



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 08:47 PM EDT

PDB ID : 7HSF / pdb\_00007hsf  
Title : PanDDA analysis group deposition – Crystal Structure of FatA in complex with Z1503180352  
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Deposited on : 2024-12-23  
Resolution : 2.13 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](#) ①) 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)	:	2.45.1

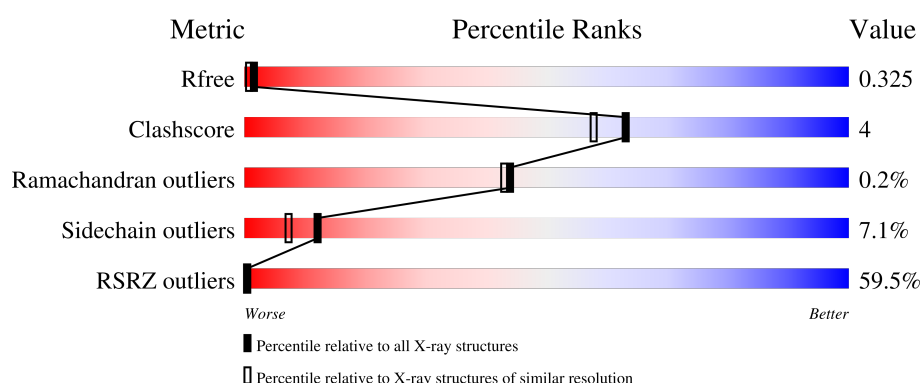
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (2.16-2.12)

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	295	<div> <div>58%</div> <div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	295	<div> <div>49%</div> <div> <div>73%</div> <div>15%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4439 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.

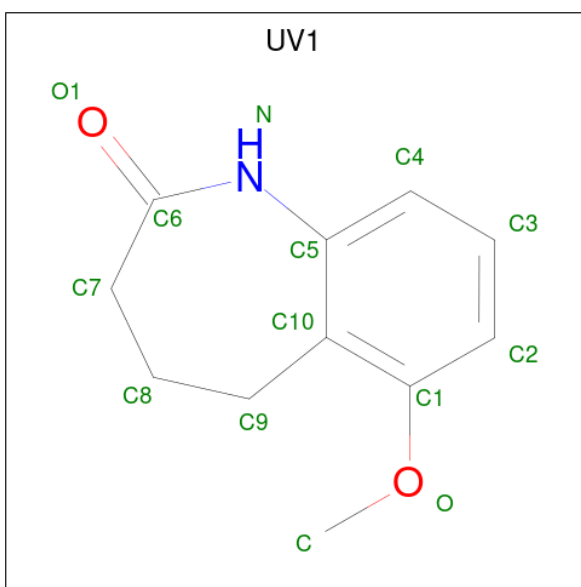
- Molecule 1 is a protein called Oleoyl-acyl carrier protein thioesterase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	4	0
			2192	1363	388	427	14			
1	B	264	Total	C	N	O	S	0	4	0
			2202	1369	392	429	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	-	initiating methionine	UNP Q42561
A	363	HIS	-	expression tag	UNP Q42561
A	364	HIS	-	expression tag	UNP Q42561
A	365	HIS	-	expression tag	UNP Q42561
A	366	HIS	-	expression tag	UNP Q42561
A	367	HIS	-	expression tag	UNP Q42561
A	368	HIS	-	expression tag	UNP Q42561
B	74	MET	-	initiating methionine	UNP Q42561
B	363	HIS	-	expression tag	UNP Q42561
B	364	HIS	-	expression tag	UNP Q42561
B	365	HIS	-	expression tag	UNP Q42561
B	366	HIS	-	expression tag	UNP Q42561
B	367	HIS	-	expression tag	UNP Q42561
B	368	HIS	-	expression tag	UNP Q42561

- Molecule 2 is 6-methoxy-1,3,4,5-tetrahydro-2H-1-benzazepin-2-one (CCD ID: UV1) (formula: C<sub>11</sub>H<sub>13</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	11	1	2		
2	B	1	Total	C	N	O	0	0
			14	11	1	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

