



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:48 AM UTC

PDB ID : 6H7U / pdb_00006h7u
Title : Crystal structure of a POT family transporter in complex with 5-aminolevulinic acid
Authors : Minhas, G.S.; Newstead, S.
Deposited on : 2018-07-31
Resolution : 2.80 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 Phenix2.0
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

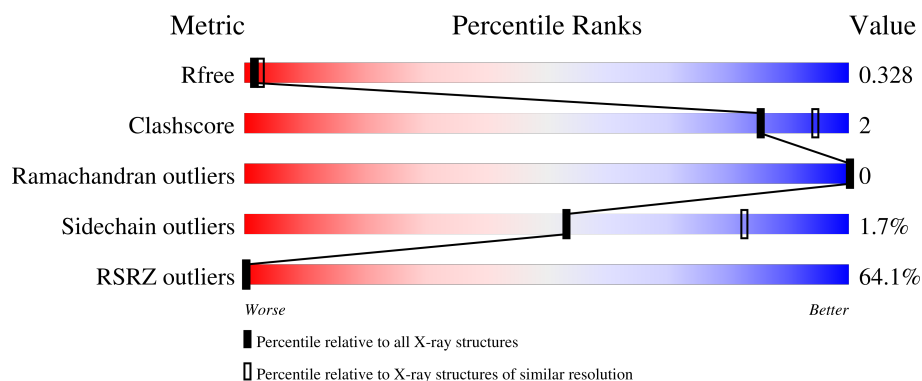
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	487	64% 96% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3816 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.

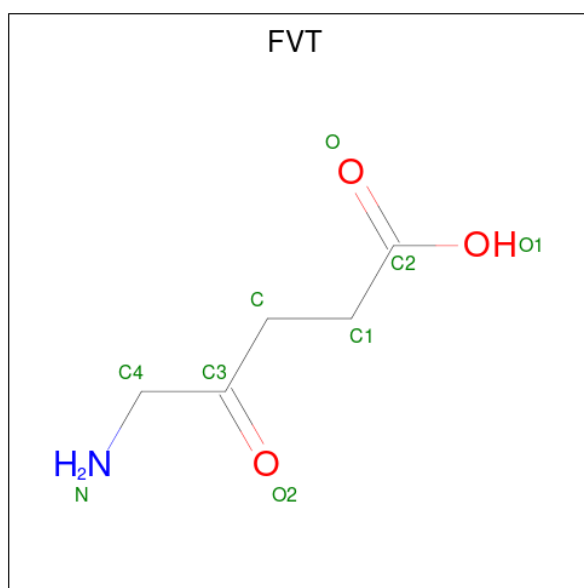
- Molecule 1 is a protein called Peptide ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3790	2526	605	637	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ASP	ASN	conflict	UNP A0A1L8Y4Q3
A	288	GLY	VAL	conflict	UNP A0A1L8Y4Q3

- Molecule 2 is 5-azanyl-4-oxidanylidene-pentanoic acid (CCD ID: FVT) (formula: C₅H₉NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	5	1	3	0	0

