



Full wwPDB X-ray Structure Validation Report i

Oct 13, 2021 – 12:17 pm BST

PDB ID : 6ZGT
Title : Crystal structure of a MFS transporter with bound 2-naphthoic acid at 2.39 Angstroem resolution
Authors : Kalbermatter, D.; Bosshart, P.; Bonetti, S.; Fotiadis, D.
Deposited on : 2020-06-19
Resolution : 2.23 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 i symbol.

The following versions of software and data (see [references](#) i) 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	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

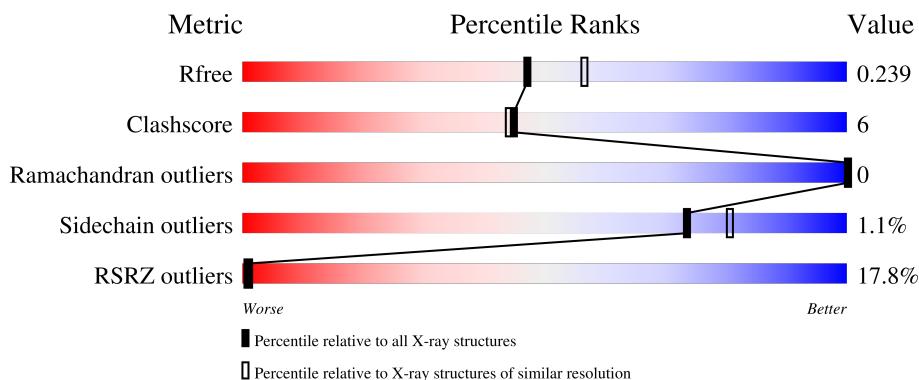
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

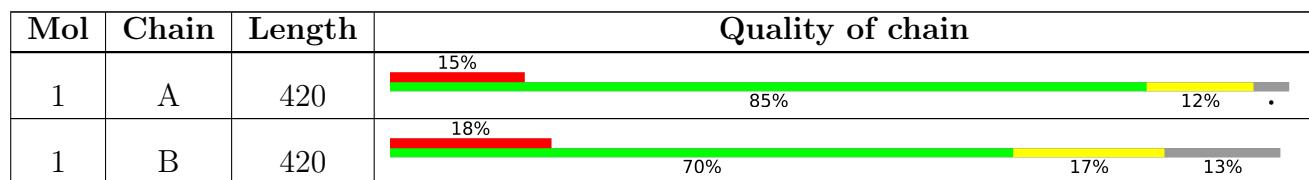
The reported resolution of this entry is 2.23 Å.

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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5822 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.

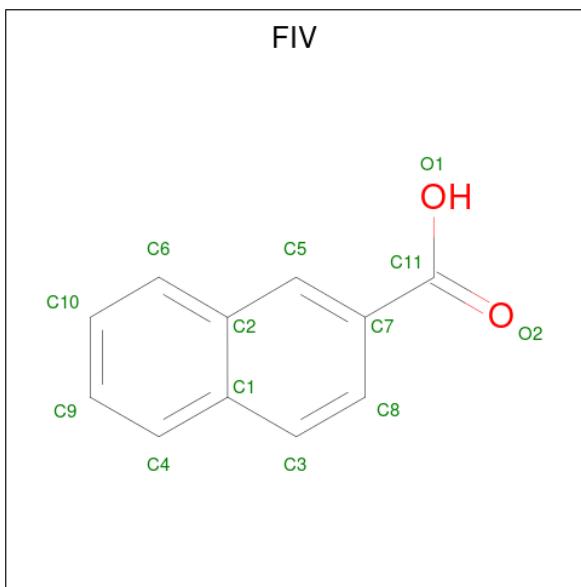
- Molecule 1 is a protein called L-lactate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C 3055	N 2044	O 481	S 505	25	0	0
1	B	364	Total	C 2735	N 1832	O 428	S 452	23	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	LEU	-	expression tag	UNP A0LNN5
A	414	GLU	-	expression tag	UNP A0LNN5
A	415	LEU	-	expression tag	UNP A0LNN5
A	416	GLU	-	expression tag	UNP A0LNN5
A	417	VAL	-	expression tag	UNP A0LNN5
A	418	LEU	-	expression tag	UNP A0LNN5
A	419	PHE	-	expression tag	UNP A0LNN5
A	420	GLN	-	expression tag	UNP A0LNN5
B	413	LEU	-	expression tag	UNP A0LNN5
B	414	GLU	-	expression tag	UNP A0LNN5
B	415	LEU	-	expression tag	UNP A0LNN5
B	416	GLU	-	expression tag	UNP A0LNN5
B	417	VAL	-	expression tag	UNP A0LNN5
B	418	LEU	-	expression tag	UNP A0LNN5
B	419	PHE	-	expression tag	UNP A0LNN5
B	420	GLN	-	expression tag	UNP A0LNN5

