



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:38 am BST

PDB ID : 6CX0
Title : Structure of AtTPC1 D376A
Authors : Kintzer, A.F.; Stroud, R.M.
Deposited on : 2018-04-02
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

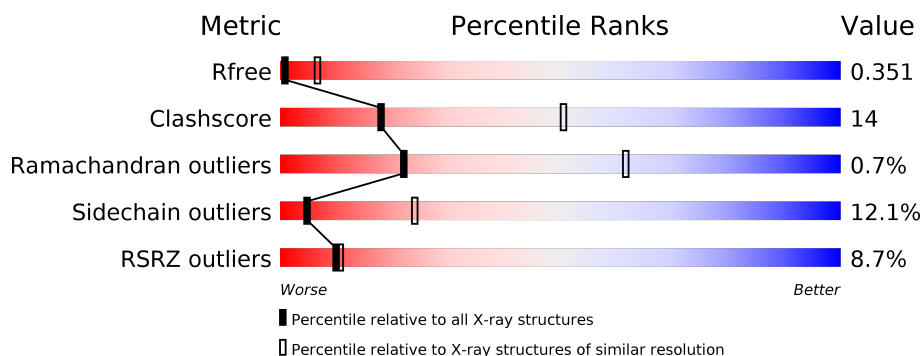
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	727	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FJ7	A	806	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5092 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 Two pore calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			5049	3361	772	894	22			

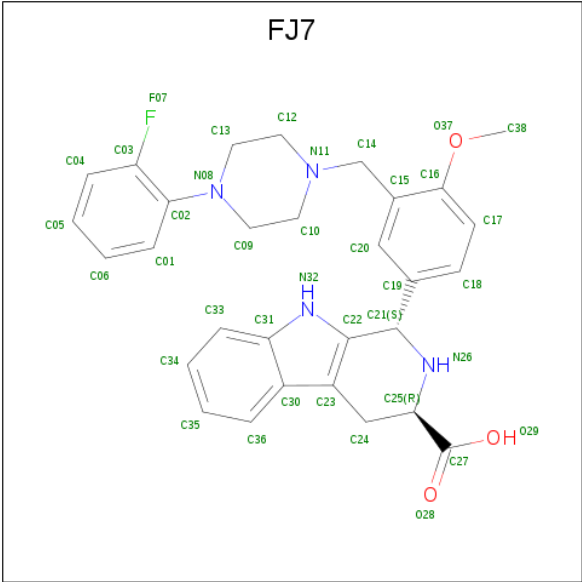
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP Q94KI8
A	734	LEU	-	expression tag	UNP Q94KI8
A	735	VAL	-	expression tag	UNP Q94KI8
A	736	PRO	-	expression tag	UNP Q94KI8
A	737	ARG	-	expression tag	UNP Q94KI8

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		

- Molecule 3 is (1S,3R)-1-(3-{[4-(2-fluorophenyl)piperazin-1-yl]methyl}-4-methoxyphenyl)-2,3,4,9-tetrahydro-1H-beta-carboline-3-carboxylic acid (three-letter code: FJ7) (formula: C₃₀H₃₁FN₄O₃).

