Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 12:18 pm GMT

PDB ID	:	9T3U / pdb_00009t3u
Title	:	Crystal structure of human soluble epoxide hydrolase C-terminal domain in complex with a TPPU-6-chlorotacrine hybrid
Authors	:	Qiu, Q.; Prischi, F.; Martinez-Conde, N.; Mullins, J.; Munoz-Torrero, D.; Vazquez, S.; Conte, M.R.
Deposited on	:	2025-10-29
Resolution	:	2.00 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 ⓘ) were used in the production of this report:

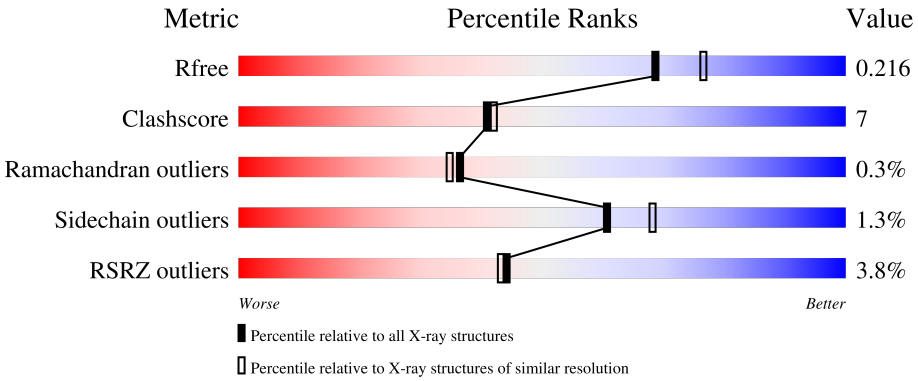
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	344	5% 82% 10% • 8%
1	B	344	2% 78% 13% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5796 atoms, of which 76 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	1	0
			2551	1639	427	462	23			
1	B	316	Total	C	N	O	S	0	0	0
			2546	1636	426	461	23			

There are 36 discrepancies between the modelled and reference sequences:

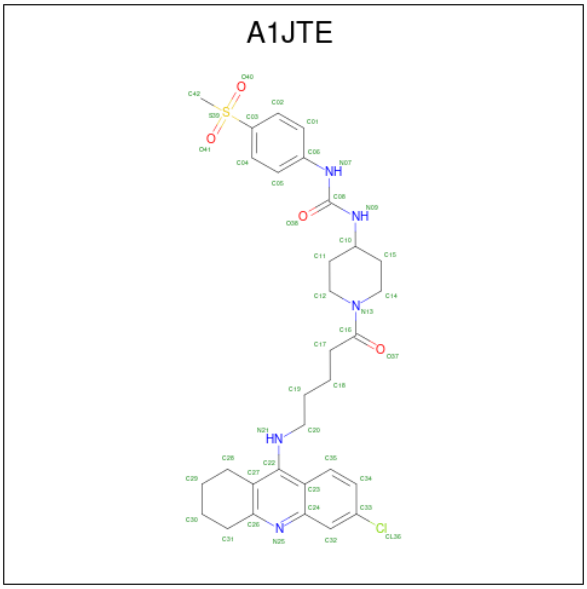
Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP P34913
A	213	HIS	-	expression tag	UNP P34913
A	214	HIS	-	expression tag	UNP P34913
A	215	HIS	-	expression tag	UNP P34913
A	216	HIS	-	expression tag	UNP P34913
A	217	HIS	-	expression tag	UNP P34913
A	218	HIS	-	expression tag	UNP P34913
A	219	SER	-	expression tag	UNP P34913
A	220	THR	-	expression tag	UNP P34913
A	221	GLU	-	expression tag	UNP P34913
A	222	ASN	-	expression tag	UNP P34913
A	223	LEU	-	expression tag	UNP P34913
A	224	TYR	-	expression tag	UNP P34913
A	225	PHE	-	expression tag	UNP P34913
A	226	GLN	-	expression tag	UNP P34913
A	227	GLY	-	expression tag	UNP P34913
A	228	SER	-	expression tag	UNP P34913
A	229	SER	-	expression tag	UNP P34913
B	212	MET	-	initiating methionine	UNP P34913
B	213	HIS	-	expression tag	UNP P34913
B	214	HIS	-	expression tag	UNP P34913
B	215	HIS	-	expression tag	UNP P34913
B	216	HIS	-	expression tag	UNP P34913
B	217	HIS	-	expression tag	UNP P34913
B	218	HIS	-	expression tag	UNP P34913