- Molecule 2 is naphthalene-2-carboxylic acid (three-letter code: FIV) (formula: C₁₁H₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 11 2	0	0
2	B	1	Total C O 13 11 2	0	0

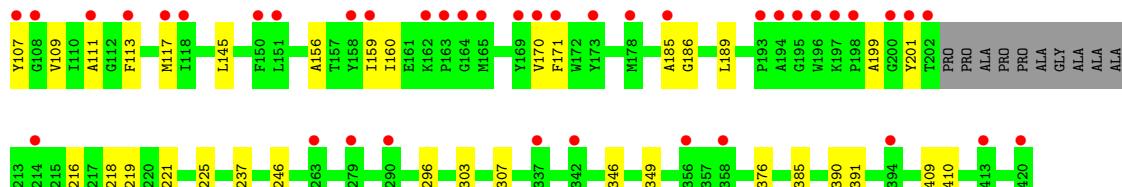
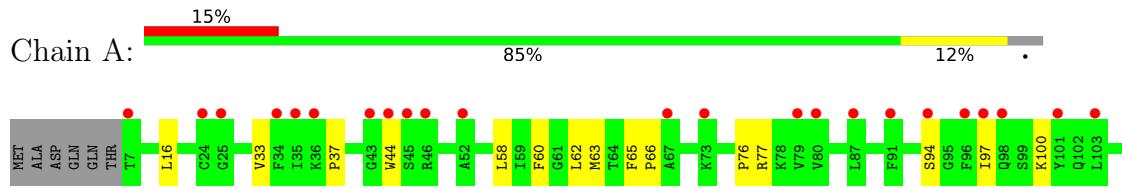
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	1	Total O 1 1	0	0

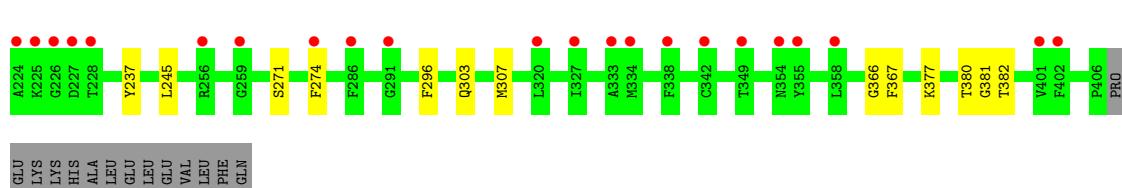
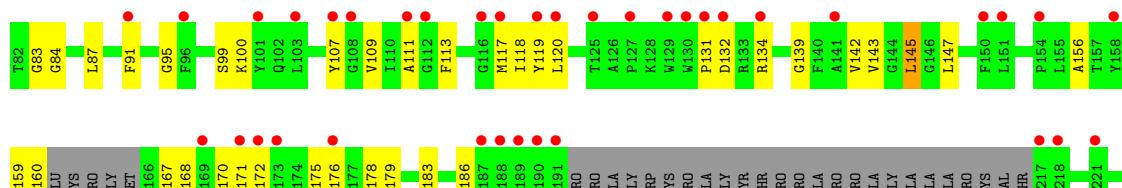
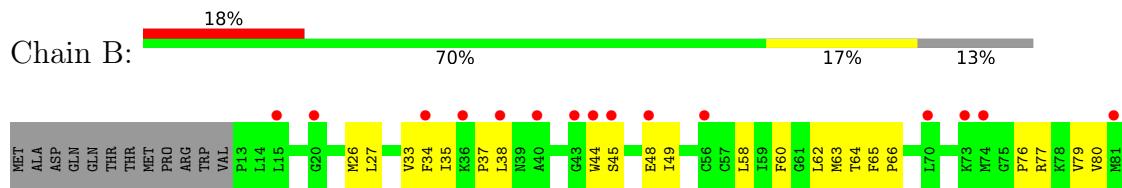
3 Residue-property plots [\(i\)](#)

