



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:16 PM UTC

PDB ID : 7HSF / pdb_00007hsf
Title : PanDDA analysis group deposition – Crystal Structure of FatA in complex with Z1503180352
Authors : Kot, E.; Ni, X.; Tomlinson, C.W.E.; Fearon, D.; Aschenbrenner, J.C.; Fairhead, M.; Koekemoer, L.; Marx, M.L.; Wright, N.D.; Mulholland, N.P.; Montgomery, M.G.; von Delft, F.
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

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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

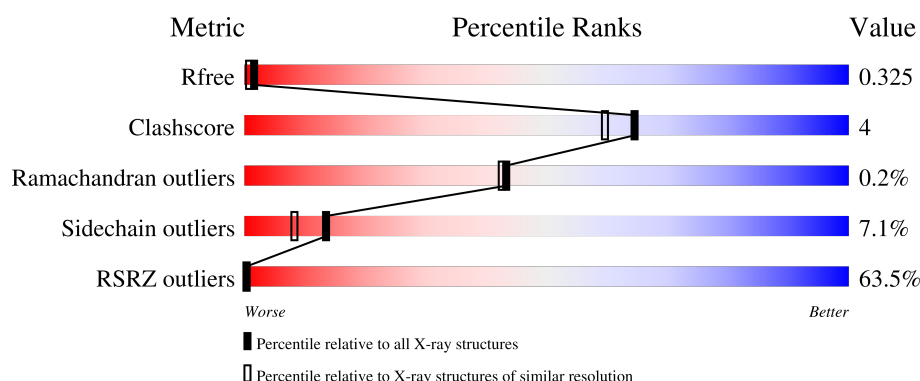
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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 ≥ 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>62%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	295	<div> <div>52%</div> <div> <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.

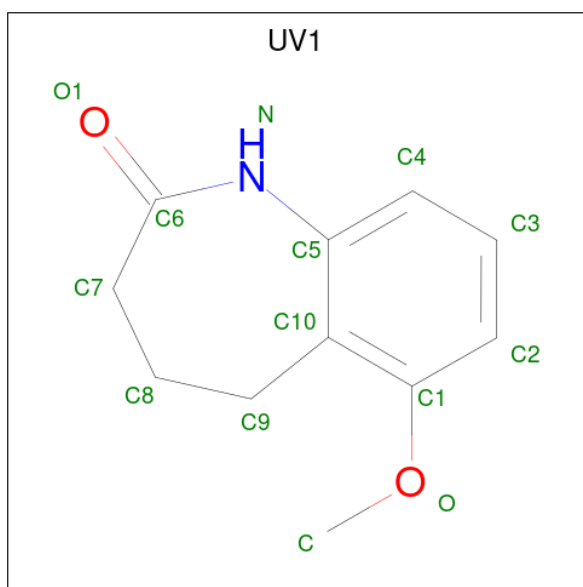
- Molecule 1 is a protein called Oleoyl-acyl carrier protein thioesterase 1, chloroplastic.

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: C₁₁H₁₃NO₂) (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: O₄S).