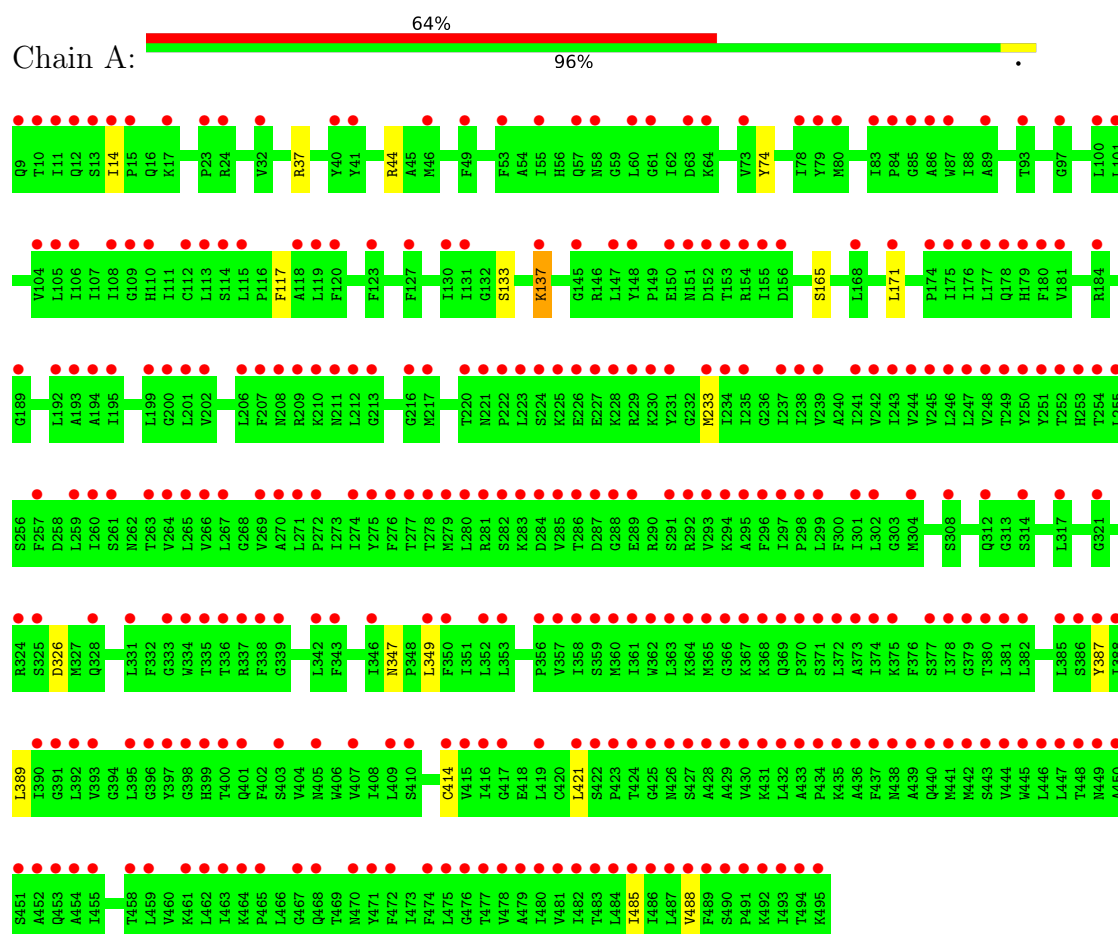
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		

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: Peptide ABC transporter permease



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.54Å 57.03Å 99.95Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	40.29 – 2.80 40.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.29-2.80) 98.3 (40.29-2.80)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.293 , 0.320 0.300 , 0.328	Depositor DCC
R_{free} test set	873 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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: FVT

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	0.85	0/3882	1.44	7/5269 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	117	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	14	ILE	N-CA-C	5.40	114.93	108.45
1	A	165	SER	CA-C-N	5.16	127.06	120.56
1	A	165	SER	C-N-CA	5.16	127.06	120.56
1	A	74	TYR	CA-C-N	5.05	125.55	119.94
1	A	74	TYR	C-N-CA	5.05	125.55	119.94

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	3790	0	3963	17	0
2	A	9	0	0	0	0
3	A	17	0	0	1	0
All	All	3816	0	3963	17	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 2.

All (17) 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:37:ARG:CZ	1:A:137:LYS:HZ2	1.13	1.59
1:A:37:ARG:NH2	1:A:137:LYS:NZ	1.66	1.42
1:A:37:ARG:CZ	1:A:137:LYS:NZ	1.87	1.34
1:A:37:ARG:NH1	1:A:137:LYS:NZ	1.80	1.29
1:A:37:ARG:NH2	1:A:137:LYS:HZ2	1.31	1.17
1:A:37:ARG:NH1	1:A:137:LYS:HZ2	1.50	1.00
1:A:37:ARG:HH22	1:A:137:LYS:NZ	1.34	0.99
1:A:37:ARG:HH12	1:A:137:LYS:NZ	1.51	0.97
1:A:37:ARG:NH1	1:A:137:LYS:HZ1	1.49	0.93
1:A:37:ARG:HH12	1:A:137:LYS:HZ1	0.86	0.85
1:A:37:ARG:HH22	1:A:137:LYS:HZ3	0.85	0.83
1:A:37:ARG:NH2	1:A:137:LYS:HZ3	1.48	0.74
1:A:414:CYS:HB3	3:A:601:HOH:O	1.95	0.65
1:A:133:SER:O	1:A:137:LYS:HB2	2.03	0.58
1:A:37:ARG:NH1	1:A:137:LYS:CE	2.73	0.49
1:A:171:LEU:HD13	1:A:349:LEU:HB2	2.01	0.42
1:A:485:ILE:O	1:A:488:VAL:HG22	2.20	0.42

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	485/487 (100%)	470 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	409/411 (100%)	402 (98%)	7 (2%)	53 83