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



SER  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.25Å 99.29Å 128.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.39 – 2.13 39.39 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.39-2.13) 98.8 (39.39-2.13)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.4 (23-JAN-2024)	Depositor
R, $R_{free}$	0.315 , 0.343 0.286 , 0.325	Depositor DCC
$R_{free}$ test set	1722 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 263.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.467 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	4439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	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.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UV1, 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	0.71	0/2230	1.00	0/3017
1	B	0.71	0/2240	1.00	0/3030
All	All	0.71	0/4470	1.00	0/6047

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

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	2192	0	2152	11	0
1	B	2202	0	2158	24	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
All	All	4439	0	4310	34	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 4.

All (34) 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:95:VAL:HG11	1:A:156:TRP:HB2	1.57	0.87
1:B:95:VAL:HG11	1:B:156:TRP:HB2	1.58	0.84
1:B:134:MET:HE1	1:B:141:TRP:NE1	1.99	0.76
1:B:131:THR:HG23	1:B:134:MET:HE3	1.68	0.74
1:B:134:MET:HE1	1:B:141:TRP:HE1	1.52	0.73
1:B:149[B]:GLU:HG2	1:B:292:VAL:HG13	1.82	0.62
1:B:137:LEU:HB3	1:B:139:LEU:HD22	1.84	0.59
1:A:89:VAL:HG22	1:A:159:VAL:HG22	1.90	0.53
1:B:240:ILE:HD13	1:B:352:GLY:HA2	1.91	0.53
1:A:240:ILE:HD13	1:A:352:GLY:HA2	1.91	0.52
1:B:171:ARG:HD2	1:B:214:ARG:NH1	2.25	0.51
1:B:89:VAL:HG22	1:B:159:VAL:HG22	1.91	0.51
1:B:340:LEU:HB2	1:B:350:ASN:HB2	1.92	0.51
1:A:98:ASN:HD21	1:A:359:LYS:NZ	2.09	0.51
1:A:280:ILE:HD11	1:A:338:HIS:HE1	1.76	0.50
1:B:166[C]:CYS:SG	1:B:176:ARG:NH1	2.84	0.50
1:B:280:ILE:HD11	1:B:338:HIS:HE1	1.77	0.49
1:B:166[A]:CYS:SG	1:B:176:ARG:NH1	2.84	0.49
1:A:269:ASN:HA	1:A:272:TYR:HD2	1.78	0.47
1:A:166[B]:CYS:SG	1:A:176:ARG:NH1	2.88	0.46
1:B:198:MET:HG3	1:B:209:VAL:HG22	1.98	0.46
1:A:276:VAL:HG21	1:A:295:LEU:HD11	1.98	0.46
1:B:166[C]:CYS:SG	1:B:176:ARG:CZ	3.04	0.46
1:B:276:VAL:HG21	1:B:295:LEU:HD11	1.97	0.45
1:B:166[A]:CYS:SG	1:B:176:ARG:CZ	3.04	0.45
1:B:166[B]:CYS:SG	1:B:176:ARG:NH1	2.90	0.44
1:B:147:HIS:HB3	1:B:193:THR:HG22	1.99	0.44
1:A:147:HIS:HB3	1:A:193:THR:HG22	2.00	0.42
1:B:280:ILE:HD11	1:B:338:HIS:CE1	2.53	0.42
1:A:280:ILE:HD11	1:A:338:HIS:CE1	2.53	0.42
1:B:234:ASN:ND2	1:B:236:SER:OG	2.54	0.41
1:B:198:MET:HE1	1:B:213:VAL:HG21	2.03	0.41
1:A:115:CYS:SG	1:B:156:TRP:HZ2	2.44	0.40
1:B:208:LYS:H	1:B:208:LYS:HG3	1.78	0.40

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	267/295 (90%)	260 (97%)	6 (2%)	1 (0%)	30	26
1	B	266/295 (90%)	257 (97%)	9 (3%)	0	100	100
All	All	533/590 (90%)	517 (97%)	15 (3%)	1 (0%)	44	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLU

### 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	248/263 (94%)	233 (94%)	15 (6%)	16	11
1	B	247/263 (94%)	226 (92%)	21 (8%)	8	4
All	All	495/526 (94%)	459 (93%)	36 (7%)	12	6

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	120[A]	SER
1	A	120[B]	SER
1	A	120[C]	SER
1	A	133	THR

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	198	MET
1	A	204	ARG
1	A	217	TYR
1	A	231	GLU
1	A	235	ARG
1	A	280	ILE
1	A	291	GLN
1	A	343	SER
1	A	349	ILE
1	B	98	ASN
1	B	119	GLN
1	B	137	LEU
1	B	139	LEU
1	B	142	VAL
1	B	145	ARG
1	B	160	VAL
1	B	172	ILE
1	B	206	LEU
1	B	208	LYS
1	B	211	ASP
1	B	217	TYR
1	B	231	GLU
1	B	232	GLU
1	B	235	ARG
1	B	268	ASN
1	B	280	ILE
1	B	283	GLU
1	B	291	GLN
1	B	343	SER
1	B	349	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	111	GLN
1	A	233	ASN
1	A	268	ASN
1	A	303	GLN
1	B	111	GLN
1	B	234	ASN

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Mol	Chain	Res	Type
1	B	268	ASN
1	B	303	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 ⓘ

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	SO4	B	402	-	4,4,4	0.28	0	6,6,6	0.46	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.36	0
2	UV1	A	401	-	15,15,15	0.28	0	18,20,20	0.75	0
2	UV1	B	401	-	15,15,15	0.25	0	18,20,20	0.75	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	UV1	A	401	-	-	0/2/12/12	0/2/2/2
2	UV1	B	401	-	-	0/2/12/12	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

