



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:16 AM UTC

PDB ID : 2WJ1 / pdb_00002wj1
Title : 3D-crystal structure of humanized-rat fatty acid amide hydrolase (FAAH) conjugated with 7-phenyl-1-(4-(pyridin-2-yl)oxazol-2-yl)heptan- 1-one, an alpha-ketooxazole
Authors : Mileni, M.; Garfunkle, J.; DeMartino, J.K.; Cravatt, B.F.; Boger, D.L.; Stevens, R.C.
Deposited on : 2009-05-19
Resolution : 1.84 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)
Xtrriage (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

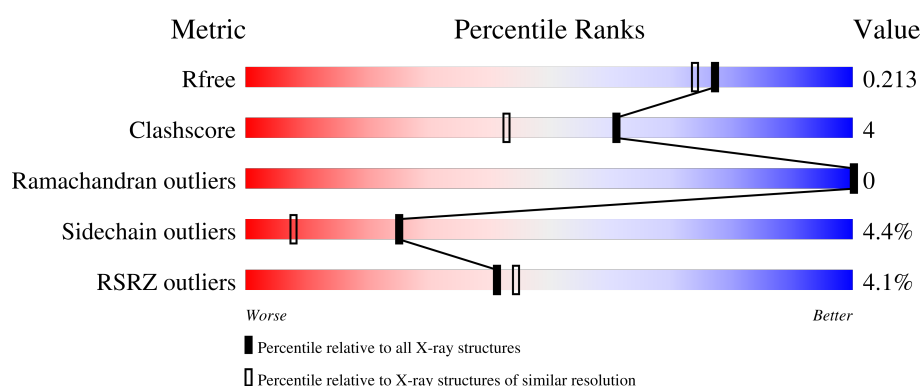
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	573	4% 83% 10% 5%
1	B	573	4% 82% 11% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9038 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.

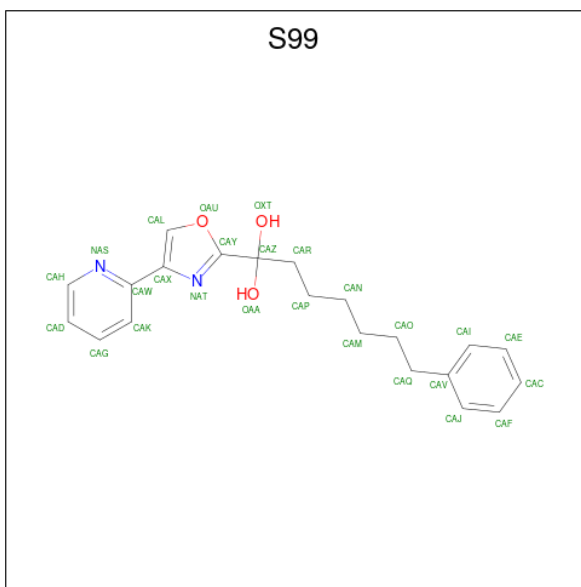
- Molecule 1 is a protein called FATTY-ACID AMIDE HYDROLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	1	0
			4199	2681	716	771	31			
1	B	544	Total	C	N	O	S	0	1	0
			4208	2686	718	773	31			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	PHE	LEU	engineered mutation	UNP P97612
A	194	TYR	PHE	engineered mutation	UNP P97612
A	377	THR	ALA	engineered mutation	UNP P97612
A	435	ASN	SER	engineered mutation	UNP P97612
A	491	VAL	ILE	engineered mutation	UNP P97612
A	495	MET	VAL	engineered mutation	UNP P97612
B	192	PHE	LEU	engineered mutation	UNP P97612
B	194	TYR	PHE	engineered mutation	UNP P97612
B	377	THR	ALA	engineered mutation	UNP P97612
B	435	ASN	SER	engineered mutation	UNP P97612
B	491	VAL	ILE	engineered mutation	UNP P97612
B	495	MET	VAL	engineered mutation	UNP P97612

- Molecule 2 is 7-phenyl-1-(4-pyridin-2-yl-1,3-oxazol-2-yl)heptane-1,1-diol (CCD ID: S99) (formula: C₂₁H₂₄N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	2	2		
2	B	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