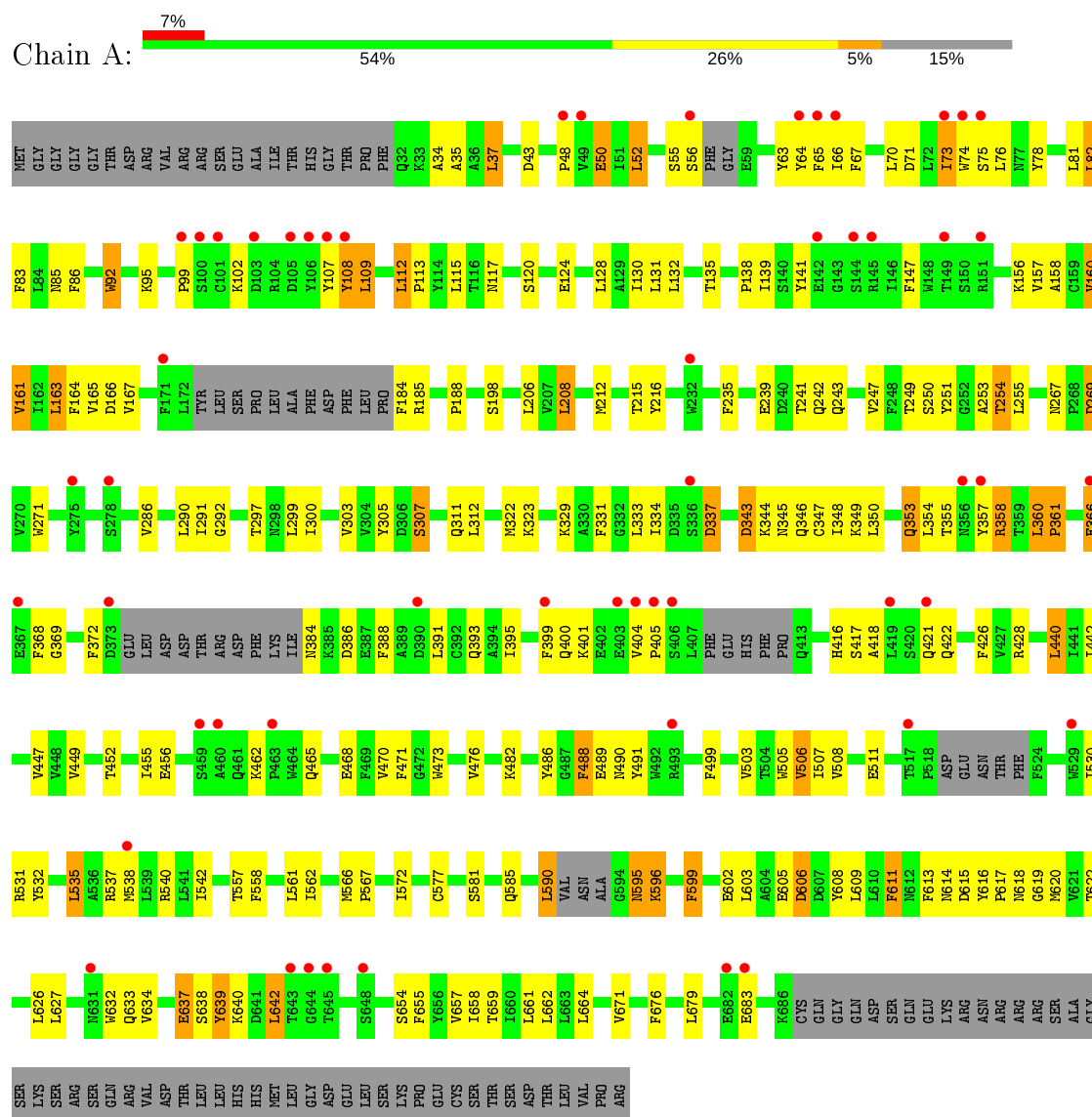


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	38	30	1	4	3	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Two pore calcium channel protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.47Å 154.42Å 218.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 3.50 41.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	46.5 (41.00-3.50) 46.5 (41.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.318 , 0.352 0.319 , 0.351	Depositor DCC
R_{free} test set	445 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	109.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.054 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.077 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5092	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FJ7

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	0.27	0/5175	0.44	0/7036

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	5049	0	5036	137	0
2	A	5	0	0	0	0
3	A	38	0	0	0	0
All	All	5092	0	5036	137	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 14.