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: L-lactate transporter



- Molecule 1: L-lactate transporter



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.53Å 199.62Å 61.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.23 19.96 – 2.23	Depositor EDS
% Data completeness (in resolution range)	67.0 (19.96-2.23) 67.0 (19.96-2.23)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.21 (at 2.23Å)	Xtriage
Refinement program	PHENIX 1.14_3228	Depositor
R , R_{free}	0.215 , 0.240 0.215 , 0.239	Depositor DCC
R_{free} test set	1995 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5822	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: FIV

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	0.53	0/3152	0.66	0/4290
1	B	0.43	0/2817	0.60	0/3830
All	All	0.48	0/5969	0.63	0/8120

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	3055	0	3094	29	0
1	B	2735	0	2766	47	0
2	A	13	0	7	3	0
2	B	13	0	7	3	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
All	All	5822	0	5874	76	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 6.

All (76) 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:26:MET:HB3	1:B:178:MET:HE2	1.68	0.76
1:B:119:TYR:CE1	1:B:145:LEU:HD11	2.25	0.71
1:B:33:VAL:HG11	1:B:156:ALA:HB1	1.75	0.68
1:A:33:VAL:HG11	1:A:156:ALA:HB1	1.76	0.66
1:A:60:PHE:CE1	2:A:501:FIV:H3	2.31	0.66
1:B:119:TYR:HE1	1:B:145:LEU:HD11	1.62	0.65
1:B:37:PRO:HG2	1:B:160:ILE:HD13	1.81	0.62
1:B:60:PHE:CE1	2:B:501:FIV:H3	2.36	0.61
1:A:199:ALA:HB1	1:A:201:TYR:O	2.04	0.57
1:A:94:SER:O	1:A:97:ILE:HG12	2.04	0.57
1:B:58:LEU:O	1:B:62:LEU:HG	2.04	0.57
1:B:119:TYR:HE1	1:B:145:LEU:CD1	2.17	0.57
1:A:303:GLN:O	1:A:307:MET:HG2	2.05	0.56
1:A:159:ILE:HB	1:A:170:VAL:HG22	1.87	0.56
1:A:94:SER:HA	1:A:97:ILE:HG23	1.88	0.54
1:B:131:PRO:HA	1:B:134:ARG:HE	1.72	0.54
1:B:145:LEU:HD13	2:B:501:FIV:O1	2.08	0.54
1:B:91:PHE:CE2	1:B:171:PHE:O	2.64	0.52
1:B:34:PHE:HB3	1:B:38:LEU:HG	1.92	0.51
1:B:271:SER:HA	1:B:274:PHE:HD2	1.76	0.51
1:B:45:SER:HB3	1:B:48:GLU:HG3	1.92	0.51
1:B:65:PHE:HB3	1:B:66:PRO:HD3	1.93	0.50
1:A:145:LEU:HD22	2:A:501:FIV:H2	1.92	0.50
1:B:91:PHE:CD2	1:B:171:PHE:O	2.65	0.50