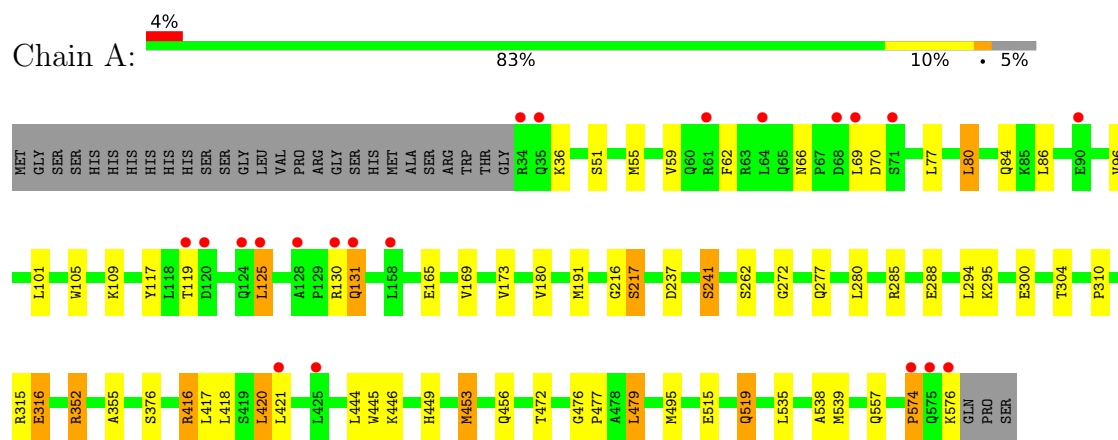
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	288	Total	O	0	0
			288	288		
4	B	292	Total	O	0	0
			292	292		

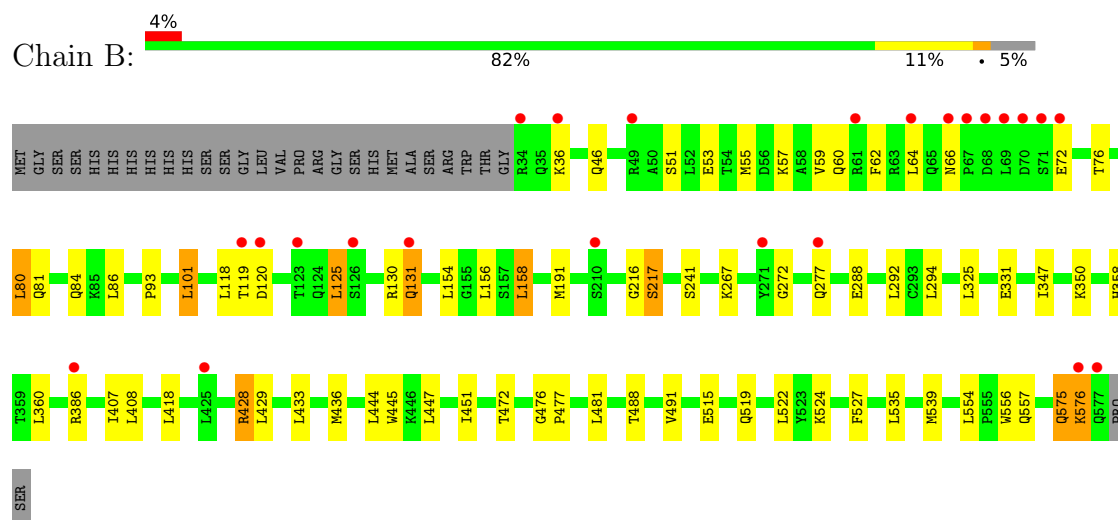
3 Residue-property plots [i](#)

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: FATTY-ACID AMIDE HYDROLASE 1



• Molecule 1: FATTY-ACID AMIDE HYDROLASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.83Å 106.21Å 79.39Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	36.31 – 1.84 36.31 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.31-1.84) 99.1 (36.31-1.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.84Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.186 , 0.214 0.186 , 0.213	Depositor DCC
R_{free} test set	5311 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.096 for l,k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9038	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: CL, S99