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	SER	-	expression tag	UNP P34913
B	220	THR	-	expression tag	UNP P34913
B	221	GLU	-	expression tag	UNP P34913
B	222	ASN	-	expression tag	UNP P34913
B	223	LEU	-	expression tag	UNP P34913
B	224	TYR	-	expression tag	UNP P34913
B	225	PHE	-	expression tag	UNP P34913
B	226	GLN	-	expression tag	UNP P34913
B	227	GLY	-	expression tag	UNP P34913
B	228	SER	-	expression tag	UNP P34913
B	229	SER	-	expression tag	UNP P34913

- Molecule 2 is 1-[1-[5-[(6-chloranyl-1,2,3,4-tetrahydroacridin-9-yl)amino]pentanoyl]piperidin-4-yl]-3-(4-methylsulfonylphenyl)urea (CCD ID: A1JTE) (formula: $C_{31}H_{38}ClN_5O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	S	0	0
			80	31	1	38	5	4	1		
2	B	1	Total	C	Cl	H	N	O	S	0	0
			80	31	1	38	5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	236	Total	O	0	0
			236	236		

Continued on next page...

Continued from previous page...

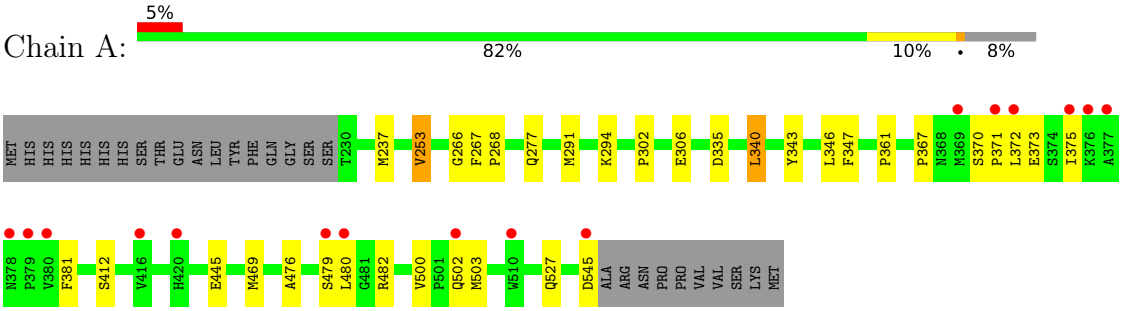
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	303	Total	O	0	0
			303	303		

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.

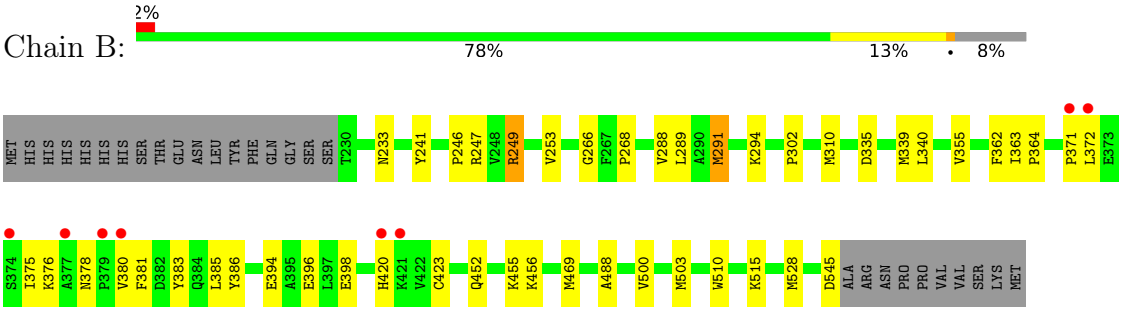
• Molecule 1: Bifunctional epoxide hydrolase 2

Chain A:



• Molecule 1: Bifunctional epoxide hydrolase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.97Å 80.50Å 105.18Å 90.00° 91.34° 90.00°	Depositor
Resolution (Å)	52.58 – 2.00 52.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.58-2.00) 99.9 (52.58-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.167 , 0.214 0.168 , 0.216	Depositor DCC
R_{free} test set	2587 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5796	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JTE

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	0.32	0/2627	0.48	0/3564
1	B	0.37	0/2622	0.52	0/3557
All	All	0.35	0/5249	0.50	0/7121

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	B	249	ARG	Sidechain
1	B	291	MET	Peptide

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	2551	0	2474	31	0
1	B	2546	0	2473	35	0
2	A	42	38	0	0	0
2	B	42	38	0	0	0
3	A	236	0	0	1	0
3	B	303	0	0	5	0
All	All	5720	76	4947	66	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 7.

All (66) 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:469:MET:HG2	3:A:834:HOH:O	1.71	0.91
1:A:371:PRO:HB2	1:A:469:MET:HE3	1.60	0.81
1:A:367:PRO:HG3	1:A:480:LEU:CD1	2.14	0.78
1:A:371:PRO:CB	1:A:469:MET:HE3	2.18	0.72
1:B:380:VAL:HA	1:B:420:HIS:HE1	1.54	0.72
1:B:372:LEU:HG	1:B:376:LYS:HD2	1.73	0.70
1:A:371:PRO:HG2	1:A:469:MET:HE3	1.73	0.69
1:B:241:TYR:HB3	1:B:249:ARG:HD2	1.73	0.69
1:A:371:PRO:CG	1:A:469:MET:HE3	2.23	0.68
1:B:500:VAL:HG22	1:B:503:MET:HG3	1.76	0.67
1:B:378:ASN:OD1	1:B:380:VAL:HB	1.94	0.66
1:A:372:LEU:HG	1:A:469:MET:HE2	1.77	0.64
1:A:306:GLU:H	1:A:306:GLU:CD	2.06	0.62
1:A:361:PRO:HG3	1:A:503:MET:HE2	1.81	0.62
1:A:347:PHE:CZ	1:A:479:SER:HB3	2.35	0.62
1:B:380:VAL:HA	1:B:420:HIS:CE1	2.35	0.62
1:A:479:SER:O	1:A:482:ARG:HG2	2.02	0.60
1:B:339:MET:HG3	3:B:752:HOH:O	2.02	0.59
1:A:367:PRO:HG3	1:A:480:LEU:HD11	1.82	0.59
1:B:394:GLU:O	1:B:398:GLU:HG3	2.03	0.59
1:A:371:PRO:HB2	1:A:469:MET:CE	2.31	0.57