All (137) 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:603:LEU:HD13	1:A:606:ASP:HB2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:LEU:HG	1:A:642:LEU:HG	1.64	0.80
1:A:404:VAL:HA	1:A:490:ASN:HD21	1.55	0.71
1:A:64:TYR:HA	1:A:67:PHE:HD2	1.57	0.69
1:A:112:LEU:HG	1:A:617:PRO:HG2	1.75	0.68
1:A:606:ASP:N	1:A:606:ASP:OD1	2.25	0.67
1:A:135:THR:HG22	1:A:156:LYS:HE2	1.75	0.67
1:A:250:SER:OG	1:A:251:TYR:N	2.26	0.67
1:A:37:LEU:HD13	1:A:334:ILE:HB	1.76	0.66
1:A:117:ASN:HA	1:A:120:SER:HB3	1.78	0.66
1:A:95:LYS:NZ	1:A:184:PHE:O	2.28	0.66
1:A:247:VAL:HG12	1:A:250:SER:HA	1.79	0.64
1:A:482:LYS:HE3	1:A:491:TYR:HE1	1.61	0.64
1:A:354:LEU:HD21	1:A:395:ILE:HG21	1.81	0.62
1:A:157:VAL:HA	1:A:160:VAL:HB	1.82	0.62
1:A:572:ILE:HD11	1:A:627:LEU:HD11	1.84	0.59
1:A:360:LEU:HD11	1:A:401:LYS:HB2	1.84	0.59
1:A:637:GLU:O	1:A:640:LYS:NZ	2.36	0.58
1:A:128:LEU:HG	1:A:163:LEU:HD21	1.86	0.58
1:A:357:TYR:HB3	1:A:358:ARG:HE	1.69	0.58
1:A:503:VAL:HG12	1:A:537:ARG:HH21	1.70	0.57
1:A:337:ASP:N	1:A:337:ASP:OD1	2.27	0.57
1:A:530:ILE:HG23	1:A:531:ARG:HG2	1.87	0.56
1:A:138:PRO:HA	1:A:141:TYR:CE2	2.40	0.56
1:A:55:SER:HA	1:A:64:TYR:CD2	2.39	0.56
1:A:37:LEU:HD22	1:A:333:LEU:HB2	1.88	0.55
1:A:505:TRP:HA	1:A:508:VAL:HG22	1.88	0.54
1:A:626:LEU:HD23	1:A:632:TRP:HB2	1.89	0.54
1:A:395:ILE:HG23	1:A:399:PHE:HB2	1.90	0.54
1:A:269:ASP:N	1:A:269:ASP:OD1	2.40	0.54
1:A:71:ASP:O	1:A:75:SER:N	2.35	0.53
1:A:50:GLU:N	1:A:50:GLU:OE2	2.41	0.53
1:A:109:LEU:H	1:A:109:LEU:HD12	1.74	0.53
1:A:473:TRP:HA	1:A:476:VAL:HG12	1.91	0.53
1:A:138:PRO:HG2	1:A:147:PHE:HE2	1.74	0.52
1:A:561:LEU:HD11	1:A:671:VAL:HG13	1.90	0.52
1:A:655:PHE:O	1:A:659:THR:HG22	2.10	0.52
1:A:34:ALA:C	1:A:353:GLN:HE22	2.13	0.52
1:A:109:LEU:HD22	1:A:611:PHE:HD2	1.74	0.52
1:A:303:VAL:O	1:A:307:SER:OG	2.24	0.51
1:A:449:VAL:HA	1:A:452:THR:HG22	1.92	0.51
1:A:212:MET:HB2	1:A:307:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:O	1:A:353:GLN:HG3	2.10	0.51
1:A:73:ILE:HA	1:A:76:LEU:HD12	1.93	0.51
1:A:86:PHE:HZ	1:A:577:CYS:SG	2.33	0.51
1:A:603:LEU:HD21	1:A:638:SER:HB3	1.92	0.51
