRP:CE2	2.51	0.46
1:A:177:TYR:HE1	1:B:223:VAL:HG21	1.81	0.46
1:B:20:LEU:HD11	1:B:35:ARG:HB2	1.98	0.45
1:D:25:GLY:HA2	1:D:30:GLU:HG2	1.97	0.45
1:B:81:TYR:HB2	1:B:88:TRP:HB2	1.98	0.44
1:C:33:LYS:HE2	1:C:42:LEU:HD22	1.99	0.44
1:C:129:HIS:CD2	1:C:194:GLU:HB2	2.52	0.44
1:D:81:TYR:HB2	1:D:88:TRP:HB2	2.00	0.44
1:C:99:LEU:HD11	1:C:117:VAL:HG11	2.00	0.44
1:C:223:VAL:O	1:C:227:MET:HG3	2.18	0.43
1:B:102:ILE:HG23	1:B:291:LEU:HD12	2.00	0.43
1:C:133:LYS:HG3	4:C:579:HOH:O	2.19	0.42
1:D:235:PRO:HD2	1:D:255:LEU:HD13	2.00	0.42
1:C:48:VAL:HG11	1:C:59:LEU:HD21	2.01	0.42
1:D:102:ILE:O	1:D:106:THR:HB	2.19	0.42
1:C:285:LEU:HD13	1:D:281:ARG:HG3	2.02	0.42
1:A:38:VAL:HG23	1:A:39:SER:H	1.85	0.42
1:B:235:PRO:HD2	1:B:255:LEU:HD13	2.01	0.41
1:A:165:GLU:HA	1:A:168:ARG:HH11	1.85	0.41
1:C:121:VAL:HG13	1:C:153:LEU:HD21	2.03	0.41
1:D:219:HIS:CE1	1:D:221:LEU:HB2	2.56	0.41
1:C:235:PRO:HD2	1:C:255:LEU:HD13	2.03	0.41
1:D:182:GLU:O	1:D:186:VAL:HG13	2.21	0.41
1:A:102:ILE:O	1:A:106:THR:HB	2.22	0.40
1:B:121:VAL:HG11	1:B:201:LEU:HD13	2.02	0.40
1:C:59:LEU:O	1:C:63:ILE:HG23	2.20	0.40
1:D:108:SER:N	1:D:211:LEU:HD21	2.36	0.40
1:A:121:VAL:HG11	1:A:201:LEU:HD13	2.03	0.40
1:A:162:ILE:O	1:A:166:LEU:HB2	2.21	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	288/309 (93%)	281 (98%)	6 (2%)	1 (0%)	37	25
1	B	276/309 (89%)	264 (96%)	12 (4%)	0	100	100
1	C	284/309 (92%)	271 (95%)	13 (5%)	0	100	100
1	D	279/309 (90%)	269 (96%)	10 (4%)	0	100	100
All	All	1127/1236 (91%)	1085 (96%)	41 (4%)	1 (0%)	48	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	VAL

### 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	247/262 (94%)	223 (90%)	24 (10%)	6	1
1	B	239/262 (91%)	225 (94%)	14 (6%)	16	5
1	C	245/262 (94%)	232 (95%)	13 (5%)	19	7
1	D	240/262 (92%)	223 (93%)	17 (7%)	12	3
All	All	971/1048 (93%)	903 (93%)	68 (7%)	12	3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET
1	A	50	MET
1	A	56	VAL
1	A	59	LEU
1	A	63	ILE
1	A	70	ARG
1	A	75	VAL
1	A	87	LEU
1	A	106	THR
1	A	132	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	136	ARG
1	A	139	LYS
1	A	152	ARG
1	A	173	ILE
1	A	186	VAL
1	A	212	GLN
1	A	221	LEU
1	A	238	LYS
1	A	257	LYS
1	A	260	LYS
1	A	275	SER
1	A	280	ASN
1	A	281	ARG
1	A	291	LEU
1	B	8	ILE
1	B	47	MET
1	B	49	LYS
1	B	70	ARG
1	B	87	LEU
1	B	106	THR
1	B	136	ARG
1	B	152	ARG
1	B	165	GLU
1	B	166	LEU
1	B	260	LYS
1	B	267	LYS
1	B	275	SER
1	B	281	ARG
1	C	19	LEU
1	C	47	MET
1	C	61	LYS
1	C	63	ILE
1	C	64	LEU
1	C	70	ARG
1	C	106	THR
1	C	131	GLN
1	C	136	ARG
1	C	203	ILE
1	C	221	LEU
1	C	260	LYS
1	C	291	LEU
1	D	10	ASN