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	0.84	4/4296 (0.1%)	0.92	5/5827 (0.1%)
1	B	0.79	1/4305 (0.0%)	0.93	4/5839 (0.1%)
All	All	0.82	5/8601 (0.1%)	0.92	9/11666 (0.1%)

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	1	4
1	B	0	4
All	All	1	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	GLN	C-O	-6.37	1.15	1.24
1	A	453[A]	MET	C-O	-5.91	1.17	1.24
1	A	453[B]	MET	C-O	-5.91	1.17	1.24
1	A	574	PRO	C-O	-5.41	1.17	1.24
1	B	277	GLN	C-O	-5.05	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	SER	N-CA-C	-10.99	99.44	113.72
1	A	217	SER	N-CA-C	-10.78	99.70	113.72
1	A	574	PRO	N-CA-C	8.18	129.31	112.47
1	A	574	PRO	CB-CA-C	7.75	124.34	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	SER	N-CA-C	7.16	121.46	112.87
1	B	576	LYS	N-CA-C	-6.72	104.03	111.82
1	B	477	PRO	N-CA-C	-6.11	99.88	112.47
1	A	477	PRO	N-CA-C	-5.27	101.61	112.47
1	A	241	SER	N-CA-C	5.24	119.15	112.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	574	PRO	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	GLY	Mainchain,Peptide
1	A	476	GLY	Mainchain,Peptide
1	B	216	GLY	Mainchain,Peptide
1	B	476	GLY	Mainchain,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	4199	0	4259	39	0
1	B	4208	0	4267	37	0
2	A	25	0	23	0	0
2	B	25	0	23	0	0
3	A	1	0	0	0	0
4	A	288	0	0	5	0
4	B	292	0	0	1	0
All	All	9038	0	8572	72	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 (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:H	1:B:358:HIS:HD2	1.27	0.81
1:B:60:GLN:O	1:B:64:LEU:HD13	1.86	0.75
1:B:55:MET:HE3	1:B:101:LEU:CD2	2.23	0.68
1:A:80:LEU:O	1:A:84:GLN:HG3	1.95	0.67
1:A:416:ARG:NH1	1:A:420:LEU:HD21	2.12	0.65
1:B:557:GLN:HG2	4:B:2285:HOH:O	1.98	0.64
1:B:131:GLN:HE21	1:B:131:GLN:N	1.97	0.63
1:B:53:GLU:OE2	1:B:57:LYS:HE3	1.98	0.61
1:A:86:LEU:HD21	1:A:96:VAL:HG21	1.83	0.61
1:A:131:GLN:HE21	1:A:131:GLN:N	1.99	0.60
1:B:119:THR:OG1	1:B:120:ASP:N	2.31	0.60
1:B:80:LEU:HD13	1:B:288:GLU:HG3	1.84	0.58
1:B:515:GLU:O	1:B:519:GLN:HG2	2.03	0.57
1:A:125:LEU:HD23	1:A:180:VAL:HG21	1.87	0.56
1:A:117:TYR:O	1:A:119:THR:HG23	2.06	0.55
1:A:456:GLN:HG2	4:A:2257:HOH:O	2.07	0.55
1:B:407:ILE:HG23	1:B:433:LEU:HD21	1.89	0.55
1:A:55:MET:HE3	1:A:101:LEU:HD12	1.89	0.54
1:B:447:LEU:C	1:B:447:LEU:HD23	2.33	0.53
1:A:80:LEU:HG	1:A:288:GLU:HG2	1.90	0.53
1:A:285:ARG:O	1:A:576:LYS:HE3	2.08	0.52
1:B:191:MET:O	1:B:217:SER:HB3	2.09	0.52
1:A:262:SER:O	1:A:280:LEU:HD21	2.10	0.52