1:B:95:GLY:O	1:B:168:ARG:NH2	2.44	0.50
1:A:37:PRO:HG2	1:A:160:ILE:HD13	1.95	0.49
1:A:221:TYR:O	1:A:225:LYS:HB3	2.12	0.49
1:B:58:LEU:HB2	1:B:367:PHE:HB2	1.94	0.49
1:B:159:ILE:HB	1:B:170:VAL:HG22	1.94	0.49
1:B:132:ASP:OD1	1:B:132:ASP:N	2.45	0.49
1:A:376:LEU:HD22	1:A:385:LEU:HD23	1.94	0.48
1:B:44:TRP:HA	1:B:48:GLU:OE1	2.14	0.48
1:B:63:MET:HG3	1:B:113:PHE:HA	1.94	0.48
1:B:145:LEU:HD22	2:B:501:FIV:C11	2.43	0.48
1:B:99:SER:OG	1:B:100:LYS:N	2.46	0.48
1:B:64:THR:HB	1:B:120:LEU:HD13	1.96	0.48
1:A:218:ASP:OD2	1:A:349:THR:HG23	2.14	0.48
1:A:145:LEU:HD22	2:A:501:FIV:C8	2.44	0.47
1:B:160:ILE:HG12	1:B:167:TRP:HA	1.96	0.47
1:B:245:LEU:HD13	1:B:366:GLY:HA2	1.95	0.47
1:B:143:VAL:O	1:B:147:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:HA	1:A:409:LYS:HD2	1.77	0.46
1:B:91:PHE:CE2	1:B:171:PHE:HA	2.51	0.46
1:B:84:GLY:HA2	1:B:118:ILE:HD11	1.98	0.46
1:A:107:TYR:O	1:A:111:ALA:HB3	2.15	0.46
1:A:65:PHE:HB3	1:A:66:PRO:HD3	1.98	0.46
1:B:172:TRP:O	1:B:176:VAL:HG23	2.16	0.46
1:B:35:ILE:HA	1:B:49:ILE:HD13	1.98	0.45
1:B:107:TYR:O	1:B:111:ALA:HB3	2.16	0.45
1:A:246:MET:HE3	1:A:390:ALA:HB2	1.98	0.45
1:B:380:THR:HB	1:B:382:THR:HG22	1.99	0.45
1:A:58:LEU:O	1:A:62:LEU:HG	2.16	0.44
1:B:91:PHE:CD2	1:B:175:GLY:HA3	2.52	0.44
1:B:377:LYS:O	1:B:381:GLY:N	2.44	0.44
1:A:63:MET:C	1:A:66:PRO:HD2	2.37	0.44
1:A:77:ARG:HG3	1:A:186:GLY:O	2.17	0.43
1:A:16:LEU:HD22	1:A:185:ALA:HA	2.00	0.43
1:B:91:PHE:CD2	1:B:175:GLY:CA	3.02	0.43
1:A:307:MET:HB2	1:A:391:ALA:HB2	2.00	0.43
1:B:77:ARG:HG3	1:B:186:GLY:O	2.19	0.43
1:A:219:TRP:HB2	1:A:346:TYR:HB3	2.01	0.42
1:B:27:LEU:HD13	1:B:87:LEU:HD11	2.00	0.42
1:B:109:VAL:O	1:B:113:PHE:HB2	2.19	0.42
1:A:76:PRO:HB2	1:A:189:LEU:HD23	2.01	0.42
1:A:216:THR:HA	1:A:410:LYS:O	2.19	0.42
1:A:109:VAL:O	1:A:113:PHE:HB2	2.21	0.41
1:A:44:TRP:CE2	1:A:100:LYS:HG3	2.55	0.41
1:B:167:TRP:O	1:B:170:VAL:HB	2.21	0.41
1:B:303:GLN:O	1:B:307:MET:HG2	2.21	0.41
1:B:139:GLY:HA2	1:B:142:VAL:HG22	2.02	0.41
1:A:113:PHE:O	1:A:117:MET:HG3	2.21	0.40
1:B:79:VAL:O	1:B:117:MET:HE2	2.21	0.40
1:B:83:GLY:HA3	1:B:117:MET:HB2	2.03	0.40
1:B:179:GLY:O	1:B:183:LEU:HG	2.22	0.40
1:A:94:SER:HA	1:A:97:ILE:CG2	2.51	0.40
1:B:76:PRO:O	1:B:80:VAL:HG23	2.21	0.40