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Mol	Chain	Res	Type
1	D	30	GLU
1	D	47	MET
1	D	49	LYS
1	D	61	LYS
1	D	70	ARG
1	D	106	THR
1	D	136	ARG
1	D	152	ARG
1	D	166	LEU
1	D	168	ARG
1	D	186	VAL
1	D	221	LEU
1	D	240	LYS
1	D	260	LYS
1	D	275	SER
1	D	280	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	123	GLN
1	A	131	GLN
1	A	142	ASN
1	A	280	ASN
1	B	60	GLN
1	B	104	GLN
1	B	142	ASN
1	B	212	GLN
1	B	280	ASN
1	C	104	GLN
1	C	142	ASN
1	D	142	ASN
1	D	280	ASN

### 5.3.3 RNA

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](#)

5 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	A1A1D	B	401	-	31,36,36	0.52	0	42,53,53	1.11	4 (9%)
3	A1A1D	A	402	-	31,36,36	0.53	0	42,53,53	1.04	2 (4%)
3	A1A1D	D	401	-	31,36,36	0.53	0	42,53,53	1.07	3 (7%)
2	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.12	0
3	A1A1D	C	401	-	31,36,36	0.54	1 (3%)	42,53,53	1.01	3 (7%)

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	A1A1D	D	401	-	-	0/20/34/34	0/4/4/4
3	A1A1D	A	402	-	-	1/20/34/34	0/4/4/4
3	A1A1D	C	401	-	-	0/20/34/34	0/4/4/4
3	A1A1D	B	401	-	-	0/20/34/34	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	A1A1D	C19-N6	2.02	1.49	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	A1A1D	C7-N3-C6	-4.62	103.31	108.66
3	C	401	A1A1D	C7-N3-C6	-4.45	103.51	108.66
3	A	402	A1A1D	C7-N3-C6	-4.45	103.52	108.66
3	D	401	A1A1D	C7-N3-C6	-4.42	103.55	108.66
3	B	401	A1A1D	C19-C18-C13	-3.22	116.68	122.71
3	A	402	A1A1D	C19-C18-C13	-2.97	117.15	122.71
3	D	401	A1A1D	C19-C18-C13	-2.94	117.21	122.71
3	C	401	A1A1D	C19-C18-C13	-2.54	117.97	122.71
3	B	401	A1A1D	C15-C14-C13	-2.29	121.13	123.27
3	D	401	A1A1D	C15-C14-C13	-2.22	121.19	123.27
3	B	401	A1A1D	C19-C18-C17	2.15	124.47	120.34
3	C	401	A1A1D	C15-C14-C13	-2.02	121.38	123.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