1:A:444:LEU:HD23	1:B:444:LEU:HD23	1.91	0.52
1:B:488:THR:O	1:B:491:VAL:HG22	2.10	0.51
1:A:557:GLN:HG2	4:A:2165:HOH:O	2.10	0.51
1:B:156:LEU:HB3	1:B:158:LEU:HD23	1.93	0.50
1:A:69:LEU:HD13	1:A:70:ASP:C	2.37	0.50
1:B:575:GLN:CD	1:B:575:GLN:H	2.18	0.49
1:A:105:TRP:CZ3	1:A:109:LYS:HE2	2.47	0.49
1:A:295:LYS:NZ	1:A:316:GLU:HG2	2.28	0.48
1:B:447:LEU:HD21	1:B:451:ILE:HD11	1.95	0.48
1:A:191:MET:O	1:A:217:SER:HB3	2.14	0.47
1:B:93:PRO:HB2	1:B:125:LEU:CD2	2.45	0.47
1:B:554:LEU:HB2	1:B:557:GLN:OE1	2.15	0.46
1:A:310:PRO:HG3	1:B:556:TRP:CZ2	2.50	0.46
1:A:169:VAL:O	1:A:173:VAL:HG23	2.15	0.46
1:A:515:GLU:O	1:A:519:GLN:HG3	2.16	0.46
1:A:300:GLU:O	1:A:304:THR:HG23	2.16	0.45
1:B:55:MET:O	1:B:59:VAL:HG23	2.16	0.45
1:B:535:LEU:HG	1:B:539:MET:HE2	1.98	0.45
1:A:295:LYS:HD3	1:A:316:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.85	0.45
1:A:376:SER:HB2	1:A:495:MET:HE3	1.99	0.45
1:A:55:MET:HE3	1:A:101:LEU:CD1	2.47	0.44
1:A:62:PHE:CE1	1:A:66:ASN:ND2	2.86	0.44
1:B:62:PHE:CD1	1:B:66:ASN:ND2	2.85	0.44
1:A:315:ARG:NH2	4:A:2166:HOH:O	2.50	0.44
1:B:515:GLU:O	1:B:519:GLN:CG	2.66	0.44
1:B:81:GLN:HA	1:B:84:GLN:HG2	1.99	0.44
1:B:331:GLU:CG	1:B:347:ILE:HD11	2.48	0.44
1:A:417:LEU:O	1:A:421:LEU:HD13	2.18	0.43
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.78	0.43
1:B:93:PRO:HB2	1:B:125:LEU:HD21	2.00	0.43
1:A:445:TRP:O	1:B:272:GLY:HA3	2.17	0.43
1:A:272:GLY:HA3	1:B:445:TRP:O	2.19	0.43
1:B:350:LYS:HG2	1:B:360:LEU:HG	2.01	0.43
1:A:535:LEU:HG	1:A:539:MET:HE2	2.01	0.42
1:A:479:LEU:HB3	1:A:538:ALA:HB1	2.02	0.42
1:B:408:LEU:HD21	1:B:436:MET:HE2	2.00	0.42
1:A:574:PRO:C	1:A:576:LYS:H	2.28	0.42
1:A:355:ALA:HB3	4:A:2194:HOH:O	2.20	0.41
1:B:118:LEU:C	1:B:119:THR:HG1	2.29	0.41
1:A:237:ASP:HA	1:A:241:SER:HB2	2.02	0.41
1:B:62:PHE:CE1	1:B:66:ASN:ND2	2.89	0.41
1:B:72:GLU:O	1:B:76:THR:HG23	2.20	0.41
1:A:55:MET:O	1:A:59:VAL:HG23	2.21	0.41
1:A:352:ARG:NH2	4:A:2194:HOH:O	2.54	0.41
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.84	0.40
1:B:428:ARG:HG3	1:B:527:PHE:CE2	2.55	0.40
1:A:449:HIS:CE1	1:A:453[B]:MET:SD	3.15	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	542/573 (95%)	527 (97%)	15 (3%)	0	100	100
1	B	543/573 (95%)	529 (97%)	14 (3%)	0	100	100
All	All	1085/1146 (95%)	1056 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	440/487 (90%)	423 (96%)	17 (4%)	28	11
1	B	464/487 (95%)	441 (95%)	23 (5%)	22	6
All	All	904/974 (93%)	864 (96%)	40 (4%)	25	8