1:B:385:LEU:HD23	1:B:423:CYS:SG	2.46	0.55
1:B:371:PRO:HG2	1:B:469:MET:HG2	1.91	0.53
1:B:386:TYR:OH	1:B:396:GLU:OE1	2.25	0.53
1:B:364:PRO:HG2	1:B:510:TRP:NE1	2.23	0.53
1:A:370:SER:HB2	1:A:371:PRO:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502[B]:GLN:O	1:A:502[B]:GLN:HG2	2.09	0.52
1:A:371:PRO:O	1:A:375:ILE:HG12	2.08	0.52
1:B:452:GLN:HE22	1:B:455:LYS:NZ	2.08	0.52
1:A:340:LEU:C	1:A:340:LEU:HD13	2.35	0.51
1:B:249:ARG:HH11	1:B:249:ARG:HB3	1.75	0.51
1:A:445:GLU:CD	1:A:445:GLU:H	2.19	0.51
1:B:528:MET:HG3	3:B:862:HOH:O	2.09	0.51
1:B:364:PRO:HG2	1:B:510:TRP:CE2	2.47	0.50
1:A:500:VAL:HG22	1:A:503:MET:HG3	1.94	0.49
1:B:381:PHE:HA	1:B:383:TYR:CE1	2.48	0.49
1:A:370:SER:OG	1:A:373:GLU:OE1	2.29	0.49
1:B:362:PHE:O	1:B:363:ILE:HD13	2.13	0.49
1:B:378:ASN:HD21	1:B:380:VAL:HB	1.78	0.48
1:B:233:ASN:OD1	3:B:701:HOH:O	2.20	0.48
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.96	0.48
1:A:375:ILE:HG23	1:A:381:PHE:HB3	1.96	0.48
1:B:455:LYS:NZ	3:B:711:HOH:O	2.47	0.47
1:B:310:MET:HE3	1:B:339:MET:SD	2.55	0.47
1:A:502[A]:GLN:H	1:A:502[A]:GLN:CD	2.22	0.46
1:B:372:LEU:O	1:B:376:LYS:HG3	2.15	0.46
1:B:378:ASN:ND2	1:B:380:VAL:HB	2.30	0.46
1:B:378:ASN:CG	1:B:380:VAL:HB	2.40	0.46
1:B:372:LEU:HD11	1:B:376:LYS:HZ2	1.81	0.45
1:A:343:TYR:OH	1:A:476:ALA:HB2	2.18	0.44
1:B:515:LYS:NZ	1:B:545:ASP:OD2	2.41	0.44
1:B:456:LYS:NZ	3:B:713:HOH:O	2.51	0.43
1:A:266:GLY:HA3	1:A:335:ASP:HB3	2.01	0.43
1:B:291:MET:HE3	1:B:291:MET:HB3	1.82	0.43
1:A:277:GLN:OE1	1:A:527:GLN:HB3	2.19	0.43
1:B:294:LYS:HE2	1:B:302:PRO:HG3	2.01	0.43
1:A:294:LYS:HE2	1:A:302:PRO:CG	2.49	0.42
1:B:355:VAL:O	1:B:488:ALA:HA	2.20	0.42
1:A:237:MET:HE2	1:A:253:VAL:HG11	2.01	0.41
1:A:370:SER:HB2	1:A:371:PRO:CD	2.49	0.41
1:A:237:MET:HE3	1:A:237:MET:HB3	1.92	0.41
1:B:246:PRO:O	1:B:247:ARG:HB2	2.20	0.41
1:B:288:VAL:C	1:B:289:LEU:HD23	2.45	0.41
1:B:371:PRO:O	1:B:375:ILE:HG12	2.21	0.41
1:A:371:PRO:HG2	1:A:469:MET:CE	2.47	0.41
1:A:267:PHE:CD1	1:A:267:PHE:C	2.99	0.41