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	400/420 (95%)	389 (97%)	11 (3%)	0	100 100
1	B	358/420 (85%)	355 (99%)	3 (1%)	0	100 100
All	All	758/840 (90%)	744 (98%)	14 (2%)	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	298/307 (97%)	295 (99%)	3 (1%)	76 82
1	B	264/307 (86%)	261 (99%)	3 (1%)	73 80
All	All	562/614 (92%)	556 (99%)	6 (1%)	73 80

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	PHE
1	A	237	TYR
1	A	296	PHE
1	B	145	LEU
1	B	237	TYR
1	B	296	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 monosaccharides 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	FIV	A	501	-	12,14,14	1.71	1 (8%)	16,19,19	1.49	2 (12%)
2	FIV	B	501	-	12,14,14	2.15	1 (8%)	16,19,19	0.85	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	FIV	A	501	-	-	0/0/4/4	0/2/2/2
2	FIV	B	501	-	-	0/0/4/4	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FIV	C7-C11	6.84	1.54	1.47
2	A	501	FIV	C7-C11	5.13	1.52	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FIV	C5-C7-C11	-3.60	115.62	120.36
2	A	501	FIV	C8-C7-C11	2.91	124.28	120.37

There are no chirality outliers.

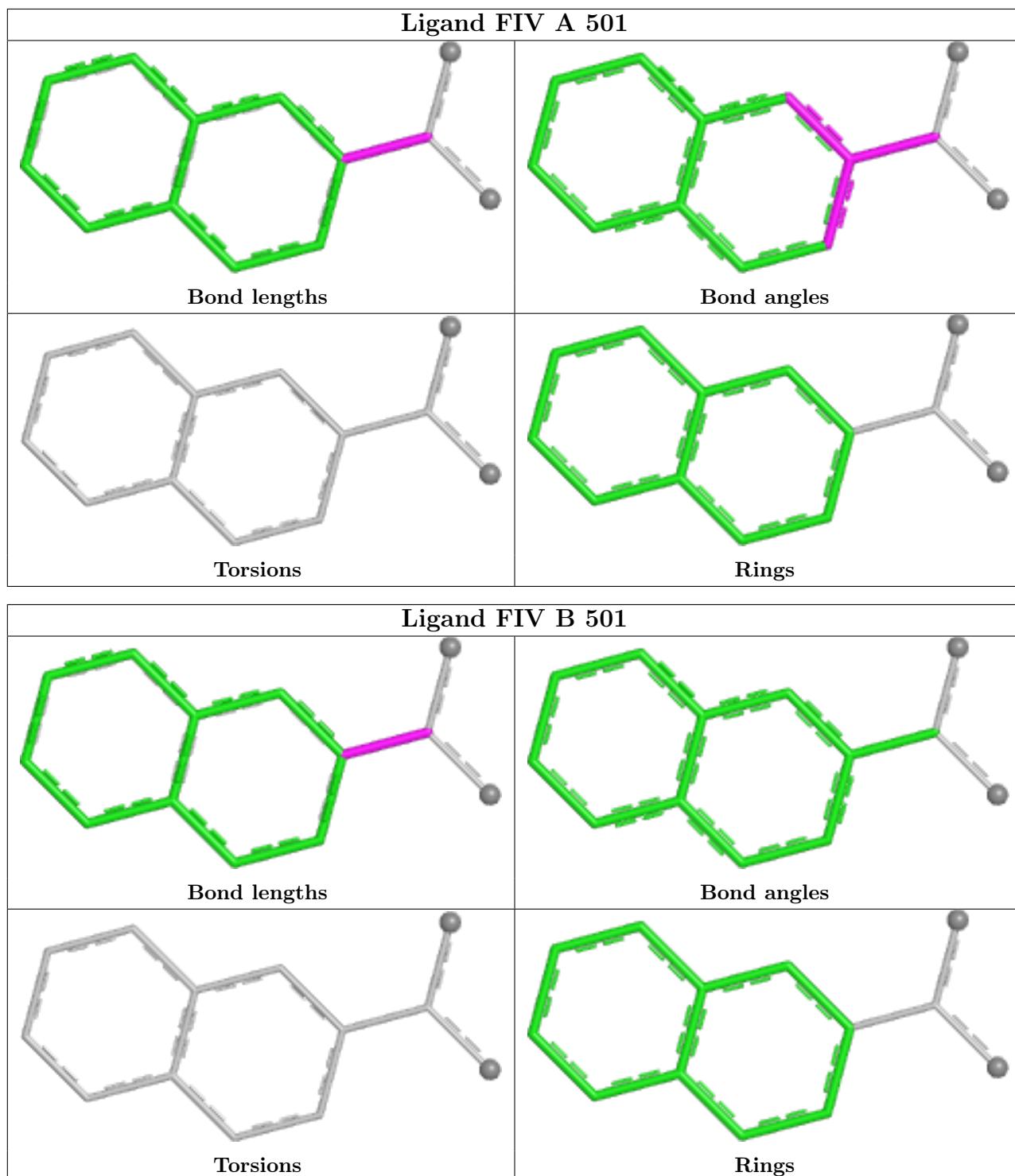
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FIV	3	0
2	B	501	FIV	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	404/420 (96%)	0.87	63 (15%) 2 1	47, 83, 146, 186	0
1	B	364/420 (86%)	0.99	74 (20%) 1 1	53, 109, 157, 190	0
All	All	768/840 (91%)	0.93	137 (17%) 1 1	47, 96, 155, 190	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	TYR	10.0
1	B	96	PHE	8.4
1	B	70	LEU	8.4
1	B	74	MET	7.9
1	A	194	ALA	7.8
1	A	196	TRP	7.7
1	A	171	PHE	7.7
1	A	91	PHE	7.6
1	B	91	PHE	7.4
1	B	225	LYS	7.0
1	B	158	TYR	6.6
1	B	188	PHE	6.5
1	B	190	GLU	6.4
1	A	107	TYR	6.3
1	A	158	TYR	6.2
1	B	226	GLY	6.1
1	A	164	GLY	6.1
1	B	107	TYR	5.9
1	A	169	TYR	5.9
1	B	125	THR	5.9
1	B	173	TYR	5.8
1	A	163	PRO	5.7
1	B	150	PHE	5.6
1	B	73	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	5.4