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

Mol	Chain	Res	Type
1	A	44	ARG
1	A	137	LYS
1	A	233	MET
1	A	347	ASN
1	A	387	TYR
1	A	389	LEU
1	A	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	208	ASN
1	A	221	ASN
1	A	253	HIS
1	A	344	GLN
1	A	453	GLN
1	A	468	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](#)

1 ligand is 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	FVT	A	501	-	8,8,8	0.16	0	6,9,9	0.53	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	FVT	A	501	-	-	4/6/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

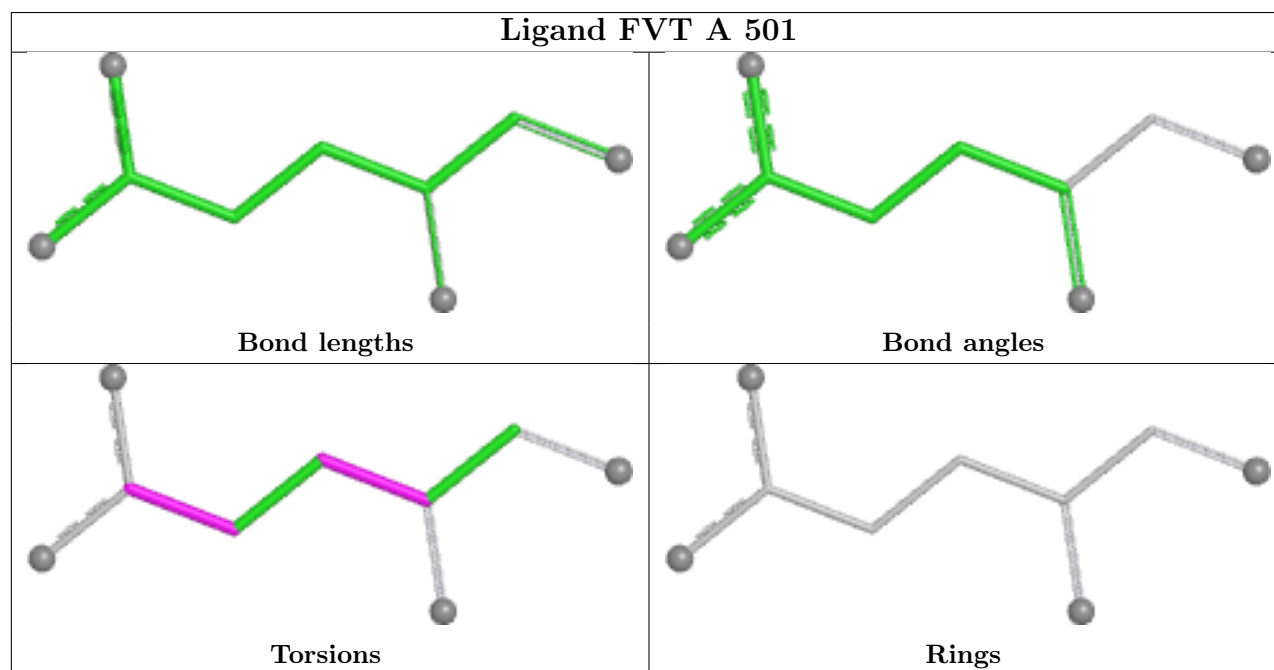
Mol	Chain	Res	Type	Atoms
2	A	501	FVT	C1-C-C3-O2
2	A	501	FVT	C1-C-C3-C4
2	A	501	FVT	C-C1-C2-O
2	A	501	FVT	C-C1-C2-O1