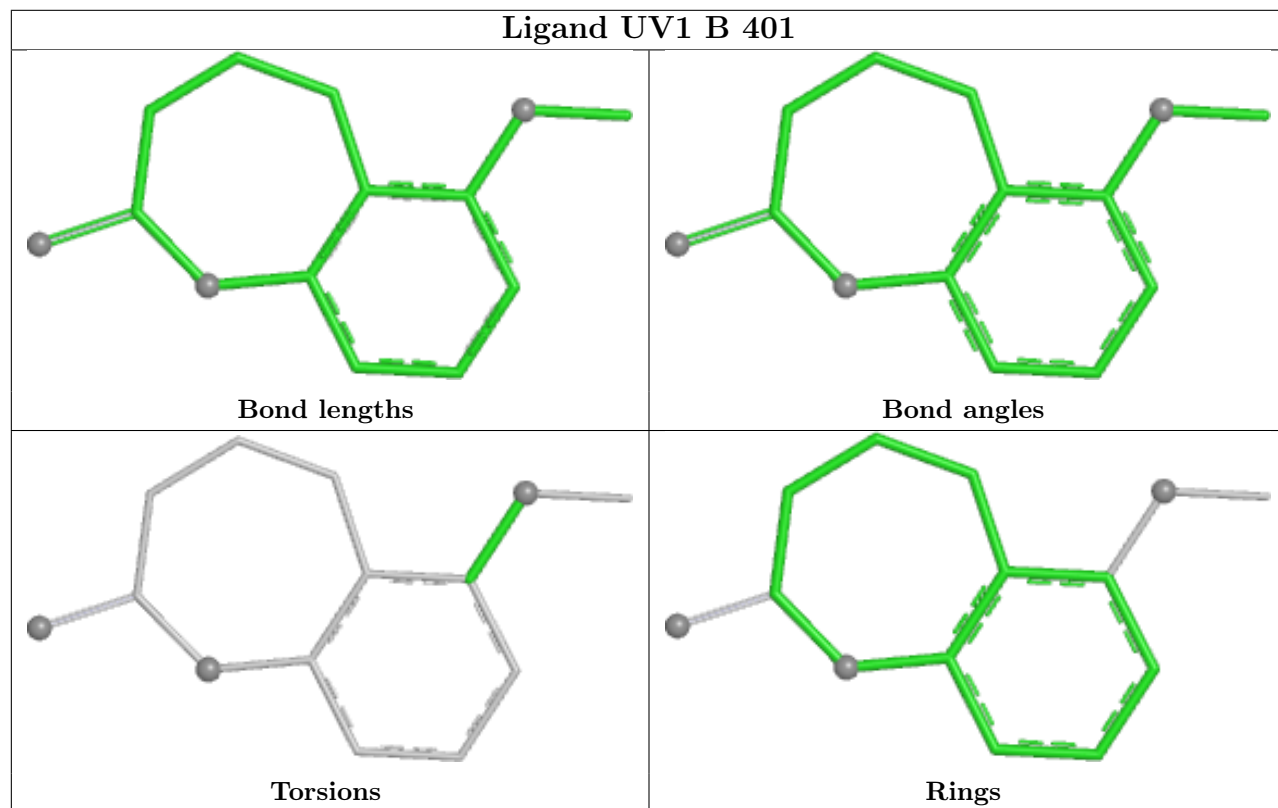
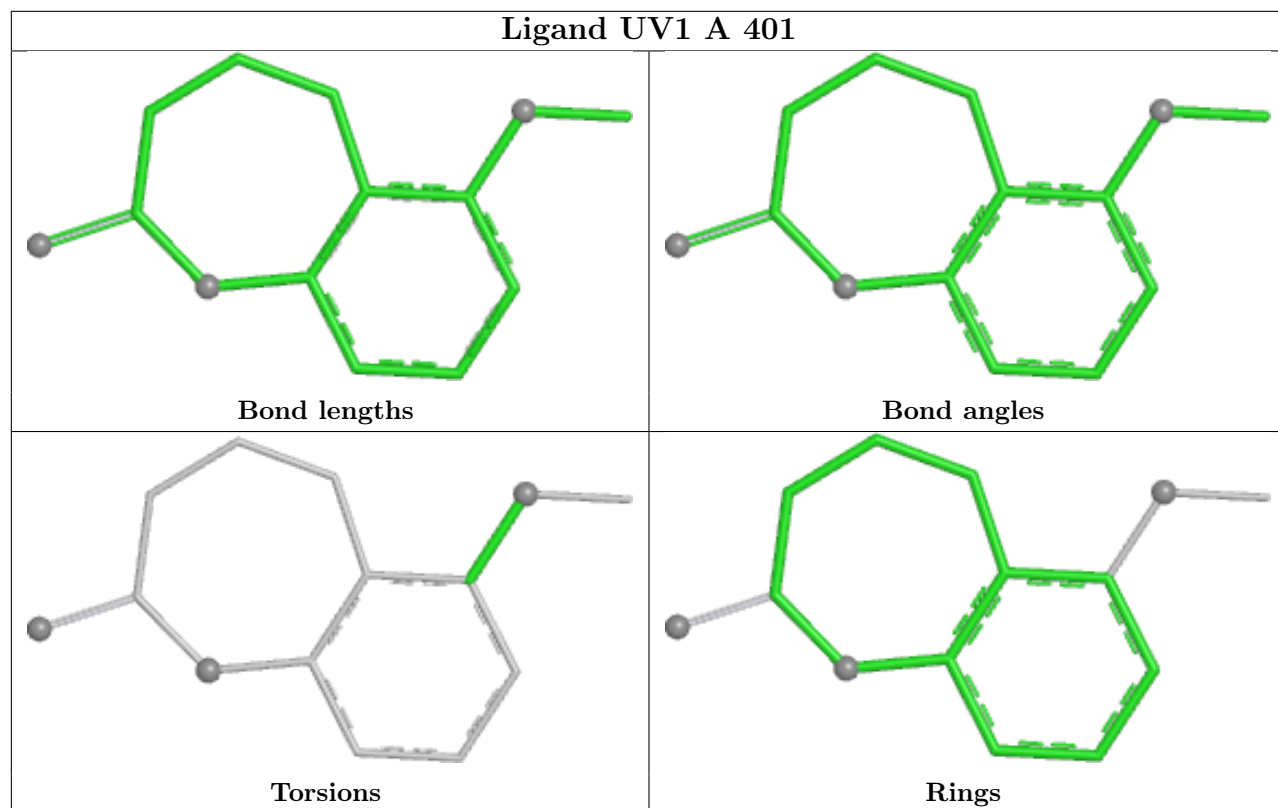
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