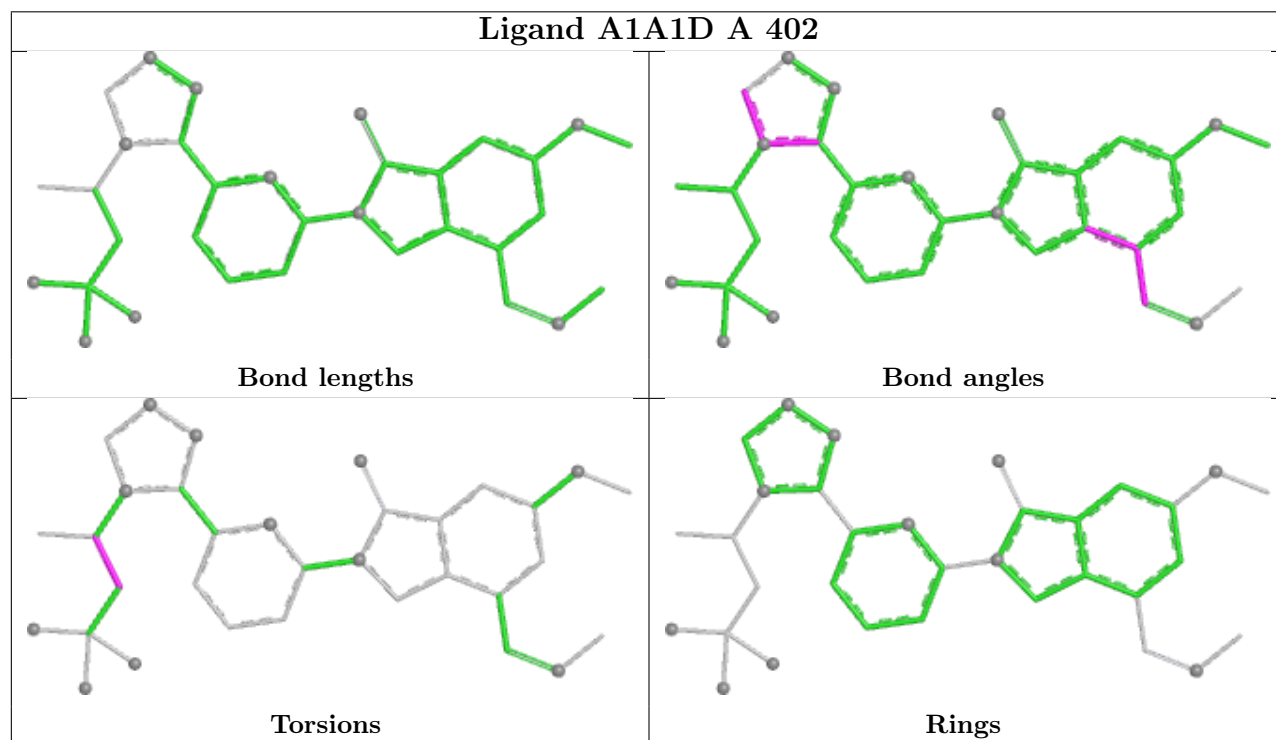
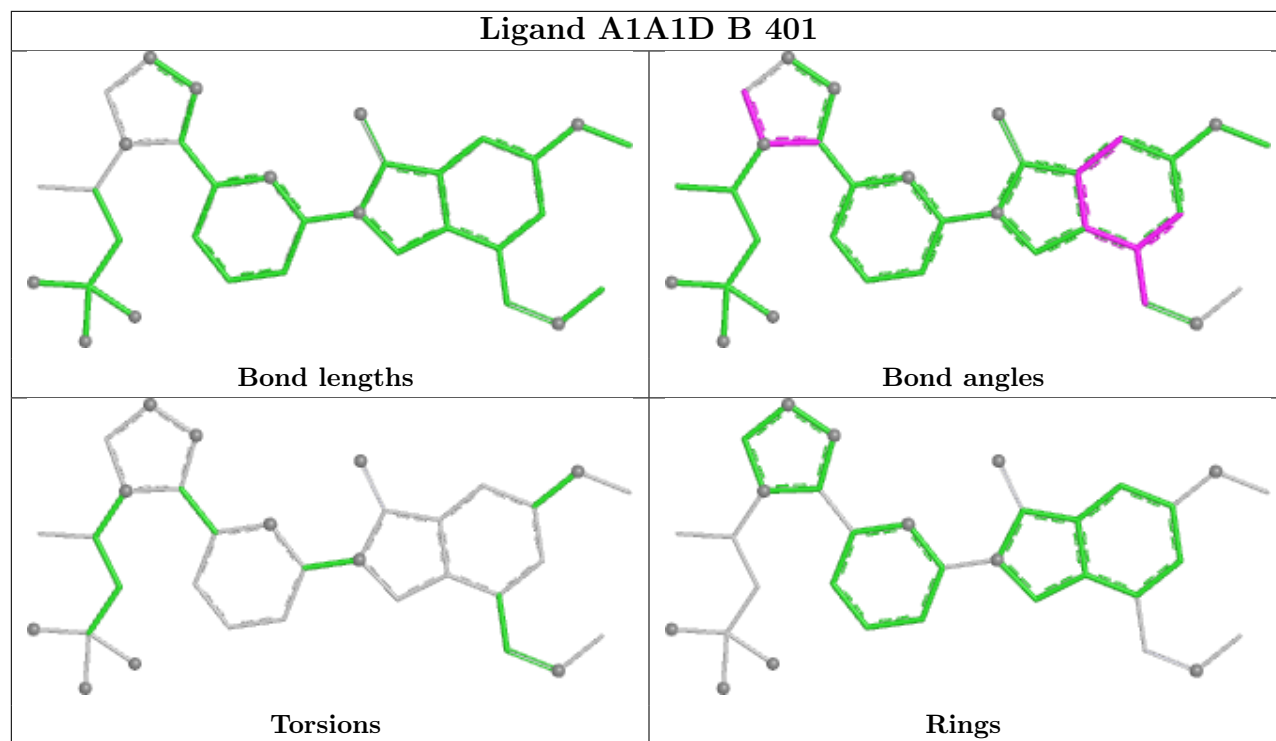
Mol	Chain	Res	Type	Atoms
3	A	402	A1A1D	C22-C10-C8-N3