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		

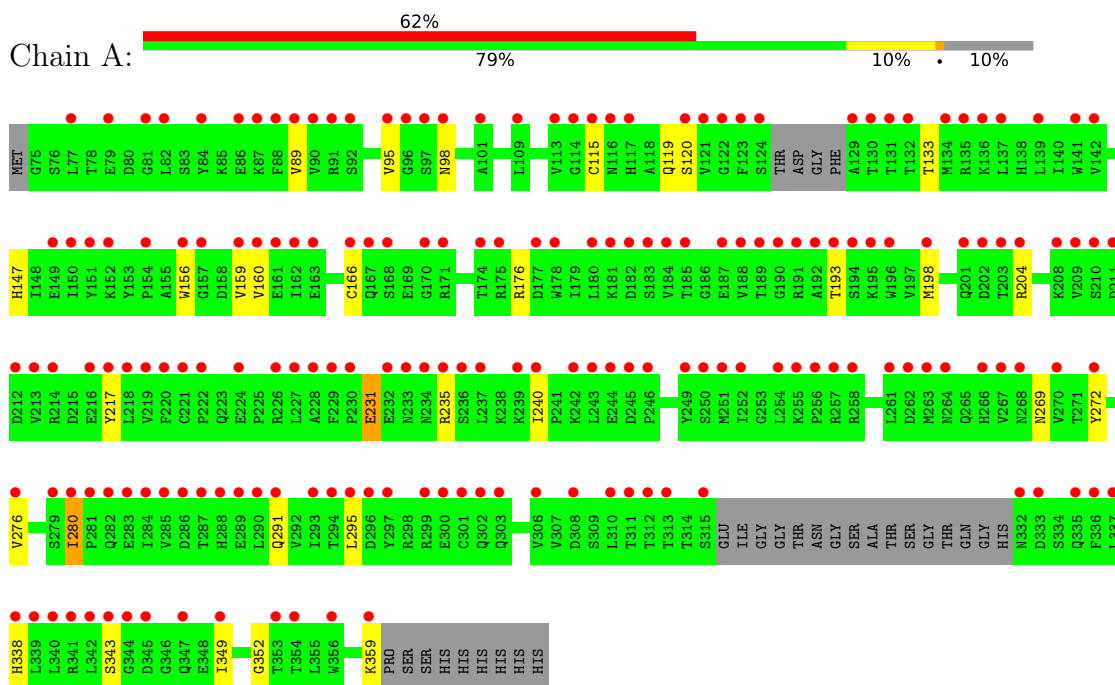
- Molecule 4 is water.

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

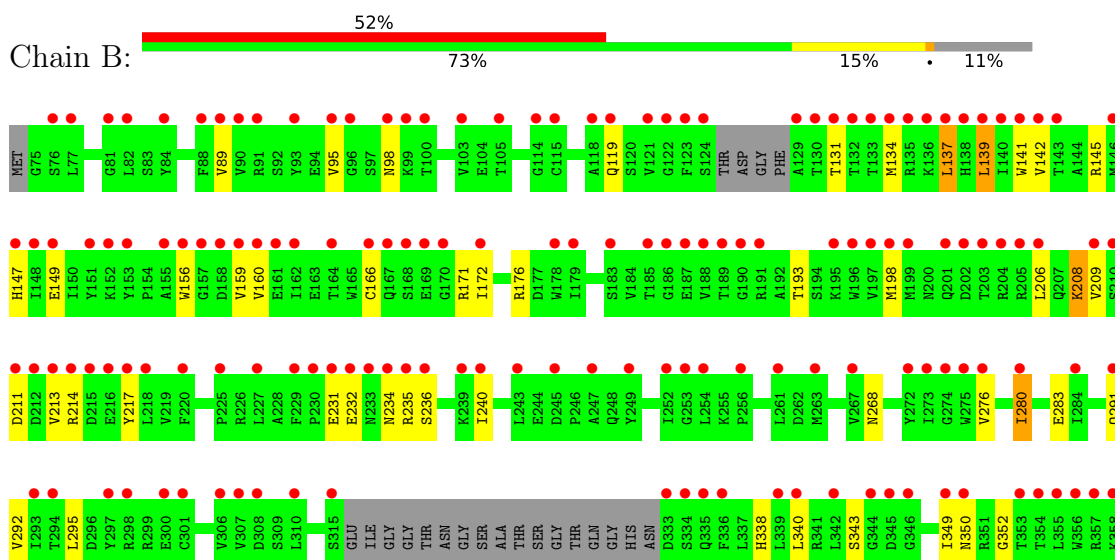
3 Residue-property plots

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: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic



- Molecule 1: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic



K359
PRO
SER
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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	33.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 263.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: 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%)	43	42

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%)	17	12
1	B	247/263 (94%)	226 (92%)	21 (8%)	10	5
All	All	495/526 (94%)	459 (93%)	36 (7%)	13	8

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UV1	B	401	-	15,15,15	0.25	0	18,20,20	0.75	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.36	0
3	SO4	B	402	-	4,4,4	0.28	0	6,6,6	0.46	0
2	UV1	A	401	-	15,15,15	0.28	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	B	401	-	-	0/2/12/12	0/2/2/2
2	UV1	A	401	-	-	0/2/12/12	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