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	487/487 (100%)	2.57	312 (64%) 0 0	42, 63, 121, 150	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	430	VAL	6.7
1	A	429	ALA	6.2
1	A	244	VAL	6.0
1	A	487	LEU	5.9
1	A	495	LYS	5.8
1	A	488	VAL	5.7
1	A	368	LYS	5.7
1	A	114	SER	5.6
1	A	432	LEU	5.6
1	A	10	THR	5.5
1	A	428	ALA	5.4
1	A	426	ASN	5.4
1	A	233	MET	5.4
1	A	13	SER	5.4
1	A	435	LYS	5.4
1	A	416	ILE	5.3
1	A	486	ILE	5.2
1	A	283	LYS	5.2
1	A	369	GLN	5.2
1	A	424	THR	5.1
1	A	245	VAL	5.0
1	A	425	GLY	5.0
1	A	177	LEU	5.0
1	A	484	LEU	4.9
1	A	361	ILE	4.9
1	A	252	THR	4.8
1	A	359	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	302	LEU	4.7
1	A	367	LYS	4.7
1	A	235	ILE	4.6
1	A	131	ILE	4.6
1	A	446	LEU	4.6
1	A	434	PRO	4.6
1	A	148	TYR	4.5
1	A	489	PHE	4.5
1	A	387	TYR	4.5
1	A	493	ILE	4.5
1	A	423	PRO	4.5
1	A	150	GLU	4.5
1	A	464	LYS	4.5
1	A	482	ILE	4.4
1	A	485	ILE	4.4
1	A	364	LYS	4.4
1	A	365	MET	4.4
1	A	374	ILE	4.4
1	A	439	ALA	4.4
1	A	284	ASP	4.4
1	A	382	LEU	4.3
1	A	12	GLN	4.3
1	A	211	ASN	4.2
1	A	363	LEU	4.2
1	A	285	VAL	4.2
1	A	395	LEU	4.2
1	A	274	ILE	4.2
1	A	253	HIS	4.1
1	A	444	VAL	4.1
1	A	189	GLY	4.1
1	A	246	LEU	4.0
1	A	179	HIS	4.0
1	A	491	PRO	4.0
1	A	362	TRP	4.0
1	A	438	ASN	4.0
1	A	492	LYS	3.9
1	A	431	LYS	3.9
1	A	481	VAL	3.9
1	A	281	ARG	3.9
1	A	292	ARG	3.9
1	A	494	THR	3.9
1	A	247	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	3.9
1	A	449	ASN	3.8
1	A	286	THR	3.8
1	A	9	GLN	3.8
1	A	64	LYS	3.8
1	A	209	ARG	3.7
1	A	237	ILE	3.7
1	A	251	TYR	3.7
1	A	447	LEU	3.7
1	A	379	GLY	3.7
1	A	436	ALA	3.7
1	A	475	LEU	3.7
1	A	372	LEU	3.7
1	A	471	TYR	3.7
1	A	255	LEU	3.6
1	A	333	GLY	3.6
1	A	250	TYR	3.6
1	A	239	VAL	3.6
1	A	248	VAL	3.6
1	A	259	LEU	3.6
1	A	221	ASN	3.6
1	A	470	ASN	3.6
1	A	294	LYS	3.6
1	A	127	PHE	3.6
1	A	213	GLY	3.6
1	A	243	ILE	3.6
1	A	393	VAL	3.6
1	A	346	ILE	3.5
1	A	451	SER	3.5
1	A	490	SER	3.5
1	A	378	ILE	3.5
1	A	334	TRP	3.5
1	A	210	LYS	3.5
1	A	297	ILE	3.5
1	A	301	ILE	3.5
1	A	254	THR	3.5
1	A	373	ALA	3.5
1	A	433	ALA	3.5
1	A	181	VAL	3.4
1	A	220	THR	3.4
1	A	458	THR	3.4
1	A	271	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	3.4
1	A	11	ILE	3.4
1	A	155	ILE	3.4
1	A	78	ILE	3.4
1	A	85	GLY	3.4
1	A	422	SER	3.4
1	A	380	THR	3.4
1	A	377	SER	3.3
1	A	400	THR	3.3
1	A	58	ASN	3.3
1	A	358	ILE	3.3
1	A	60	LEU	3.3
1	A	275	TYR	3.3
1	A	288	GLY	3.3
1	A	151	ASN	3.3
1	A	296	PHE	3.3
1	A	357	VAL	3.3
1	A	477	THR	3.3
1	A	476	GLY	3.3
1	A	15	PRO	3.2
1	A	366	GLY	3.2
1	A	46	MET	3.2
1	A	113	LEU	3.2
1	A	437	PHE	3.2
1	A	272	PRO	3.2
1	A	443	SER	3.2
1	A	299	LEU	3.2
1	A	264	VAL	3.2
1	A	293	VAL	3.2
1	A	308	SER	3.2
1	A	381	LEU	3.2
1	A	399	HIS	3.2
1	A	260	ILE	3.1
1	A	328	GLN	3.1
1	A	461	LYS	3.1
1	A	79	TYR	3.1
1	A	207	PHE	3.1
1	A	108	ILE	3.1
1	A	119	LEU	3.1
1	A	192	LEU	3.1
1	A	483	THR	3.1