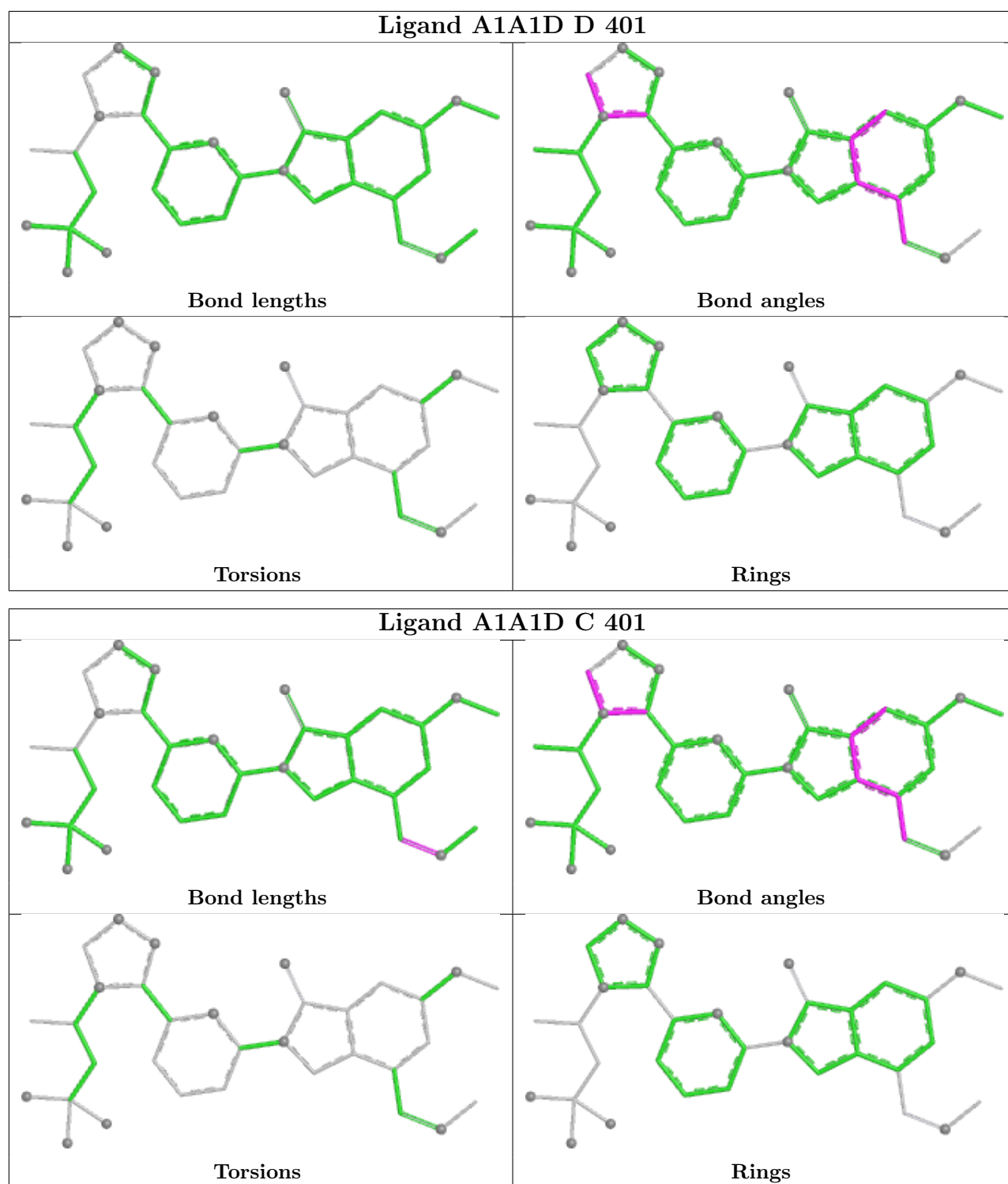
There are no ring outliers.