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	315/344 (92%)	308 (98%)	6 (2%)	1 (0%)	36 35
1	B	314/344 (91%)	306 (98%)	7 (2%)	1 (0%)	36 35
All	All	629/688 (91%)	614 (98%)	13 (2%)	2 (0%)	36 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	PRO
1	A	268	PRO

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	278/304 (91%)	273 (98%)	5 (2%)	51 58
1	B	278/304 (91%)	276 (99%)	2 (1%)	76 82
All	All	556/608 (91%)	549 (99%)	7 (1%)	61 68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	VAL
1	A	340	LEU
1	A	346	LEU
1	A	412	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	545	ASP
1	B	253	VAL
1	B	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	399	GLN
1	A	505	GLN
1	B	452	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1JTE	A	601	-	46,46,46	1.88	12 (26%)	62,65,65	2.23	15 (24%)
2	A1JTE	B	601	-	46,46,46	1.84	12 (26%)	62,65,65	2.14	18 (29%)

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	A1JTE	A	601	-	-	4/26/43/43	0/5/5/5
2	A1JTE	B	601	-	-	5/26/43/43	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	A1JTE	C08-N07	5.15	1.48	1.37
2	A	601	A1JTE	C08-N07	5.08	1.48	1.37
2	A	601	A1JTE	C16-N13	4.51	1.44	1.35
2	A	601	A1JTE	C08-N09	4.33	1.44	1.35
2	B	601	A1JTE	C08-N09	3.99	1.44	1.35
2	B	601	A1JTE	C26-N25	3.60	1.36	1.32
2	A	601	A1JTE	C23-C24	-3.59	1.36	1.42
2	B	601	A1JTE	C28-C27	3.53	1.57	1.51
2	A	601	A1JTE	C28-C27	3.50	1.57	1.51
2	B	601	A1JTE	C16-N13	3.32	1.42	1.35
2	A	601	A1JTE	C20-N21	-3.19	1.39	1.45
2	B	601	A1JTE	C23-C24	-3.05	1.37	1.42
2	B	601	A1JTE	C20-N21	-2.78	1.40	1.45
2	B	601	A1JTE	C33-CL36	2.71	1.80	1.74
2	A	601	A1JTE	C26-N25	2.69	1.35	1.32
2	B	601	A1JTE	C31-C26	2.46	1.54	1.50
2	A	601	A1JTE	C33-CL36	2.38	1.79	1.74
2	A	601	A1JTE	C14-N13	2.33	1.51	1.47
2	A	601	A1JTE	C15-C10	-2.27	1.46	1.52
2	A	601	A1JTE	C31-C26	2.25	1.54	1.50
2	B	601	A1JTE	C32-C33	2.22	1.40	1.36
2	A	601	A1JTE	C12-N13	2.14	1.50	1.47
2	B	601	A1JTE	C32-C24	2.12	1.45	1.41
2	B	601	A1JTE	C03-S39	2.10	1.79	1.77

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	A1JTE	O41-S39-O40	-10.63	99.62	117.92
2	B	601	A1JTE	O41-S39-O40	-9.35	101.82	117.92
2	B	601	A1JTE	C42-S39-C03	6.44	112.19	104.58
2	A	601	A1JTE	O40-S39-C42	4.27	114.64	108.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	A1JTE	C10-N09-C08	4.12	131.73	123.02
2	A	601	A1JTE	C11-C10-C15	4.08	117.89	110.82
2	B	601	A1JTE	C12-C11-C10	3.57	116.76	110.50
2	A	601	A1JTE	O41-S39-C42	3.48	113.49	108.49
2	A	601	A1JTE	C27-C26-N25	-3.44	120.75	123.68
2	A	601	A1JTE	C15-C14-N13	3.37	115.94	110.82
2	B	601	A1JTE	C26-N25-C24	3.31	121.76	117.67
2	A	601	A1JTE	O41-S39-C03	3.25	110.90	108.25
2	A	601	A1JTE	N07-C08-N09	-3.13	109.39	113.76
2	B	601	A1JTE	C11-C10-C15	3.11	116.20	110.82
2	B	601	A1JTE	C27-C26-N25	-3.10	121.03	123.68
2	A	601	A1JTE	C26-N25-C24	3.06	121.44	117.67
2	A	601	A1JTE	C17-C16-N13	3.02	122.73	118.01
2	B	601	A1JTE	C32-C33-CL36	2.89	123.26	119.64
2	B	601	A1JTE	O40-S39-C03	2.82	110.55	108.25
2	B	601	A1JTE	C23-C24-N25	-2.72	119.93	122.81
2	A	601	A1JTE	O40-S39-C03	2.71	110.45	108.25
2	A	601	A1JTE	C42-S39-C03	2.59	107.65	104.58
2	B	601	A1JTE	C35-C23-C22	-2.51	120.25	124.78
2	B	601	A1JTE	C06-N07-C08	-2.50	121.50	126.61
2	A	601	A1JTE	O38-C08-N09	2.42	127.03	122.62
2	B	601	A1JTE	C31-C26-C27	-2.33	119.08	121.49
2	B	601	A1JTE	C34-C33-C32	-2.27	119.30	121.99
2	B	601	A1JTE	O37-C16-N13	-2.25	117.67	122.05
2	A	601	A1JTE	C05-C06-C01	2.22	122.07	119.03
2	B	601	A1JTE	O40-S39-C42	2.11	111.53	108.49
2	B	601	A1JTE	C15-C10-N09	-2.08	106.26	110.56
2	B	601	A1JTE	C11-C10-N09	-2.07	106.28	110.56
2	B	601	A1JTE	O41-S39-C03	2.03	109.90	108.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1JTE	C11-C10-N09-C08
2	B	601	A1JTE	C16-C17-C18-C19
2	B	601	A1JTE	C18-C19-C20-N21
2	A	601	A1JTE	C18-C19-C20-N21
2	B	601	A1JTE	C23-C22-N21-C20
2	B	601	A1JTE	C17-C18-C19-C20
2	A	601	A1JTE	C16-C17-C18-C19
2	B	601	A1JTE	C19-C20-N21-C22

Continued on next page...