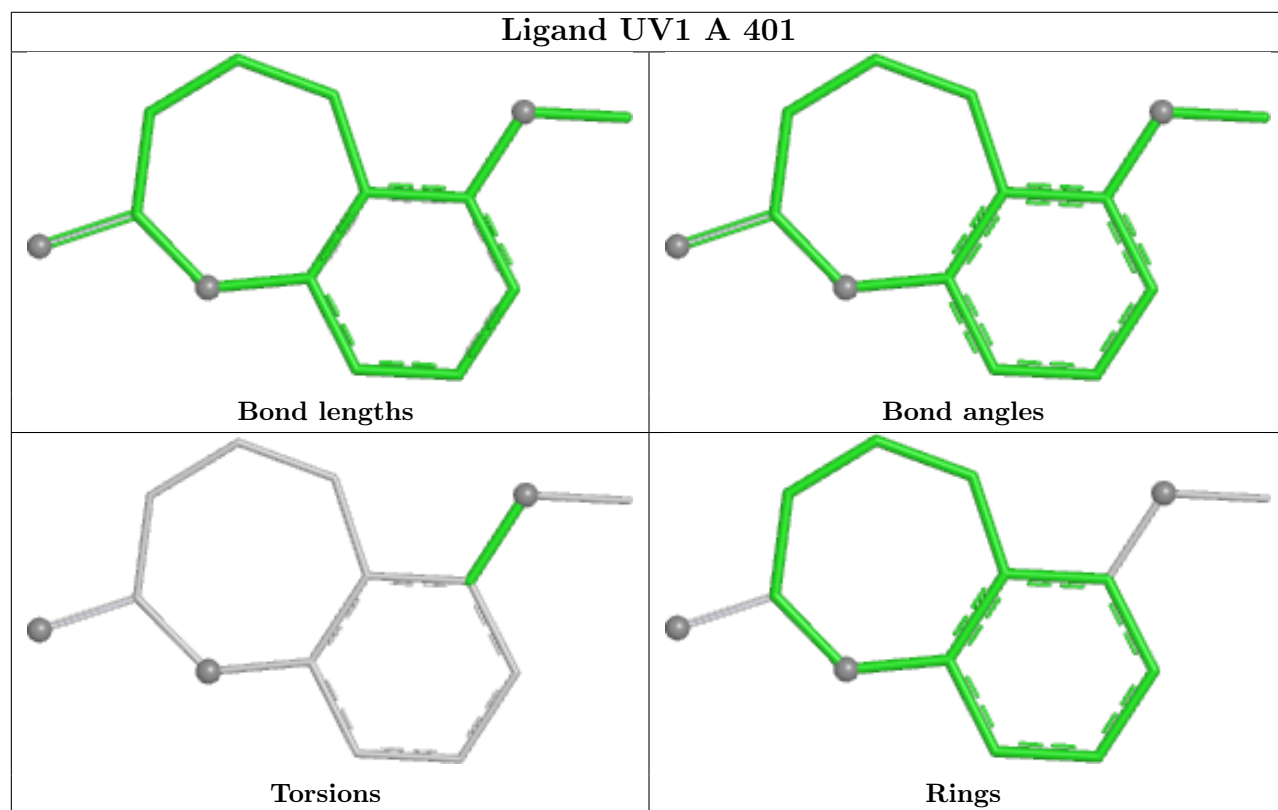
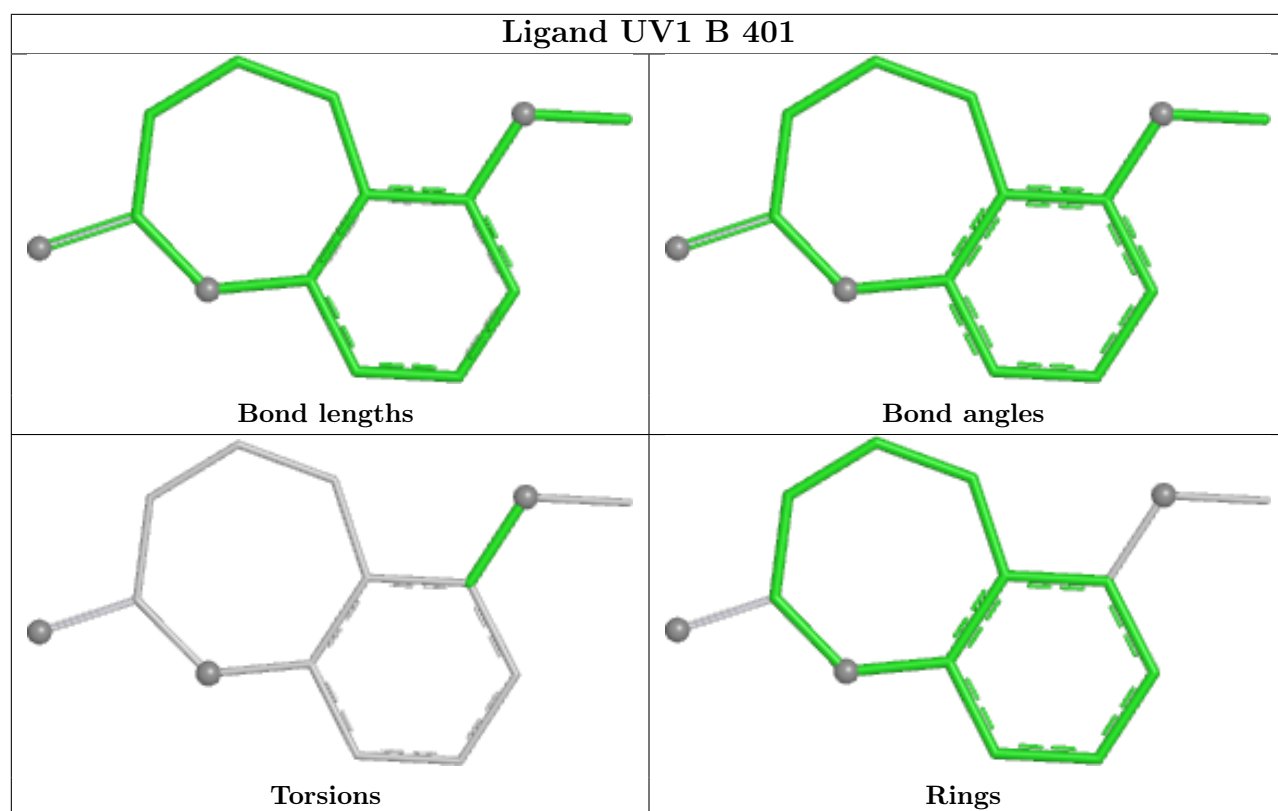
There are no chirality outliers.