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 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	289/309 (93%)	0.39	22 (7%) 21 22	23, 38, 70, 98	1 (0%)
1	B	281/309 (90%)	0.44	23 (8%) 19 20	22, 38, 64, 116	1 (0%)
1	C	287/309 (92%)	0.75	35 (12%) 10 9	22, 44, 83, 122	1 (0%)
1	D	282/309 (91%)	0.62	26 (9%) 16 16	22, 42, 73, 106	1 (0%)
All	All	1139/1236 (92%)	0.55	106 (9%) 16 16	22, 40, 74, 122	4 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216[A]	PHE	5.0
1	D	8	ILE	4.9
1	A	173	ILE	4.7
1	C	170	LEU	4.7
1	A	52	PRO	4.6
1	C	225	PHE	4.5
1	D	50	MET	4.4
1	D	63	ILE	4.2
1	A	84	LEU	4.1
1	C	173	ILE	4.0
1	B	291	LEU	4.0
1	B	50	MET	3.8
1	C	167	ALA	3.7
1	D	49	LYS	3.6
1	D	38	VAL	3.6
1	B	63	ILE	3.5
1	B	173	ILE	3.5
1	C	166	LEU	3.4
1	D	169	ARG	3.4
1	C	172	PHE	3.3
1	B	168	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	3.3
1	B	292	LYS	3.2
1	C	229	LYS	3.2
1	A	56	VAL	3.2
1	C	3	VAL	3.1
1	A	50	MET	3.1
1	D	225[A]	PHE	3.1
1	B	293	ASN	3.1
1	C	291	LEU	3.0
1	D	293	ASN	3.0
1	B	56	VAL	3.0
1	B	5	ASP	3.0
1	D	55	ASP	3.0
1	D	173	ILE	2.9
1	C	232	TYR	2.9
1	B	229	LYS	2.9
1	D	172	PHE	2.9
1	D	56	VAL	2.9
1	C	83	TRP	2.9
1	A	37	LYS	2.9
1	C	190	GLY	2.8
1	A	168	ARG	2.7
1	C	82	LEU	2.7
1	A	49	LYS	2.7
1	C	70	ARG	2.7
1	B	226	LEU	2.7
1	D	84	LEU	2.7
1	A	51	GLU	2.6
1	B	290	LYS	2.6
1	A	293	ASN	2.5
1	C	56	VAL	2.5
1	A	83	TRP	2.5
1	C	293	ASN	2.5
1	C	84	LEU	2.5
1	A	229	LYS	2.5
1	D	82	LEU	2.5
1	A	174	GLY	2.4
1	C	169	ARG	2.4
1	A	172	PHE	2.4
1	B	133	LYS	2.4
1	D	170	LEU	2.3
1	A	8	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	238	LYS	2.3
1	B	49	LYS	2.3
1	B	225	PHE	2.3
1	C	50	MET	2.3
1	B	59	LEU	2.3
1	C	226	LEU	2.3
1	D	166	LEU	2.3
1	C	292	LYS	2.3
1	C	4	VAL	2.3
1	C	149	GLY	2.2
1	C	231	GLY	2.2
1	C	6	PRO	2.2
1	D	61	LYS	2.2
1	D	83	TRP	2.2
1	D	9	PHE	2.2
1	A	170	LEU	2.2
1	B	186	VAL	2.2
1	B	216	PHE	2.2
1	D	48	VAL	2.2
1	A	63	ILE	2.2
1	C	162	ILE	2.2
1	D	11	ARG	2.2
1	D	168	ARG	2.2
1	C	38	VAL	2.1
1	D	186	VAL	2.1
1	B	172	PHE	2.1
1	C	19	LEU	2.1
1	B	189	LYS	2.1
1	B	48	VAL	2.1
1	D	25	GLY	2.1
1	B	164	ALA	2.1
1	C	277	PRO	2.1
1	C	230	SER	2.1
1	A	171	GLU	2.1
1	C	106	THR	2.1
1	A	54	ASP	2.0
1	D	188	LEU	2.0
1	A	240	LYS	2.0
1	B	167	ALA	2.0
1	C	13	PRO	2.0
1	C	20	LEU	2.0
1	C	11	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	22	ARG	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](#)