### 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<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	265/295 (89%)	2.53	171 (64%) <b>0</b> <b>0</b>	9, 35, 57, 77	166 (62%)
1	B	264/295 (89%)	2.35	144 (54%) <b>0</b> <b>0</b>	8, 47, 69, 93	86 (32%)
All	All	529/590 (89%)	2.44	315 (59%) <b>0</b> <b>0</b>	8, 42, 67, 93	252 (47%)

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	6.7
1	B	129	ALA	6.2
1	B	300[A]	GLU	6.1
1	B	168	SER	6.1
1	A	129	ALA	6.1
1	A	220	PHE	6.1
1	A	137	LEU	5.8
1	B	254	LEU	5.8
1	B	345	ASP	5.7
1	B	230	PRO	5.7
1	A	209	VAL	5.5
1	A	203	THR	5.4
1	A	353	THR	5.4
1	A	356	TRP	5.3
1	B	96	GLY	5.3
1	B	211	ASP	5.2
1	A	159	VAL	5.2
1	B	164	THR	5.1
1	A	166[A]	CYS	5.1
1	A	149	GLU	5.1
1	A	113	VAL	5.0
1	A	171	ARG	5.0
1	A	160	VAL	4.9
1	B	90	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	236	SER	4.9
1	B	209	VAL	4.8
1	A	139	LEU	4.7
1	B	236	SER	4.7
1	B	121	VAL	4.7
1	B	276	VAL	4.7
1	A	84	TYR	4.7
1	A	95	VAL	4.6
1	B	273	ILE	4.6
1	A	123	PHE	4.6
1	B	123	PHE	4.6
1	B	166[A]	CYS	4.5
1	B	122	GLY	4.5
1	B	201	GLN	4.5
1	B	148	ILE	4.4
1	A	193	THR	4.4
1	A	150	ILE	4.4
1	B	253	GLY	4.3
1	A	116	ASN	4.3
1	A	156	TRP	4.2
1	A	211	ASP	4.2
1	B	156	TRP	4.2
1	A	82	LEU	4.2
1	A	87	LYS	4.1
1	A	296	ASP	4.1
1	B	103	VAL	4.1
1	A	289	GLU	4.1
1	B	232	GLU	4.1
1	A	332	ASN	4.1
1	A	345	ASP	4.1
1	A	312	THR	4.1
1	B	215	ASP	4.0
1	A	134[A]	MET	4.0
1	A	230	PRO	4.0
1	A	151	TYR	3.9
1	A	178	TRP	3.9
1	B	349	ILE	3.9
1	A	132	THR	3.9
1	A	354	THR	3.9
1	A	217	TYR	3.9
1	B	119	GLN	3.8
1	B	267	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	301	CYS	3.8
1	A	258	ARG	3.7
1	A	114	GLY	3.7
1	A	195	LYS	3.7
1	B	153	TYR	3.7
1	B	191[A]	ARG	3.7
1	B	234	ASN	3.7
1	A	115	CYS	3.7
1	A	135	ARG	3.7
1	A	235	ARG	3.7
1	A	168	SER	3.7
1	B	139	LEU	3.7
1	B	135	ARG	3.7
1	A	141	TRP	3.7
1	B	212	ASP	3.7
1	B	95	VAL	3.6
1	A	294	THR	3.6
1	B	124	SER	3.6
1	A	263	MET	3.6
1	B	160	VAL	3.6
1	B	213	VAL	3.6
1	B	306	VAL	3.6
1	A	264	ASN	3.6
1	A	189	THR	3.6
1	A	154	PRO	3.6
1	B	233	ASN	3.6
1	B	130	THR	3.5
1	B	196	TRP	3.5
1	B	84	TYR	3.5
1	B	225	PRO	3.5
1	B	183	SER	3.5
1	A	270	VAL	3.5
1	A	131	THR	3.5
1	A	279	SER	3.5
1	B	235	ARG	3.5
1	A	97[A]	SER	3.4
1	A	340	LEU	3.4
1	B	357	ARG	3.4
1	A	339	LEU	3.4
1	B	280	ILE	3.4
1	A	306	VAL	3.4
1	B	229	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	344	GLY	3.4
1	A	268	ASN	3.4
1	B	151	TYR	3.4
1	A	337	LEU	3.3
1	B	310	LEU	3.3
1	A	262	ASP	3.3
1	A	244	GLU	3.3
1	A	284	ILE	3.3
1	A	249	TYR	3.3
1	B	336	PHE	3.3
1	A	261	LEU	3.3
1	B	157	GLY	3.2
1	A	267	VAL	3.2
1	A	245	ASP	3.2
1	A	96	GLY	3.2
1	A	359	LYS	3.2
1	A	212	ASP	3.2
1	A	190	GLY	3.2
1	A	255	LYS	3.2
1	B	199	MET	3.2
1	B	167	GLN	3.2
1	A	222	PRO	3.2
1	A	256	PRO	3.2
1	B	354	THR	3.1
1	A	286	ASP	3.1
1	B	275	TRP	3.1
1	B	356	TRP	3.1
1	B	358	LYS	3.1
1	A	101	ALA	3.1
1	A	229	PHE	3.1
1	B	149[A]	GLU	3.1
1	B	301	CYS	3.1
1	B	189	THR	3.1
1	A	251	MET	3.1
1	B	197	VAL	3.1
1	B	198	MET	3.1
1	B	252	ILE	3.0
1	A	181	LYS	3.0
1	A	239	LYS	3.0