1:A:128:LEU:HD11	1:A:164:PHE:HA	1.93	0.50
1:A:369:GLY:HA2	1:A:372:PHE:HD2	1.76	0.50
1:A:292:GLY:O	1:A:297:THR:OG1	2.22	0.50
1:A:455:ILE:HG13	1:A:456:GLU:N	2.27	0.50
1:A:92:TRP:CZ3	1:A:188:PRO:HG3	2.47	0.50
1:A:112:LEU:HD13	1:A:113:PRO:HD2	1.94	0.49
1:A:499:PHE:O	1:A:503:VAL:HG23	2.12	0.49
1:A:615:ASP:HB3	1:A:618:ASN:HB2	1.93	0.49
1:A:63:TYR:O	1:A:66:ILE:HG22	2.12	0.49
1:A:299:LEU:O	1:A:303:VAL:HG23	2.13	0.49
1:A:70:LEU:O	1:A:74:TRP:HD1	1.96	0.49
1:A:43:ASP:O	1:A:48:PRO:HD2	2.13	0.48
1:A:185:ARG:O	1:A:585:GLN:NE2	2.47	0.48
1:A:404:VAL:HG12	1:A:405:PRO:O	2.14	0.47
1:A:639:TYR:HA	1:A:642:LEU:HB2	1.96	0.47
1:A:235:PHE:HB2	1:A:254:THR:HG21	1.95	0.47
1:A:216:TYR:OH	1:A:657:VAL:O	2.27	0.47
1:A:286:VAL:O	1:A:290:LEU:HB2	2.14	0.47
1:A:344:LYS:O	1:A:348:ILE:HG23	2.15	0.46
1:A:442:ILE:HG23	1:A:471:PHE:HZ	1.80	0.46
1:A:124:GLU:HB3	1:A:167:VAL:HG22	1.97	0.46
1:A:455:ILE:HG13	1:A:456:GLU:H	1.80	0.46
1:A:615:ASP:O	1:A:619:GLY:N	2.40	0.46
1:A:422:GLN:O	1:A:426:PHE:HD1	1.98	0.46
1:A:353:GLN:H	1:A:353:GLN:HG3	1.50	0.46
1:A:139:ILE:HG12	1:A:147:PHE:CG	2.51	0.45
1:A:297:THR:HA	1:A:300:ILE:HD12	1.99	0.45
1:A:208:LEU:HG	1:A:311:GLN:HB3	1.98	0.45
1:A:619:GLY:HA2	1:A:622:THR:HG22	1.99	0.45
1:A:267:ASN:O	1:A:271:TRP:NE1	2.49	0.45
1:A:417:SER:O	1:A:421:GLN:N	2.49	0.45
1:A:241:THR:HG23	1:A:243:GLN:H	1.81	0.45
1:A:249:THR:HB	1:A:253:ALA:HB2	1.99	0.45
1:A:355:THR:OG1	1:A:361:PRO:HD2	2.17	0.45
1:A:507:ILE:HG13	1:A:537:ARG:HH22	1.82	0.45
1:A:590:LEU:O	1:A:614:ASN:ND2	2.49	0.45
1:A:616:TYR:HB3	1:A:617:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLN:O	1:A:401:LYS:HG3	2.17	0.45
1:A:488:PHE:HD1	1:A:489:GLU:HG2	1.82	0.45
1:A:558:PHE:O	1:A:562:ILE:HG13	2.17	0.45
1:A:329:LYS:O	1:A:333:LEU:HG	2.17	0.44
1:A:609:LEU:HD12	1:A:634:VAL:HG21	1.98	0.44
1:A:131:LEU:O	1:A:135:THR:HG23	2.16	0.44
1:A:81:LEU:HD22	1:A:130:ILE:HG22	1.99	0.44
1:A:676:PHE:HD1	1:A:679:LEU:HD12	1.82	0.44
1:A:440:LEU:HD13	1:A:538:MET:HB3	2.00	0.44
1:A:56:SER:HA	1:A:63:TYR:HD2	1.83	0.44
1:A:300:ILE:HG21	1:A:661:LEU:HD22	1.99	0.44