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, 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	265/295 (89%)	2.65	182 (68%) 0 0	9, 35, 57, 77	166 (62%)
1	B	264/295 (89%)	2.48	154 (58%) 0 0	8, 47, 69, 93	86 (32%)
All	All	529/590 (89%)	2.56	336 (63%) 0 0	8, 42, 67, 93	252 (47%)

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	LEU	6.9
1	B	129	ALA	6.4
1	A	220	PHE	6.3
1	A	129	ALA	6.3
1	B	168	SER	6.3
1	B	300[A]	GLU	6.2
1	A	137	LEU	6.0
1	B	254	LEU	6.0
1	B	230	PRO	5.8
1	B	345	ASP	5.8
1	A	209	VAL	5.7
1	A	356	TRP	5.6
1	A	203	THR	5.6
1	A	353	THR	5.6
1	B	96	GLY	5.5
1	A	159	VAL	5.4
1	B	211	ASP	5.3
1	A	166[A]	CYS	5.3
1	B	164	THR	5.3
1	A	113	VAL	5.2
1	A	149	GLU	5.1
1	A	160	VAL	5.1
1	B	90	VAL	5.1
1	A	171	ARG	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	236	SER	5.0
1	B	209	VAL	4.9
1	A	139	LEU	4.9
1	A	84	TYR	4.9
1	B	121	VAL	4.9
1	B	276	VAL	4.9
1	A	95	VAL	4.8
1	B	236	SER	4.8
1	A	123	PHE	4.8
1	B	123	PHE	4.8
1	B	273	ILE	4.7
1	B	166[A]	CYS	4.7
1	B	122	GLY	4.7
1	B	148	ILE	4.6
1	B	201	GLN	4.5
1	A	193	THR	4.5
1	B	253	GLY	4.5
1	A	150	ILE	4.5
1	A	156	TRP	4.5
1	B	156	TRP	4.4
1	A	116	ASN	4.4
1	A	82	LEU	4.4
1	B	103	VAL	4.3
1	A	211	ASP	4.3
1	A	296	ASP	4.2
1	A	312	THR	4.2
1	A	87	LYS	4.2
1	A	332	ASN	4.2
1	A	178	TRP	4.1
1	A	345	ASP	4.1
1	A	289	GLU	4.1
1	B	232	GLU	4.1
1	A	230	PRO	4.1
1	A	151	TYR	4.1
1	A	134[A]	MET	4.1
1	B	215	ASP	4.1
1	A	217	TYR	4.1
1	B	349	ILE	4.1
1	A	132	THR	4.0
1	A	354	THR	4.0
1	B	267	VAL	3.9
1	A	301	CYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	114	GLY	3.9
1	B	153	TYR	3.9
1	B	119	GLN	3.9
1	A	141	TRP	3.9
1	A	115	CYS	3.9
1	B	139	LEU	3.9
1	B	234	ASN	3.8
1	B	95	VAL	3.8
1	A	168	SER	3.8
1	A	258	ARG	3.8
1	A	195	LYS	3.8
1	B	191[A]	ARG	3.8
1	A	294	THR	3.8
1	B	160	VAL	3.8
1	B	213	VAL	3.8
1	B	306	VAL	3.8
1	A	135	ARG	3.8
1	A	235	ARG	3.8
1	B	196	TRP	3.7
1	B	212	ASP	3.7
1	B	135	ARG	3.7
1	B	124	SER	3.7
1	A	189	THR	3.7
1	A	154	PRO	3.7
1	A	263	MET	3.7
1	A	264	ASN	3.7
1	B	84	TYR	3.7
1	B	130	THR	3.7
1	B	233	ASN	3.7
1	A	270	VAL	3.7
1	B	225	PRO	3.6
1	A	131	THR	3.6
1	B	183	SER	3.6
1	A	340	LEU	3.6