1	A	288	HIS	3.0
1	B	170	GLY	3.0
1	A	228	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	3.0
1	A	242	LYS	3.0
1	A	202	ASP	3.0
1	A	120[A]	SER	3.0
1	A	227	LEU	3.0
1	A	341	ARG	3.0
1	A	283	GLU	3.0
1	A	98	ASN	2.9
1	B	190	GLY	2.9
1	B	346	GLY	2.9
1	A	162	ILE	2.9
1	B	249	TYR	2.9
1	A	302	GLN	2.9
1	A	299	ARG	2.9
1	A	142	VAL	2.9
1	A	219	VAL	2.9
1	B	82	LEU	2.9
1	B	188	VAL	2.9
1	B	340	LEU	2.9
1	B	263	MET	2.9
1	B	333	ASP	2.9
1	B	131	THR	2.9
1	A	281	PRO	2.9
1	B	342	LEU	2.9
1	A	343	SER	2.9
1	A	272	TYR	2.9
1	B	274	GLY	2.9
1	A	300	GLU	2.9
1	A	180	LEU	2.8
1	A	184	VAL	2.8
1	A	285	VAL	2.8
1	B	220	PHE	2.8
1	B	298	ARG	2.8
1	B	140	ILE	2.8
1	A	287	THR	2.8
1	B	152	LYS	2.8
1	A	177	ASP	2.8
1	A	88	PHE	2.8
1	B	216	GLU	2.8
1	B	185	THR	2.8
1	B	115	CYS	2.8
1	B	272	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLN	2.8
1	B	355	LEU	2.8
1	A	161	GLU	2.8
1	A	210	SER	2.8
1	B	293	ILE	2.7
1	A	201	GLN	2.7
1	B	98	ASN	2.7
1	B	195	LYS	2.7
1	A	250	SER	2.7
1	A	303	GLN	2.7
1	B	187	GLU	2.7
1	B	217	TYR	2.7
1	A	310	LEU	2.7
1	B	206	LEU	2.7
1	B	88	PHE	2.7
1	B	179	ILE	2.7
1	A	136	LYS	2.7
1	B	99	LYS	2.7
1	B	136	LYS	2.7
1	B	134	MET	2.7
1	A	117	HIS	2.7
1	A	92	SER	2.6
1	B	118	ALA	2.6
1	B	291	GLN	2.6
1	B	240	ILE	2.6
1	B	256	PRO	2.6
1	B	214	ARG	2.6
1	A	311	THR	2.6
1	B	146	MET	2.6
1	A	214	ARG	2.6
1	B	138	HIS	2.6
1	B	247	ALA	2.5
1	B	105	THR	2.5
1	B	133	THR	2.5
1	B	205	ARG	2.5
1	B	162	ILE	2.5
1	B	141	TRP	2.5
1	A	185	THR	2.5
1	A	252	ILE	2.5
1	A	77	LEU	2.5
1	B	155	ALA	2.5
1	A	191	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	204	ARG	2.5
1	A	79	GLU	2.5
1	A	240	ILE	2.5
1	B	137	LEU	2.5
1	A	226	ARG	2.5
1	A	121	VAL	2.5
1	A	183	SER	2.4
1	B	284	ILE	2.4
1	B	218	LEU	2.4
1	B	227	LEU	2.4
1	A	232	GLU	2.4
1	B	159	VAL	2.4
1	A	152	LYS	2.4
1	B	93	TYR	2.4
1	A	333	ASP	2.4
1	B	178	TRP	2.4
1	A	297	TYR	2.4
1	A	257	ARG	2.4
1	A	344	GLY	2.4
1	A	243	LEU	2.4
1	A	109	LEU	2.3
1	A	91	ARG	2.3
1	B	339	LEU	2.3
1	A	204	ARG	2.3
1	B	142	VAL	2.3
1	B	307	VAL	2.3
1	B	114	GLY	2.3
1	B	186	GLY	2.3
1	A	221	CYS	2.3
1	B	245	ASP	2.3
1	B	308	ASP	2.3
1	B	203	THR	2.3
1	A	336	PHE	2.2
1	A	280	ILE	2.2
1	A	293	ILE	2.2
1	A	130	THR	2.2
1	B	334	SER	2.2
1	A	246	PRO	2.2
1	A	170	GLY	2.2
1	B	81	GLY	2.2
1	A	188	VAL	2.2
1	B	147	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	233	ASN	2.2
1	B	100	THR	2.2
1	A	167	GLN	2.2
1	A	347	GLN	2.2
1	A	224	GLU	2.2
1	B	77	LEU	2.2
1	B	297	TYR	2.2
1	A	81	GLY	2.2
1	B	89	VAL	2.2
1	A	335	GLN	2.2
1	A	187	GLU	2.1
1	B	353	THR	2.1
1	A	194	SER	2.1
1	B	76	SER	2.1
1	A	175	ARG	2.1
1	A	234	ASN	2.1
1	A	89	VAL	2.1
1	A	182	ASP	2.1
1	A	315	SER	2.1
1	B	158	ASP	2.1
1	B	294	THR	2.1
1	A	266	HIS	2.1
1	A	198	MET	2.1
1	A	295	LEU	2.1
1	B	261	LEU	2.1
1	B	210	SER	2.1
1	B	335	GLN	2.1
1	A	86	GLU	2.1
1	A	308	ASP	2.1
1	A	174	THR	2.1
1	A	122	GLY	2.0
1	A	157	GLY	2.0
1	A	282	GLN	2.1
1	A	163	GLU	2.0
1	A	338	HIS	2.0
1	A	218	LEU	2.0
1	A	290	LEU	2.0
1	B	243	LEU	2.0
1	B	350	ASN	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