1:A:138:PRO:HB2	1:A:147:PHE:HD2	1.83	0.43
1:A:507:ILE:HG13	1:A:537:ARG:HH12	1.82	0.43
1:A:452:THR:HA	1:A:455:ILE:HG12	1.99	0.43
1:A:503:VAL:O	1:A:506:VAL:HG12	2.18	0.43
1:A:577:CYS:HA	1:A:620:MET:HE1	2.01	0.43
1:A:208:LEU:HD11	1:A:312:LEU:HA	2.00	0.43
1:A:442:ILE:HG23	1:A:471:PHE:CZ	2.53	0.43
1:A:428:ARG:HG2	1:A:486:TYR:CE1	2.54	0.43
1:A:334:ILE:HD11	1:A:346:GLN:O	2.19	0.43
1:A:35:ALA:N	1:A:353:GLN:HE22	2.17	0.42
1:A:52:LEU:HA	1:A:52:LEU:HD13	1.74	0.42
1:A:595:ASN:O	1:A:599:PHE:HB2	2.19	0.42
1:A:343:ASP:N	1:A:343:ASP:OD1	2.51	0.42
1:A:664:LEU:HA	1:A:664:LEU:HD23	1.87	0.42
1:A:290:LEU:HD22	1:A:291:ILE:HD12	2.01	0.42
1:A:78:TYR:O	1:A:82:LEU:HG	2.19	0.42
1:A:128:LEU:HD12	1:A:167:VAL:HG21	2.02	0.42
1:A:557:THR:O	1:A:561:LEU:N	2.52	0.42
1:A:658:ILE:O	1:A:662:LEU:HB3	2.20	0.42
1:A:404:VAL:HG13	1:A:490:ASN:OD1	2.20	0.41
1:A:462:LYS:O	1:A:465:GLN:HG2	2.20	0.41
1:A:109:LEU:HD13	1:A:611:PHE:O	2.20	0.41
1:A:345:ASN:HA	1:A:348:ILE:HG12	2.02	0.41
1:A:109:LEU:HD22	1:A:611:PHE:CD2	2.54	0.41
1:A:135:THR:HG21	1:A:160:VAL:HG21	2.01	0.41
1:A:95:LYS:NZ	1:A:184:PHE:HB2	2.36	0.41
1:A:92:TRP:HA	1:A:115:LEU:HD22	2.01	0.41
1:A:323:LYS:HZ1	1:A:393:GLN:HG2	1.86	0.41
1:A:366:GLU:H	1:A:366:GLU:HG3	1.62	0.41
1:A:566:MET:N	1:A:567:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:CZ	1:A:662:LEU:HB2	2.56	0.41
1:A:503:VAL:HG12	1:A:537:ARG:NH2	2.34	0.41
1:A:596:LYS:HA	1:A:596:LYS:HD3	1.73	0.41
1:A:349:LYS:HG3	1:A:350:LEU:N	2.36	0.41
1:A:428:ARG:HG2	1:A:486:TYR:HE1	1.86	0.41
1:A:447:VAL:HA	1:A:468:GLU:OE2	2.21	0.41
1:A:633:GLN:OE1	1:A:633:GLN:N	2.42	0.41
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.84	0.41
1:A:158:ALA:O	1:A:161:VAL:HG12	2.21	0.40
1:A:331:PHE:HB2	1:A:388:PHE:CD2	2.56	0.40
1:A:511:GLU:HA	1:A:531:ARG:NH1	2.36	0.40
1:A:532:TYR:O	1:A:535:LEU:HD23	2.21	0.40
1:A:602:GLU:O	1:A:603:LEU:HD23	2.22	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	605/727 (83%)	564 (93%)	37 (6%)	4 (1%)	22	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	PRO
1	A	108	TYR
1	A	99	PRO
1	A	418	ALA