1	A	279	SER	3.6
1	B	229	PHE	3.6
1	A	339	LEU	3.6
1	B	344	GLY	3.6
1	A	97[A]	SER	3.6
1	A	306	VAL	3.5
1	B	280	ILE	3.5
1	B	151	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	235	ARG	3.5
1	A	337	LEU	3.5
1	B	310	LEU	3.5
1	A	268	ASN	3.5
1	B	357	ARG	3.5
1	B	336	PHE	3.4
1	A	249	TYR	3.4
1	A	284	ILE	3.4
1	B	157	GLY	3.4
1	A	261	LEU	3.4
1	A	267	VAL	3.4
1	A	96	GLY	3.4
1	A	262	ASP	3.4
1	A	190	GLY	3.4
1	B	275	TRP	3.3
1	B	356	TRP	3.3
1	A	244	GLU	3.3
1	A	245	ASP	3.3
1	A	222	PRO	3.3
1	A	256	PRO	3.3
1	A	101	ALA	3.3
1	A	229	PHE	3.3
1	B	199	MET	3.3
1	A	212	ASP	3.3
1	B	354	THR	3.3
1	A	359	LYS	3.3
1	B	167	GLN	3.3
1	B	301	CYS	3.2
1	A	255	LYS	3.2
1	A	286	ASP	3.2
1	B	189	THR	3.2
1	B	197	VAL	3.2
1	B	170	GLY	3.2
1	B	358	LYS	3.2
1	A	228	ALA	3.2
1	B	252	ILE	3.2
1	B	149[A]	GLU	3.2
1	A	251	MET	3.2
1	B	198	MET	3.2
1	A	288	HIS	3.1
1	A	227	LEU	3.1
1	A	349	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	190	GLY	3.1
1	B	346	GLY	3.1
1	A	181	LYS	3.1
1	A	239	LYS	3.1
1	A	120[A]	SER	3.1
1	B	249	TYR	3.1
1	A	202	ASP	3.1
1	A	142	VAL	3.1
1	A	219	VAL	3.1
1	B	188	VAL	3.1
1	B	82	LEU	3.1
1	B	340	LEU	3.1
1	A	162	ILE	3.1
1	A	98	ASN	3.0
1	A	242	LYS	3.0
1	B	342	LEU	3.0
1	A	341	ARG	3.0
1	B	274	GLY	3.0
1	B	131	THR	3.0
1	A	272	TYR	3.0
1	A	281	PRO	3.0
1	A	283	GLU	3.0
1	B	220	PHE	3.0
1	B	263	MET	3.0
1	A	302	GLN	3.0
1	A	180	LEU	3.0
1	A	184	VAL	3.0
1	A	285	VAL	3.0
1	B	333	ASP	3.0
1	A	88	PHE	3.0
1	A	299	ARG	3.0
1	A	343	SER	3.0
1	B	140	ILE	3.0
1	A	287	THR	3.0
1	B	272	TYR	3.0
1	B	115	CYS	2.9
1	B	355	LEU	2.9
1	B	185	THR	2.9
1	A	300	GLU	2.9
1	A	177	ASP	2.9
1	B	298	ARG	2.9
1	B	152	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	291	GLN	2.9
1	B	293	ILE	2.9
1	B	216	GLU	2.9
1	A	210	SER	2.9
1	B	88	PHE	2.9
1	B	217	TYR	2.9
1	A	310	LEU	2.8
1	B	206	LEU	2.8
1	A	250	SER	2.8
1	B	98	ASN	2.8
1	A	201	GLN	2.8
1	A	161	GLU	2.8
1	B	179	ILE	2.8
1	A	303	GLN	2.8
1	B	118	ALA	2.8
1	B	195	LYS	2.8
1	A	117	HIS	2.8
1	B	134	MET	2.8
1	B	187	GLU	2.8
1	A	92	SER	2.7
1	A	136	LYS	2.7
1	B	99	LYS	2.7
1	B	136	LYS	2.7
1	B	256	PRO	2.7
1	B	240	ILE	2.7
1	B	141	TRP	2.7
1	B	247	ALA	2.7