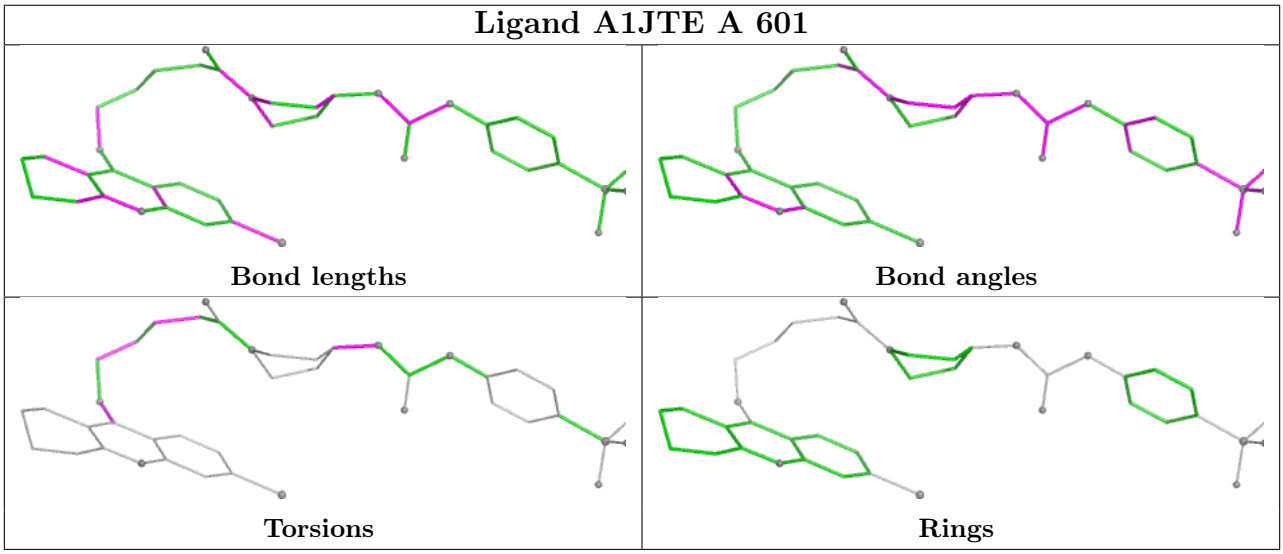
Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	601	A1JTE	C23-C22-N21-C20

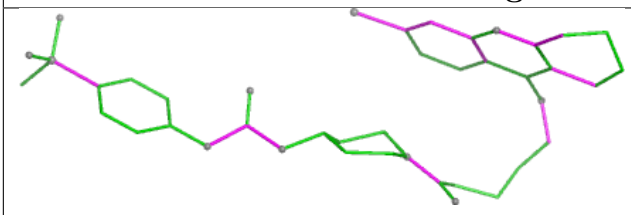
There are no ring outliers.

No monomer is involved in short contacts.

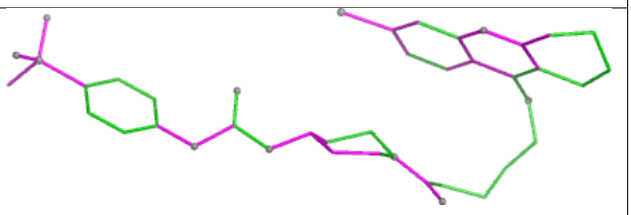
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