1	A	234	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	3.0
1	A	249	THR	3.0
1	A	270	ALA	3.0
1	A	269	VAL	3.0
1	A	208	ASN	3.0
1	A	228	LYS	3.0
1	A	241	ILE	3.0
1	A	415	VAL	3.0
1	A	261	SER	3.0
1	A	467	GLY	3.0
1	A	356	PRO	3.0
1	A	118	ALA	3.0
1	A	242	VAL	3.0
1	A	231	TYR	3.0
1	A	14	ILE	3.0
1	A	314	SER	3.0
1	A	403	SER	3.0
1	A	194	ALA	3.0
1	A	238	ILE	2.9
1	A	178	GLN	2.9
1	A	370	PRO	2.9
1	A	115	LEU	2.9
1	A	331	LEU	2.9
1	A	442	MET	2.9
1	A	392	LEU	2.9
1	A	445	TRP	2.9
1	A	17	LYS	2.9
1	A	49	PHE	2.9
1	A	257	PHE	2.9
1	A	352	LEU	2.8
1	A	391	GLY	2.8
1	A	24	ARG	2.8
1	A	291	SER	2.8
1	A	61	GLY	2.8
1	A	84	PRO	2.8
1	A	104	VAL	2.8
1	A	201	LEU	2.8
1	A	223	LEU	2.8
1	A	337	ARG	2.7
1	A	478	VAL	2.7
1	A	474	PHE	2.7
1	A	147	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	388	ILE	2.7
1	A	397	TYR	2.7
1	A	409	LEU	2.7
1	A	225	LYS	2.7
1	A	57	GLN	2.7
1	A	440	GLN	2.7
1	A	217	MET	2.7
1	A	353	LEU	2.7
1	A	463	ILE	2.7
1	A	87	TRP	2.7
1	A	335	THR	2.7
1	A	339	GLY	2.7
1	A	289	GLU	2.7
1	A	123	PHE	2.7
1	A	180	PHE	2.7
1	A	454	ALA	2.7
1	A	414	CYS	2.7
1	A	73	VAL	2.7
1	A	462	LEU	2.7
1	A	350	PHE	2.6
1	A	154	ARG	2.6
1	A	63	ASP	2.6
1	A	105	LEU	2.6
1	A	230	LYS	2.6
1	A	421	LEU	2.6
1	A	386	SER	2.6
1	A	441	MET	2.6
1	A	222	PRO	2.6
1	A	227	GLU	2.6
1	A	480	ILE	2.6
1	A	287	ASP	2.6
1	A	280	LEU	2.6
1	A	336	THR	2.6
1	A	212	LEU	2.6
1	A	267	LEU	2.6
1	A	342	LEU	2.6
1	A	80	MET	2.6
1	A	106	ILE	2.6
1	A	452	ALA	2.6
1	A	465	PRO	2.5
1	A	479	ALA	2.5
1	A	152	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	2.5
1	A	398	GLY	2.5
1	A	427	SER	2.5
1	A	265	LEU	2.5
1	A	321	GLY	2.5
1	A	360	MET	2.5
1	A	130	ILE	2.5
1	A	263	THR	2.5
1	A	200	GLY	2.5
1	A	390	ILE	2.5
1	A	229	ARG	2.5
1	A	278	THR	2.5
1	A	396	GLY	2.4
1	A	417	GLY	2.4
1	A	282	SER	2.4
1	A	101	LEU	2.4
1	A	349	LEU	2.4
1	A	277	THR	2.4
1	A	110	HIS	2.4
1	A	112	CYS	2.3
1	A	410	SER	2.3
1	A	83	ILE	2.3
1	A	195	ILE	2.3
1	A	97	GLY	2.3
1	A	468	GLN	2.3
1	A	325	SER	2.3
1	A	371	SER	2.3
1	A	385	LEU	2.3
1	A	419	LEU	2.3
1	A	55	ILE	2.3
1	A	459	LEU	2.3
1	A	338	PHE	2.3
1	A	156	ASP	2.3
1	A	23	PRO	2.3
1	A	174	PRO	2.3
1	A	279	MET	2.2
1	A	120	PHE	2.2
1	A	343	PHE	2.2
1	A	401	GLN	2.2
1	A	266	VAL	2.2
1	A	109	GLY	2.2
1	A	137	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	450	ALA	2.2
1	A	184	ARG	2.2
1	A	455	ILE	2.2
1	A	298	PRO	2.2
1	A	226	GLU	2.2
1	A	93	THR	2.2
1	A	304	MET	2.2
1	A	448	THR	2.2
1	A	145	GLY	2.2
1	A	375	LYS	2.1
1	A	40	TYR	2.1
1	A	224	SER	2.1
1	A	453	GLN	2.1
1	A	171	LEU	2.1
1	A	199	LEU	2.1
1	A	86	ALA	2.1
1	A	324	ARG	2.1
1	A	176	ILE	2.1
1	A	312	GLN	2.1
1	A	405	ASN	2.1
1	A	206	LEU	2.1
1	A	153	THR	2.1
1	A	89	ALA	2.1
1	A	295	ALA	2.1
1	A	216	GLY	2.1
1	A	32	VAL	2.0
1	A	202	VAL	2.0
1	A	193	ALA	2.0
1	A	41	TYR	2.0
1	A	317	LEU	2.0
1	A	53	PHE	2.0
1	A	276	PHE	2.0
1	A	472	PHE	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](#)