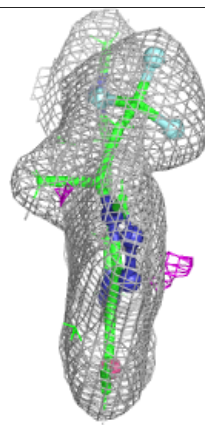
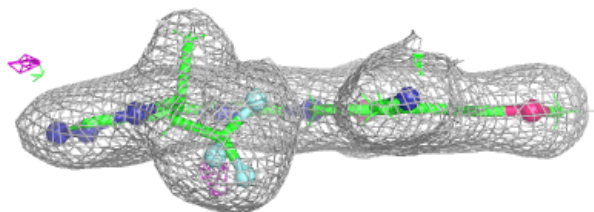
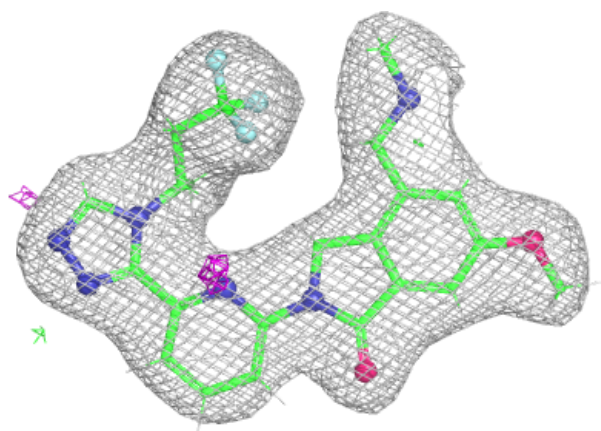
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	401	5/5	0.94	0.07	66,66,69,70	0
3	A1A1D	D	401	33/33	0.94	0.07	27,29,41,48	23
3	A1A1D	C	401	33/33	0.95	0.07	25,28,38,44	23
3	A1A1D	A	402	33/33	0.95	0.06	23,28,33,37	23
3	A1A1D	B	401	33/33	0.96	0.06	27,28,37,42	23