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	51	SER
1	A	77	LEU
1	A	80	LEU
1	A	125	LEU
1	A	130	ARG
1	A	131	GLN
1	A	165	GLU
1	A	277	GLN
1	A	316	GLU
1	A	352	ARG
1	A	416	ARG
1	A	418	LEU
1	A	420	LEU
1	A	446	LYS
1	A	472	THR
1	A	479	LEU
1	B	36	LYS

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Mol	Chain	Res	Type
1	B	46	GLN
1	B	51	SER
1	B	80	LEU
1	B	86	LEU
1	B	101	LEU
1	B	125	LEU
1	B	130	ARG
1	B	131	GLN
1	B	154	LEU
1	B	158	LEU
1	B	267	LYS
1	B	292	LEU
1	B	386	ARG
1	B	418	LEU
1	B	428	ARG
1	B	429	LEU
1	B	472	THR
1	B	481	LEU
1	B	522	LEU
1	B	524	LYS
1	B	575	GLN
1	B	576	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	66	ASN
1	A	81	GLN
1	A	131	GLN
1	A	301	HIS
1	A	351	GLN
1	A	367	ASN
1	A	449	HIS
1	A	466	ASN
1	B	66	ASN
1	B	81	GLN
1	B	131	GLN
1	B	351	GLN
1	B	358	HIS
1	B	456	GLN
1	B	466	ASN

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Mol	Chain	Res	Type
1	B	482	ASN
1	B	575	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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	S99	A	1577	1	25,27,28	1.23	3 (12%)	28,34,37	1.89	6 (21%)
2	S99	B	1578	1	25,27,28	1.30	3 (12%)	28,34,37	1.70	6 (21%)

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	S99	A	1577	1	-	2/17/17/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S99	B	1578	1	-	2/17/17/20	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1577	S99	CAW-CAX	-3.14	1.39	1.47
2	B	1578	S99	CAW-CAX	-2.92	1.40	1.47
2	B	1578	S99	CAY-NAT	2.86	1.34	1.29
2	A	1577	S99	CAY-NAT	2.55	1.33	1.29
2	B	1578	S99	CAX-NAT	-2.33	1.35	1.39
2	A	1577	S99	CAX-NAT	-2.07	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1577	S99	CAX-NAT-CAY	6.34	107.90	104.55
2	B	1578	S99	CAX-NAT-CAY	5.06	107.22	104.55
2	B	1578	S99	CAH-NAS-CAW	4.54	122.78	116.93
2	A	1577	S99	CAH-NAS-CAW	4.43	122.64	116.93
2	B	1578	S99	CAD-CAH-NAS	-2.73	119.09	123.42
2	B	1578	S99	CAW-CAX-CAL	-2.43	125.04	129.07
2	A	1577	S99	CAK-CAW-NAS	-2.34	119.58	122.74
2	A	1577	S99	CAD-CAH-NAS	-2.29	119.80	123.42
2	A	1577	S99	CAX-CAW-NAS	2.14	120.53	116.51
2	A	1577	S99	CAW-CAX-CAL	-2.07	125.63	129.07
2	B	1578	S99	CAK-CAW-NAS	-2.06	119.97	122.74
2	B	1578	S99	CAX-CAW-NAS	2.04	120.35	116.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