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	547/651 (84%)	481 (88%)	66 (12%)	5 24

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	50	GLU
1	A	52	LEU
1	A	65	PHE
1	A	73	ILE
1	A	82	LEU
1	A	83	PHE
1	A	85	ASN
1	A	92	TRP
1	A	102	LYS
1	A	107	TYR
1	A	108	TYR
1	A	109	LEU
1	A	112	LEU
1	A	132	LEU
1	A	160	VAL
1	A	161	VAL
1	A	163	LEU
1	A	165	VAL
1	A	166	ASP
1	A	198	SER
1	A	206	LEU
1	A	208	LEU
1	A	215	THR
1	A	239	GLU
1	A	242	GLN
1	A	254	THR
1	A	255	LEU
1	A	269	ASP
1	A	305	TYR

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Mol	Chain	Res	Type
1	A	307	SER
1	A	322	MET
1	A	337	ASP
1	A	343	ASP
1	A	347	CYS
1	A	353	GLN
1	A	358	ARG
1	A	360	LEU
1	A	366	GLU
1	A	368	PHE
1	A	384	ASN
1	A	386	ASP
1	A	391	LEU
1	A	416	HIS
1	A	440	LEU
1	A	470	VAL
1	A	488	PHE
1	A	506	VAL
1	A	535	LEU
1	A	540	ARG
1	A	542	ILE
1	A	581	SER
1	A	590	LEU
1	A	595	ASN
1	A	596	LYS
1	A	599	PHE
1	A	605	GLU
1	A	606	ASP
1	A	608	TYR
1	A	611	PHE
1	A	613	PHE
1	A	637	GLU
1	A	639	TYR
1	A	642	LEU
1	A	654	SER
1	A	683	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	FJ7	A	806	-	36,43,43	2.26	7 (19%)	46,62,62	1.98	12 (26%)

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	FJ7	A	806	-	-	8/14/40/40	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	FJ7	C14-N11	-8.12	1.31	1.47
3	A	806	FJ7	C10-N11	-5.52	1.31	1.46
3	A	806	FJ7	C12-N11	-5.46	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	FJ7	C23-C22	-4.52	1.32	1.39
3	A	806	FJ7	C30-C31	-3.21	1.34	1.42
3	A	806	FJ7	C21-N26	-2.27	1.45	1.48
3	A	806	FJ7	C02-N08	2.25	1.46	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	806	FJ7	C19-C21-C22	7.72	130.19	112.79
3	A	806	FJ7	F07-C03-C02	3.70	121.78	118.42
3	A	806	FJ7	O37-C16-C15	3.58	120.96	115.97
3	A	806	FJ7	O37-C16-C17	-3.19	118.91	124.37
3	A	806	FJ7	C13-N08-C02	3.07	123.55	116.27
3	A	806	FJ7	C13-C12-N11	2.94	116.68	110.64
3	A	806	FJ7	C01-C02-N08	-2.88	117.70	122.30
3	A	806	FJ7	C13-N08-C09	2.64	117.35	111.52
3	A	806	FJ7	C38-O37-C16	-2.44	113.84	117.53
3	A	806	FJ7	C18-C19-C21	-2.24	116.94	120.74
3	A	806	FJ7	C03-C02-N08	2.22	123.11	120.47
3	A	806	FJ7	C10-C09-N08	-2.02	106.77	110.70

There are no chirality outliers.

All (8) torsion outliers are listed below:

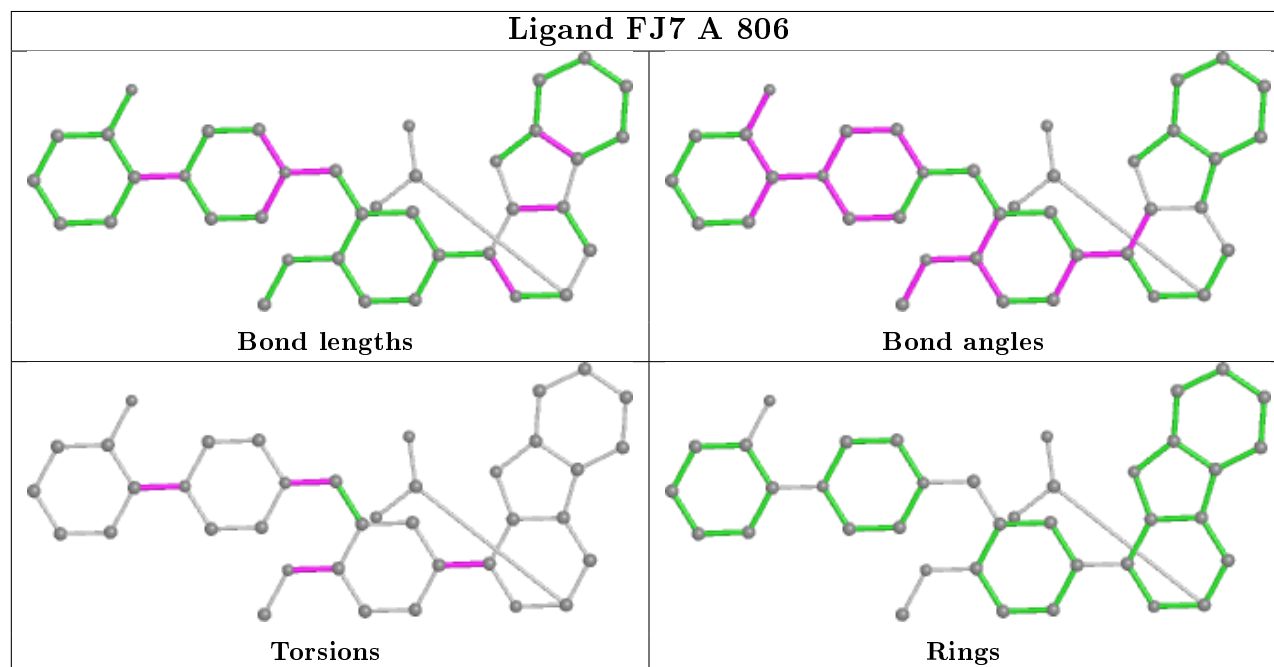
Mol	Chain	Res	Type	Atoms
3	A	806	FJ7	C18-C19-C21-N26
3	A	806	FJ7	C20-C19-C21-N26
3	A	806	FJ7	C01-C02-N08-C13
3	A	806	FJ7	C15-C16-O37-C38
3	A	806	FJ7	C03-C02-N08-C13
3	A	806	FJ7	C15-C14-N11-C10
3	A	806	FJ7	C17-C16-O37-C38
3	A	806	FJ7	C15-C14-N11-C12

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 [i](#)

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	619/727 (85%)	0.20	54 (8%) 10 11	57, 110, 162, 251	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	ASP	5.5
1	A	74	TRP	5.5
1	A	66	ILE	4.9
1	A	149	THR	4.4
1	A	105	ASP	4.1
1	A	403	GLU	4.0
1	A	405	PRO	4.0
1	A	73	ILE	4.0
1	A	106	TYR	3.6
1	A	65	PHE	3.6
1	A	100	SER	3.4
1	A	419	LEU	3.4
1	A	336	SER	3.4
1	A	406	SER	3.3
1	A	145	ARG	3.3
1	A	107	TYR	3.2
1	A	645	THR	3.1
1	A	48	PRO	3.1
1	A	517	THR	3.1
1	A	56	SER	3.1
1	A	64	TYR	3.1
1	A	643	THR	3.0
1	A	538	MET	3.0
1	A	151	ARG	3.0
1	A	103	ASP	2.9
1	A	108	TYR	2.9
1	A	232	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	648	SER	2.9
1	A	399	PHE	2.8
1	A	142	GLU	2.7
1	A	367	GLU	2.7
1	A	404	VAL	2.6
1	A	463	PRO	2.6
1	A	460	ALA	2.6
1	A	356	ASN	2.5
1	A	357	TYR	2.5
1	A	631	ASN	2.5
1	A	644	GLY	2.4
1	A	682	GLU	2.4
1	A	49	VAL	2.3
1	A	144	SER	2.3
1	A	529	TRP	2.3
1	A	99	PRO	2.2
1	A	421	GLN	2.2
1	A	75	SER	2.2
1	A	101	CYS	2.2
1	A	459	SER	2.2
1	A	275	TYR	2.1
1	A	171	PHE	2.1
1	A	278	SER	2.1
1	A	373	ASP	2.1
1	A	366	GLU	2.1
1	A	493	ARG	2.1
1	A	683	GLU	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 carbohydrates in this entry.