1	A	311	THR	2.7
1	B	291	GLN	2.7
1	B	105	THR	2.7
1	B	133	THR	2.7
1	B	138	HIS	2.7
1	B	146	MET	2.7
1	B	162	ILE	2.7
1	B	214	ARG	2.7
1	B	155	ALA	2.6
1	A	77	LEU	2.6
1	A	185	THR	2.6
1	A	252	ILE	2.6
1	A	214	ARG	2.6
1	B	137	LEU	2.6
1	B	205	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	121	VAL	2.6
1	A	240	ILE	2.6
1	B	178	TRP	2.6
1	B	218	LEU	2.6
1	B	227	LEU	2.6
1	B	93	TYR	2.6
1	B	159	VAL	2.6
1	B	284	ILE	2.6
1	A	191	ARG	2.6
1	B	204	ARG	2.6
1	A	183	SER	2.6
1	A	79	GLU	2.5
1	A	297	TYR	2.5
1	A	344	GLY	2.5
1	A	226	ARG	2.5
1	A	243	LEU	2.5
1	A	333	ASP	2.5
1	A	232	GLU	2.5
1	A	109	LEU	2.5
1	A	152	LYS	2.5
1	B	339	LEU	2.5
1	A	257	ARG	2.5
1	B	114	GLY	2.5
1	B	186	GLY	2.5
1	B	142	VAL	2.4
1	B	307	VAL	2.4
1	A	221	CYS	2.4
1	A	91	ARG	2.4
1	A	336	PHE	2.4
1	A	204	ARG	2.4
1	B	203	THR	2.4
1	A	170	GLY	2.4
1	B	81	GLY	2.4
1	B	245	ASP	2.4
1	B	308	ASP	2.4
1	A	188	VAL	2.4
1	A	280	ILE	2.4
1	A	293	ILE	2.4
1	A	130	THR	2.4
1	A	246	PRO	2.4
1	B	334	SER	2.3
1	B	147	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	100	THR	2.3
1	B	297	TYR	2.3
1	A	233	ASN	2.3
1	A	81	GLY	2.3
1	B	77	LEU	2.3
1	B	89	VAL	2.3
1	A	167	GLN	2.3
1	A	347	GLN	2.3
1	A	89	VAL	2.3
1	B	353	THR	2.3
1	A	224	GLU	2.2
1	A	194	SER	2.2
1	A	335	GLN	2.2
1	B	76	SER	2.2
1	B	294	THR	2.2
1	A	234	ASN	2.2
1	A	295	LEU	2.2
1	B	261	LEU	2.2
1	A	187	GLU	2.2
1	A	266	HIS	2.2
1	A	315	SER	2.2
1	A	175	ARG	2.2
1	A	182	ASP	2.2
1	A	198	MET	2.2
1	B	158	ASP	2.2
1	A	122	GLY	2.2
1	A	157	GLY	2.2
1	B	210	SER	2.2
1	A	174	THR	2.2
1	B	335	GLN	2.2
1	A	218	LEU	2.2
1	A	290	LEU	2.2
1	B	243	LEU	2.2
1	A	308	ASP	2.2
1	A	86	GLU	2.1
1	A	282	GLN	2.1
1	A	338	HIS	2.1
1	A	192	ALA	2.1
1	B	350	ASN	2.1
1	A	163	GLU	2.1
1	A	196	TRP	2.1
1	A	90	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	2.1
1	B	315	SER	2.1
1	B	132	THR	2.1
1	A	124	SER	2.1
1	B	161	GLU	2.1
1	B	231	GLU	2.1
1	A	313	THR	2.1
1	A	208	LYS	2.1
1	B	172	ILE	2.1
1	A	213	VAL	2.1
1	B	91	ARG	2.0
1	A	216	GLU	2.0
1	B	169	GLU	2.0
1	A	254	LEU	2.0
1	A	342	LEU	2.0
1	B	202	ASP	2.0
1	B	239	LYS	2.0
1	B	143	THR	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](#)