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 A1A1D D 401:**

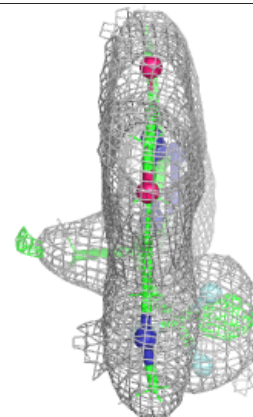
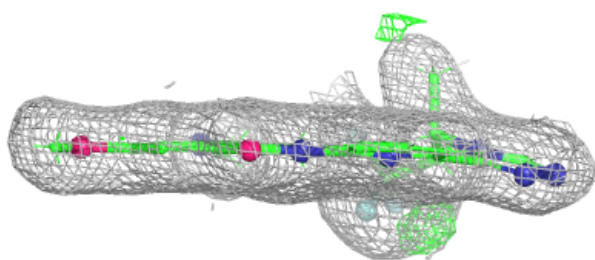
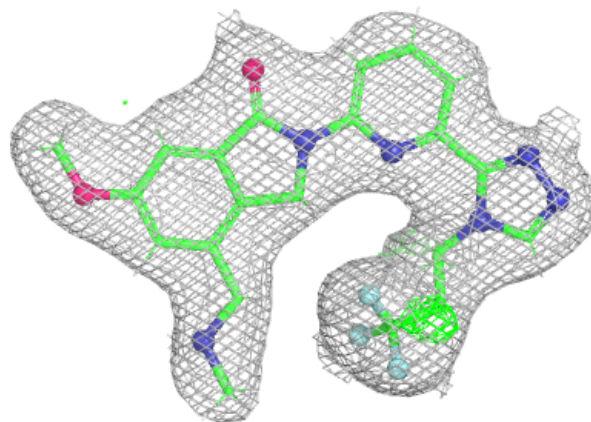
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





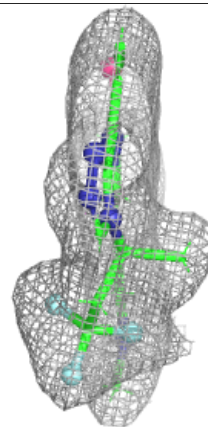
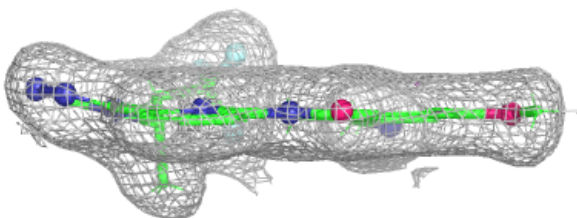
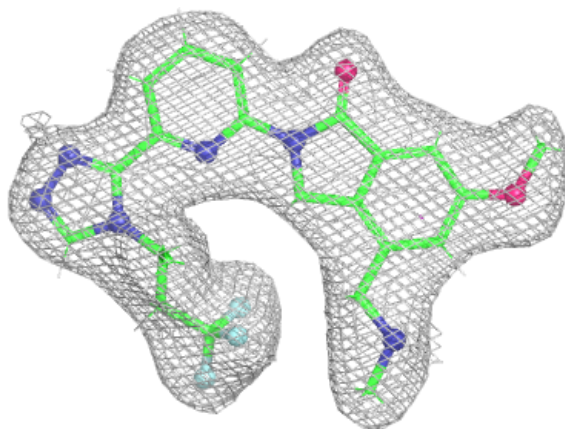
**Electron density around A1A1D C 401:**