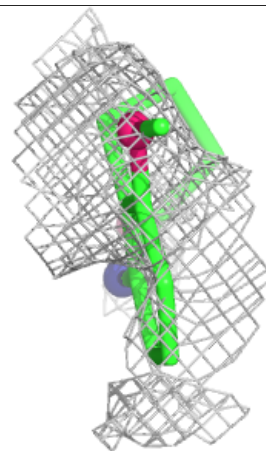
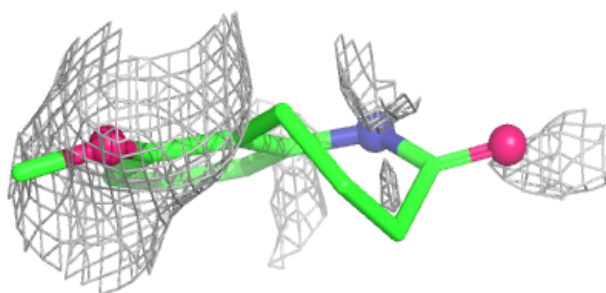
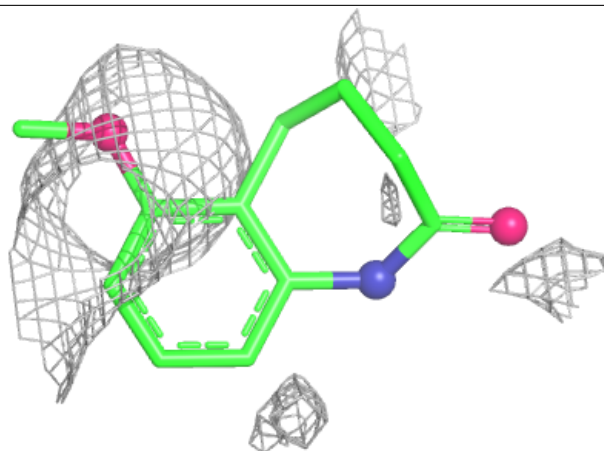
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	UV1	B	401	14/14	0.92	0.24	41,41,41,41	14
3	SO4	B	402	5/5	0.92	0.29	60,60,60,61	5
2	UV1	A	401	14/14	0.93	0.18	40,42,42,42	14
3	SO4	A	402	5/5	0.96	0.12	89,89,89,89	0