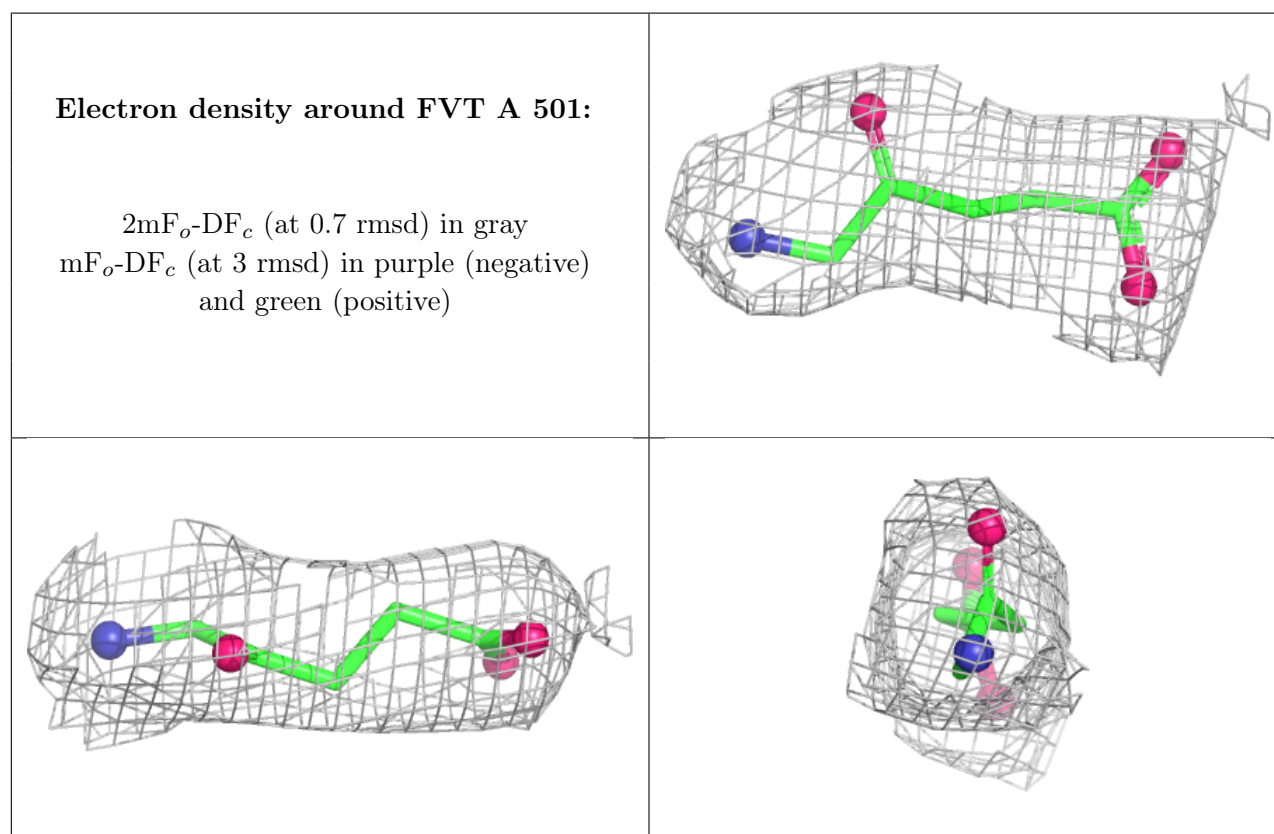
There are no oligosaccharides in this entry.

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	FVT	A	501	9/9	0.78	0.24	65,65,67,68	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.