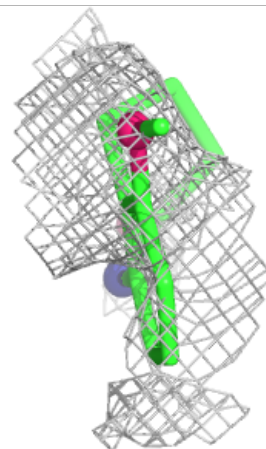
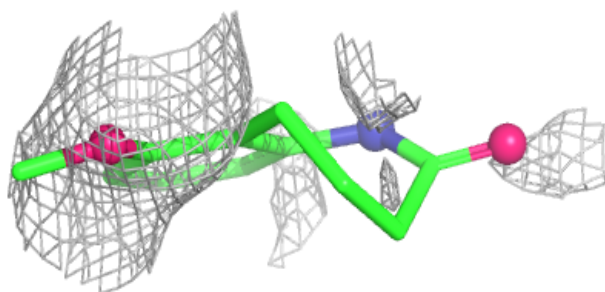
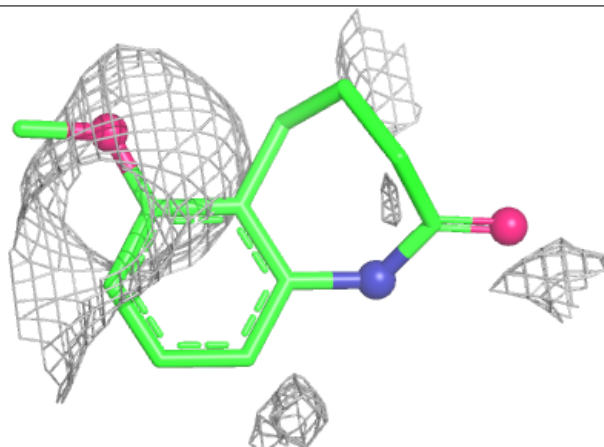
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