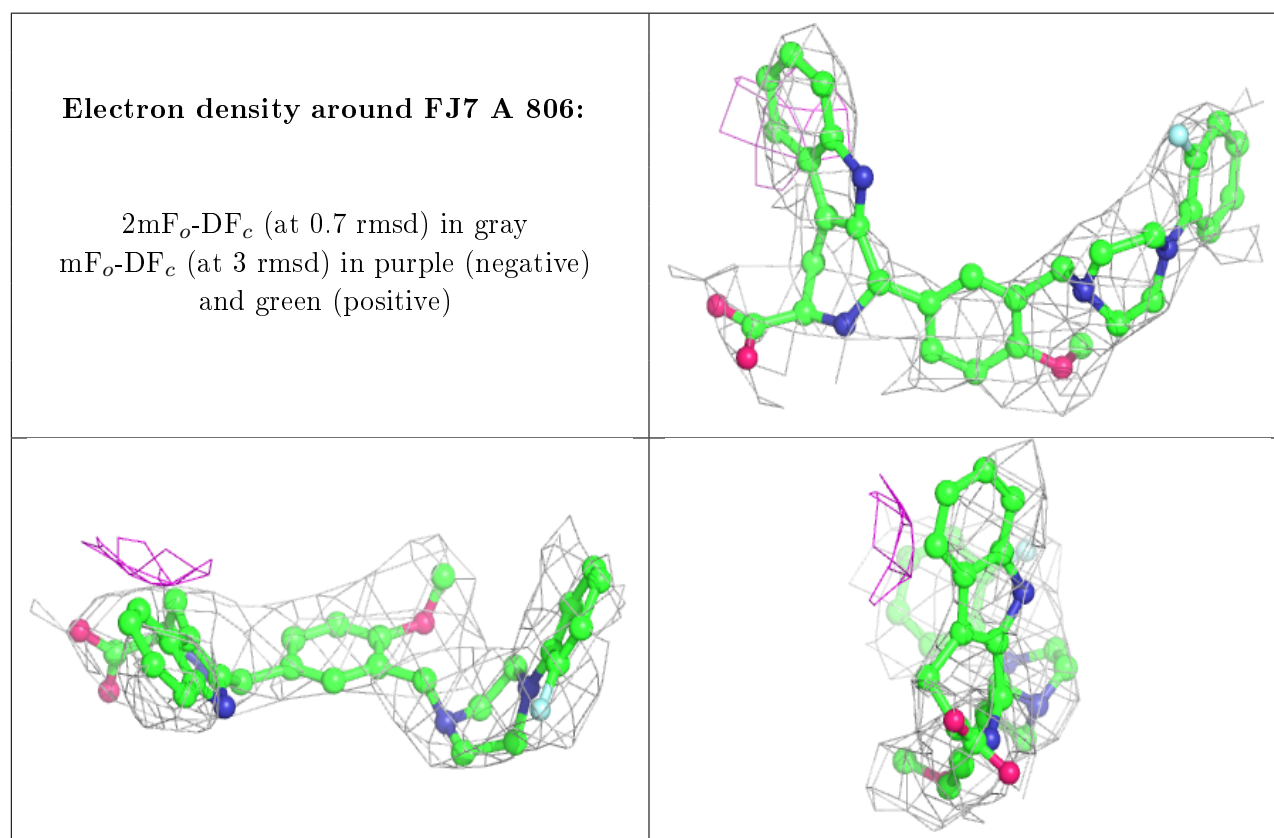
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	FJ7	A	806	38/38	0.71	0.51	101,152,176,184	0
2	CA	A	805	1/1	0.83	0.18	162,162,162,162	0
2	CA	A	801	1/1	0.88	0.74	168,168,168,168	0
2	CA	A	804	1/1	0.90	0.36	161,161,161,161	0
2	CA	A	803	1/1	0.97	0.33	141,141,141,141	0
2	CA	A	802	1/1	0.97	0.16	114,114,114,114	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.