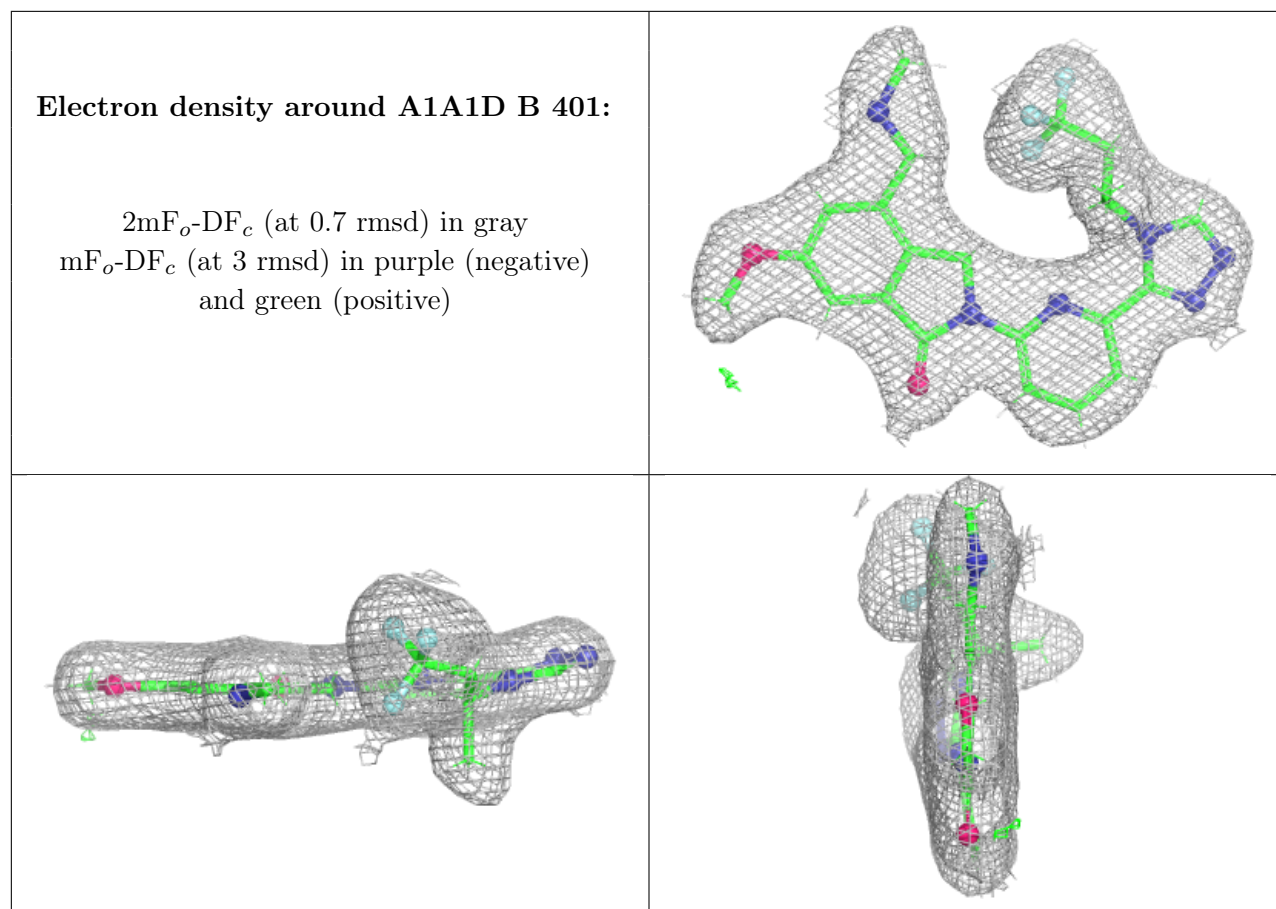
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1A1D A 402:**

$2mF_o-DF_c$  (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.