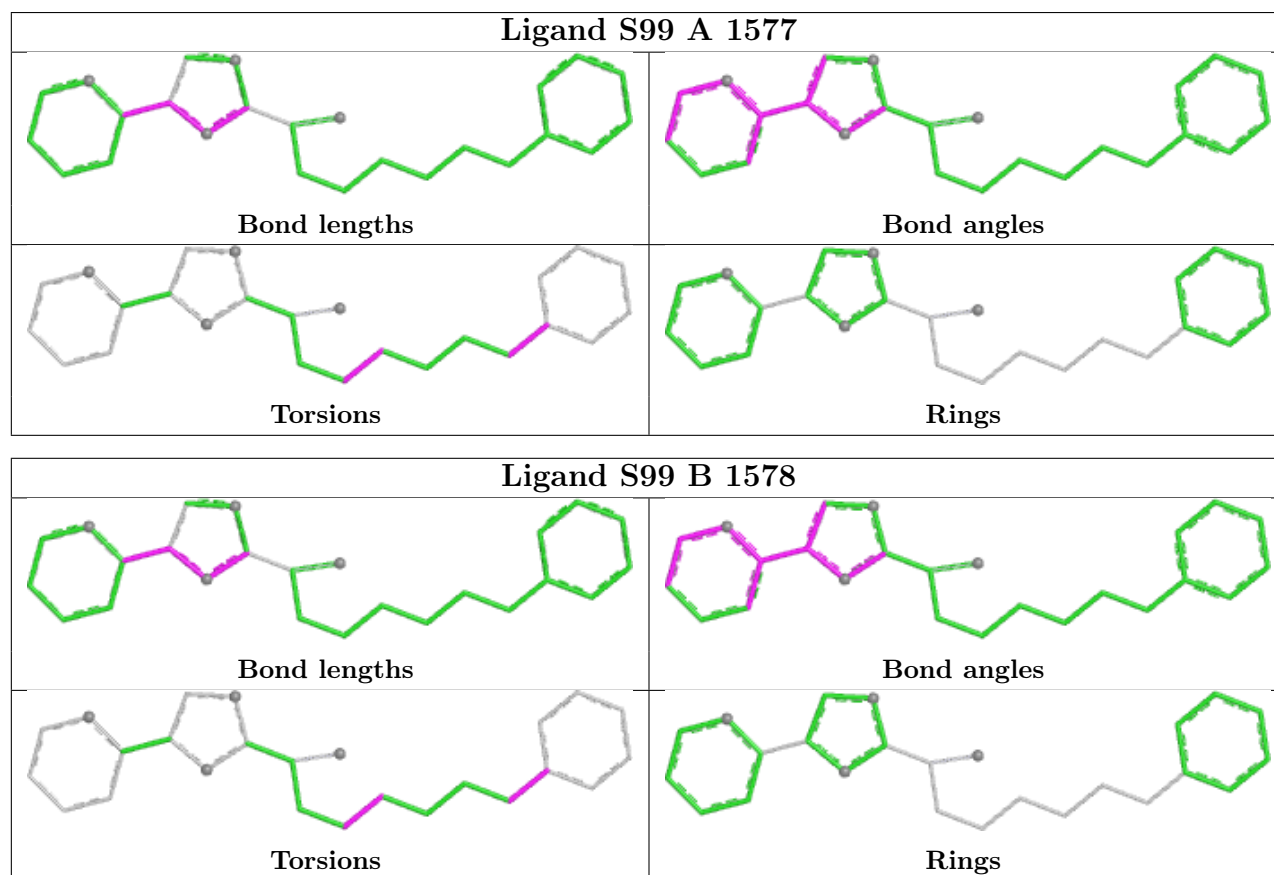
Mol	Chain	Res	Type	Atoms
2	A	1577	S99	CAM-CAN-CAP-CAR
2	B	1578	S99	CAM-CAN-CAP-CAR
2	A	1577	S99	CAO-CAQ-CAV-CAI
2	B	1578	S99	CAO-CAQ-CAV-CAI

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	543/573 (94%)	0.21	21 (3%)	43 46	13, 24, 57, 109	1 (0%)
1	B	544/573 (94%)	0.27	24 (4%)	39 42	12, 26, 59, 109	1 (0%)
All	All	1087/1146 (94%)	0.24	45 (4%)	41 44	12, 25, 58, 109	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	THR	4.0
1	A	71	SER	3.8
1	B	120	ASP	3.7
1	B	577	GLN	3.7
1	B	64	LEU	3.6
1	B	119	THR	3.5
1	B	576	LYS	3.5
1	A	125	LEU	3.4
1	A	64	LEU	3.3
1	A	131	GLN	3.1
1	B	71	SER	3.0
1	A	158	LEU	3.0
1	B	61	ARG	2.8
1	A	120	ASP	2.8
1	A	576	LYS	2.7
1	B	68	ASP	2.7
1	A	35	GLN	2.6
1	B	69	LEU	2.6
1	B	277	GLN	2.6
1	A	68	ASP	2.6
1	A	425	LEU	2.5
1	B	72	GLU	2.4
1	A	128	ALA	2.4
1	A	69	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	131	GLN	2.4
1	A	421	LEU	2.4
1	B	425	LEU	2.4
1	B	70	ASP	2.4
1	A	34	ARG	2.4
1	B	123	THR	2.4
1	A	90	GLU	2.4
1	A	574	PRO	2.3
1	B	386	ARG	2.3
1	B	271	TYR	2.2
1	B	210	SER	2.2
1	B	126	SER	2.2
1	A	61	ARG	2.2
1	A	575	GLN	2.2
1	B	67	PRO	2.2
1	B	34	ARG	2.2
1	A	130	ARG	2.1
1	B	36	LYS	2.1
1	A	124	GLN	2.1
1	B	66	ASN	2.0
1	B	49	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