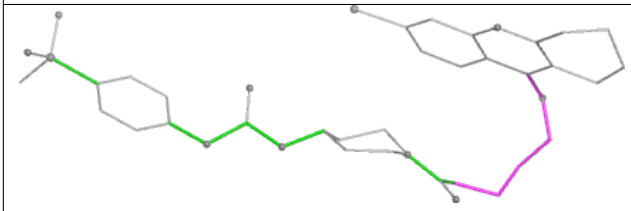
Ligand A1JTE B 601



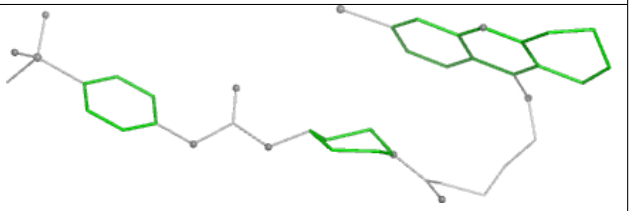
Bond lengths



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	316/344 (91%)	-0.07	16 (5%) 33 32	13, 26, 60, 83	1 (0%)
1	B	316/344 (91%)	-0.25	8 (2%) 58 58	13, 22, 51, 78	0
All	All	632/688 (91%)	-0.16	24 (3%) 44 43	13, 24, 57, 83	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	ALA	5.0
1	B	377	ALA	4.6
1	B	371	PRO	3.9
1	A	372	LEU	3.8
1	A	375	ILE	3.6
1	A	380	VAL	3.5
1	A	510	TRP	3.4
1	B	372	LEU	3.2
1	B	379	PRO	3.0
1	A	369	MET	2.9
1	A	420	HIS	2.8
1	A	479	SER	2.7
1	A	502[A]	GLN	2.7
1	B	380	VAL	2.7
1	A	371	PRO	2.6
1	A	416	VAL	2.5
1	A	480	LEU	2.5
1	A	378	ASN	2.3
1	A	545	ASP	2.3
1	A	376	LYS	2.3
1	B	374	SER	2.2
1	B	420	HIS	2.2
1	B	421	LYS	2.2
1	A	379	PRO	2.1

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)

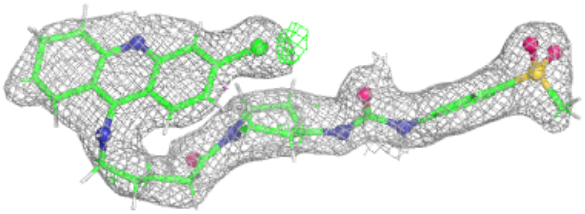
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

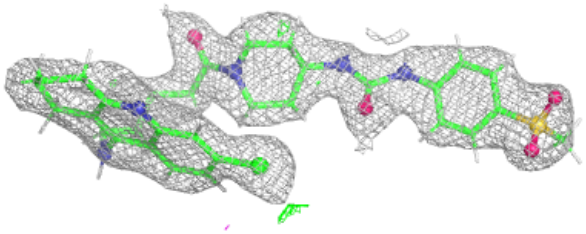
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1JTE	A	601	42/42	0.91	0.11	21,39,53,60	80
2	A1JTE	B	601	42/42	0.91	0.10	21,35,50,53	80

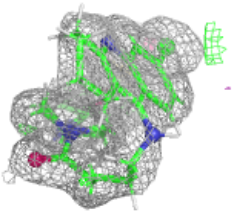
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JTE A 601:

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

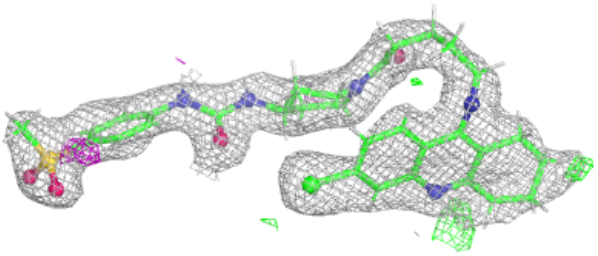


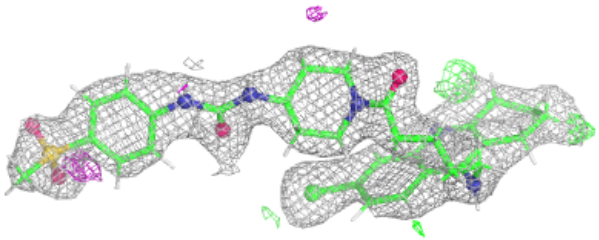


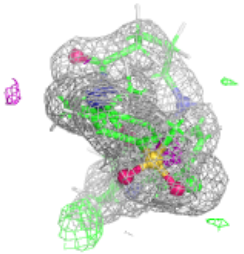


Electron density around A1JTE B 601:

$2mF_o$-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.