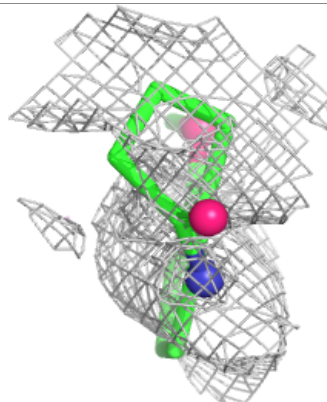
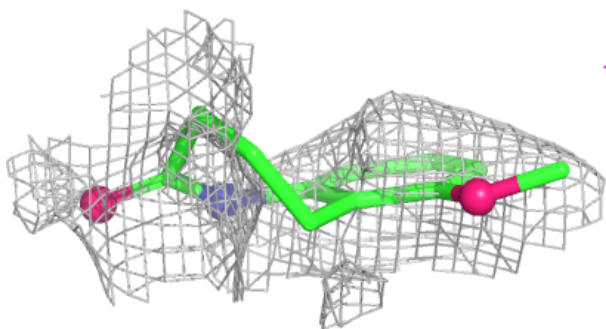
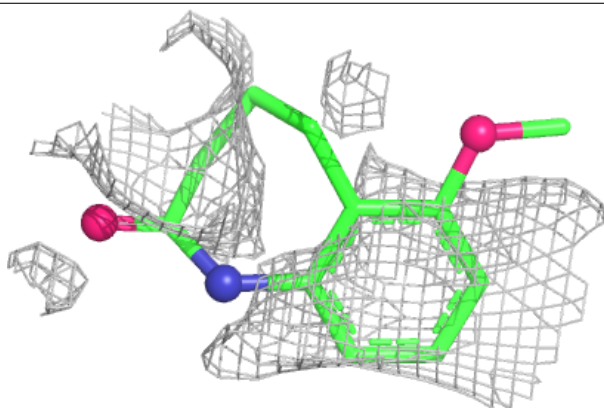
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UV1 B 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 UV1 A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.