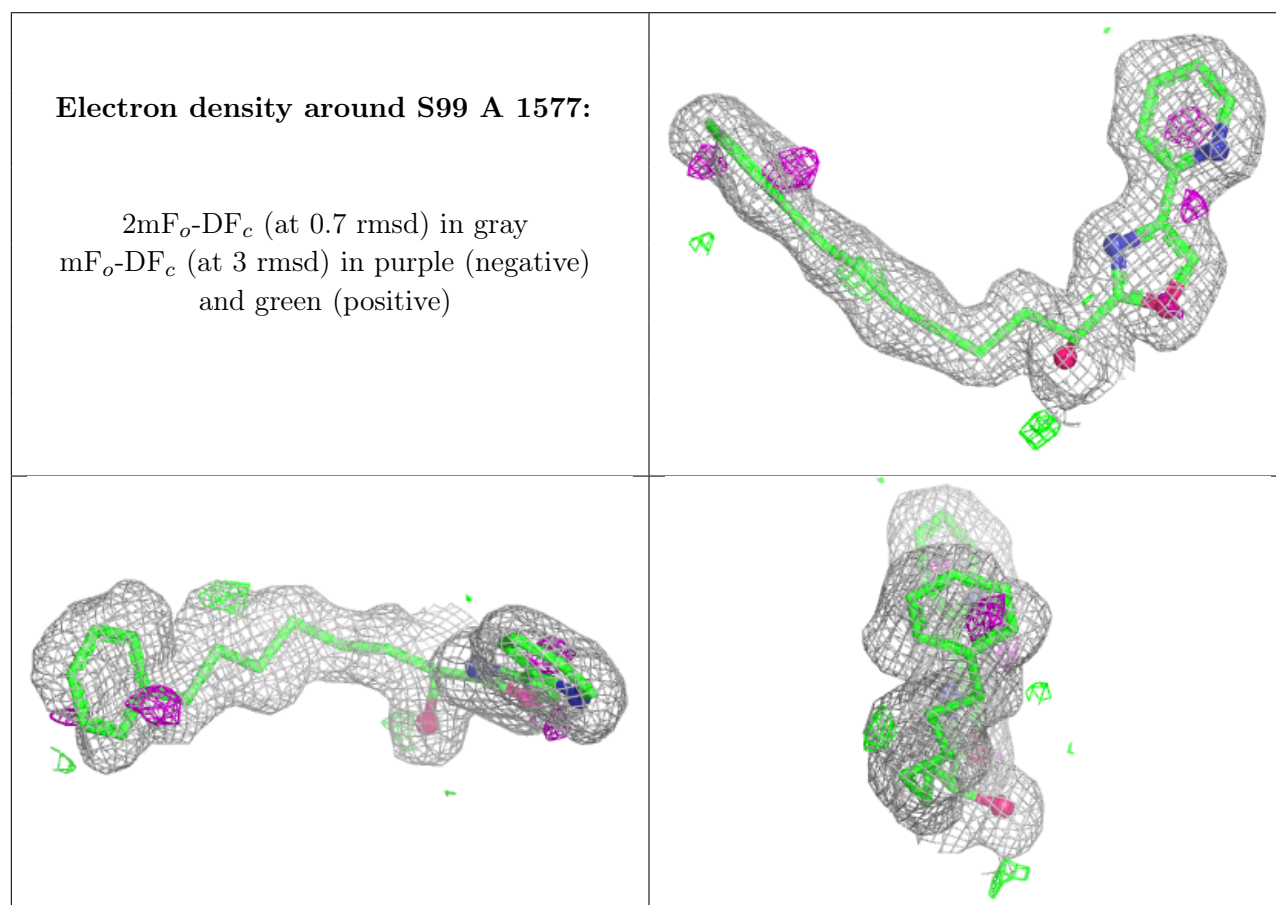
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	S99	A	1577	25/26	0.93	0.09	11,22,31,42	0
2	S99	B	1578	25/26	0.93	0.09	14,24,35,40	0