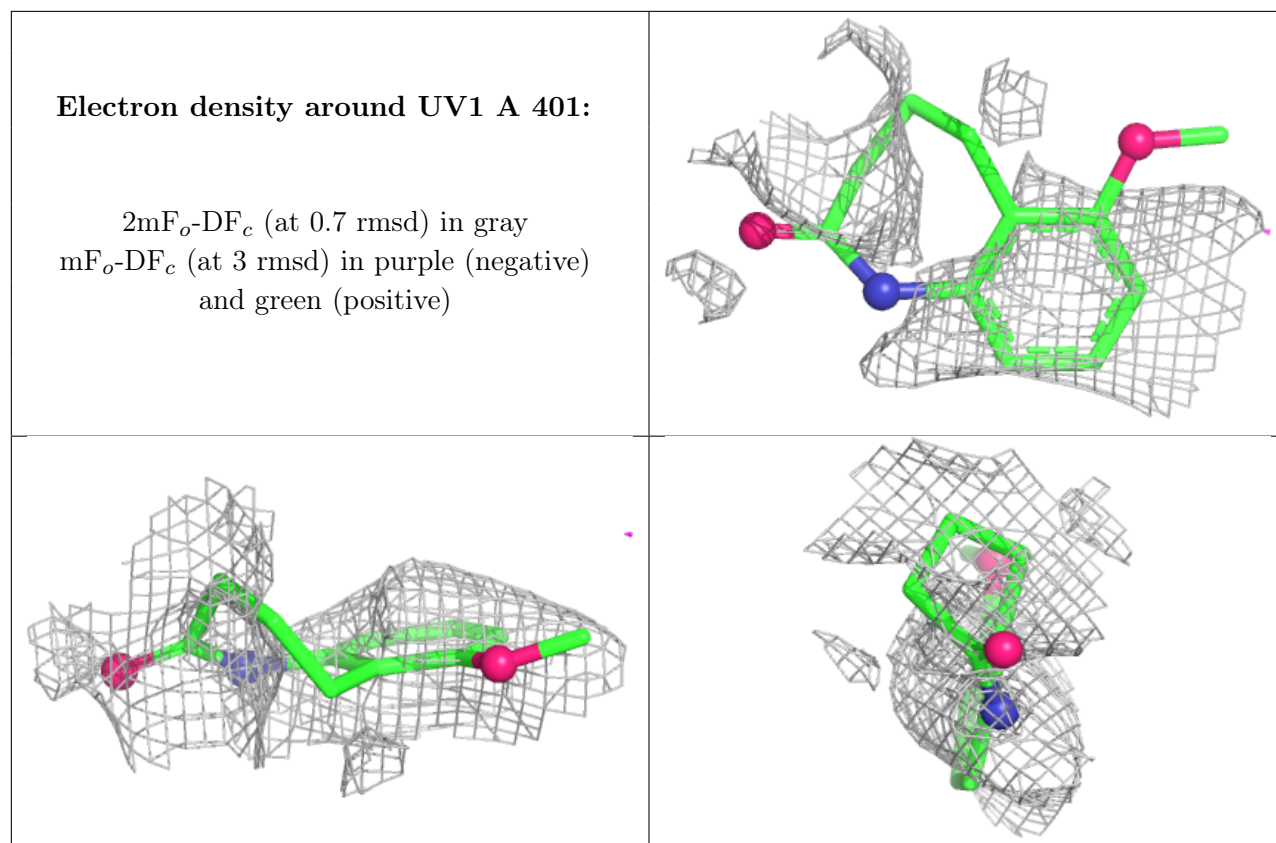
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UV1	B	401	14/14	0.92	0.24	41,41,41,41	14
3	SO4	B	402	5/5	0.92	0.29	60,60,60,61	5
2	UV1	A	401	14/14	0.93	0.18	40,42,42,42	14
3	SO4	A	402	5/5	0.96	0.12	89,89,89,89	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.