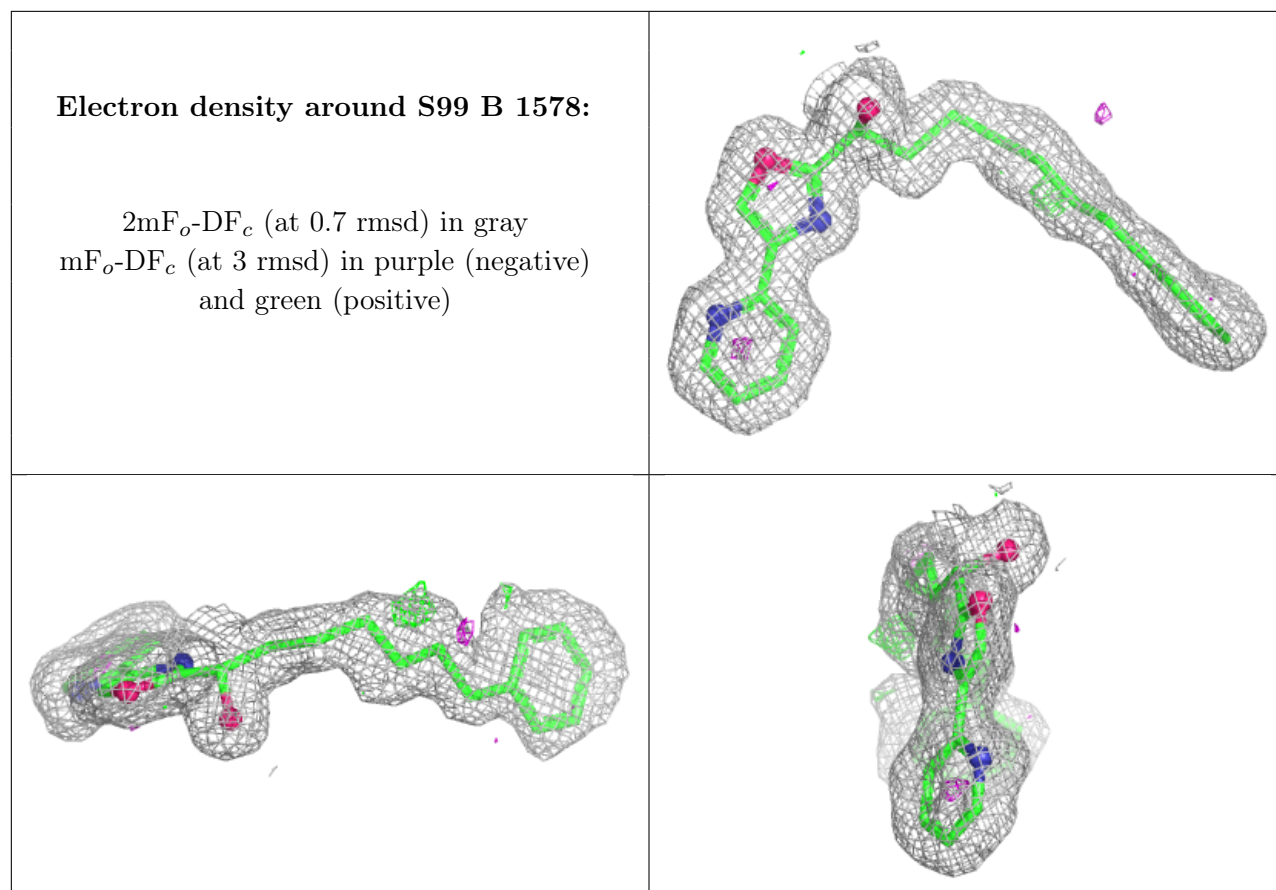
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	1578	1/1	0.95	0.07	28,28,28,28	0

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 ⓘ

There are no such residues in this entry.