1	B	101	TYR	5.3
1	A	214	LYS	5.1
1	B	172	TRP	4.9
1	B	169	TYR	4.9
1	B	129	TRP	4.9
1	A	43	GLY	4.7
1	A	170	VAL	4.7
1	B	217	ARG	4.6
1	B	176	VAL	4.6
1	B	189	LEU	4.6
1	A	96	PHE	4.4
1	B	40	ALA	4.3
1	A	24	CYS	4.3
1	A	173	TYR	4.3
1	A	7	THR	4.3
1	B	119	TYR	4.3
1	B	171	PHE	4.2
1	B	15	LEU	4.0
1	A	118	ILE	4.0
1	A	342	CYS	4.0
1	A	101	TYR	3.9
1	A	193	PRO	3.9
1	B	131	PRO	3.9
1	B	44	TRP	3.8
1	B	354	ASN	3.8
1	A	45	SER	3.8
1	B	259	GLY	3.8
1	A	111	ALA	3.8
1	B	218	ASP	3.8
1	B	402	PHE	3.7
1	A	103	LEU	3.7
1	B	45	SER	3.7
1	A	80	VAL	3.6
1	B	108	GLY	3.6
1	B	127	PRO	3.5
1	B	111	ALA	3.5
1	A	94	SER	3.5
1	A	151	LEU	3.5
1	A	202	THR	3.5
1	A	150	PHE	3.4
1	A	117	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	LYS	3.3
1	A	98	GLN	3.3
1	B	151	LEU	3.2
1	A	178	MET	3.2
1	A	263	MET	3.2
1	B	358	LEU	3.1
1	A	200	GLY	3.1
1	B	227	ASP	3.0
1	B	334	MET	3.0
1	B	134	ARG	3.0
1	B	117	MET	3.0
1	A	197	LYS	3.0
1	A	67	ALA	3.0
1	B	36	LYS	3.0
1	B	120	LEU	3.0
1	B	154	PRO	2.9
1	A	52	ALA	2.9
1	A	46	ARG	2.8
1	B	141	ALA	2.8
1	A	165	MET	2.8
1	B	112	GLY	2.8
1	B	187	ALA	2.8
1	A	34	PHE	2.8
1	A	79	VAL	2.8
1	B	103	LEU	2.8
1	B	132	ASP	2.7
1	A	394	CYS	2.7
1	A	358	LEU	2.7
1	A	25	GLY	2.7
1	B	401	VAL	2.7
1	B	191	PRO	2.6
1	A	35	ILE	2.6
1	B	34	PHE	2.6
1	A	162	LYS	2.6
1	B	327	ILE	2.6
1	A	420	GLN	2.6
1	B	116	GLY	2.5
1	A	97	ILE	2.5
1	B	130	TRP	2.5
1	A	185	ALA	2.5
1	B	349	THR	2.5
1	B	338	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	228	THR	2.5
1	A	159	ILE	2.5
1	A	198	PRO	2.5
1	B	320	LEU	2.5
1	A	195	GLY	2.5
1	B	48	GLU	2.5
1	B	20	GLY	2.5
1	B	274	PHE	2.4
1	B	286	PHE	2.4
1	A	108	GLY	2.4
1	B	43	GLY	2.4
1	A	356	GLY	2.4
1	B	224	ALA	2.4
1	B	355	TYR	2.4
1	B	81	MET	2.3
1	B	256	ARG	2.3
1	A	413	LEU	2.3
1	A	44	TRP	2.2
1	B	38	LEU	2.2
1	A	279	THR	2.2
1	B	342	CYS	2.2
1	B	56	CYS	2.1
1	A	36	LYS	2.1
1	A	337	LEU	2.1
1	B	221	TYR	2.1
1	A	113	PHE	2.1
1	A	290	ILE	2.0
1	B	333	ALA	2.0
1	B	291	GLY	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 [\(i\)](#)

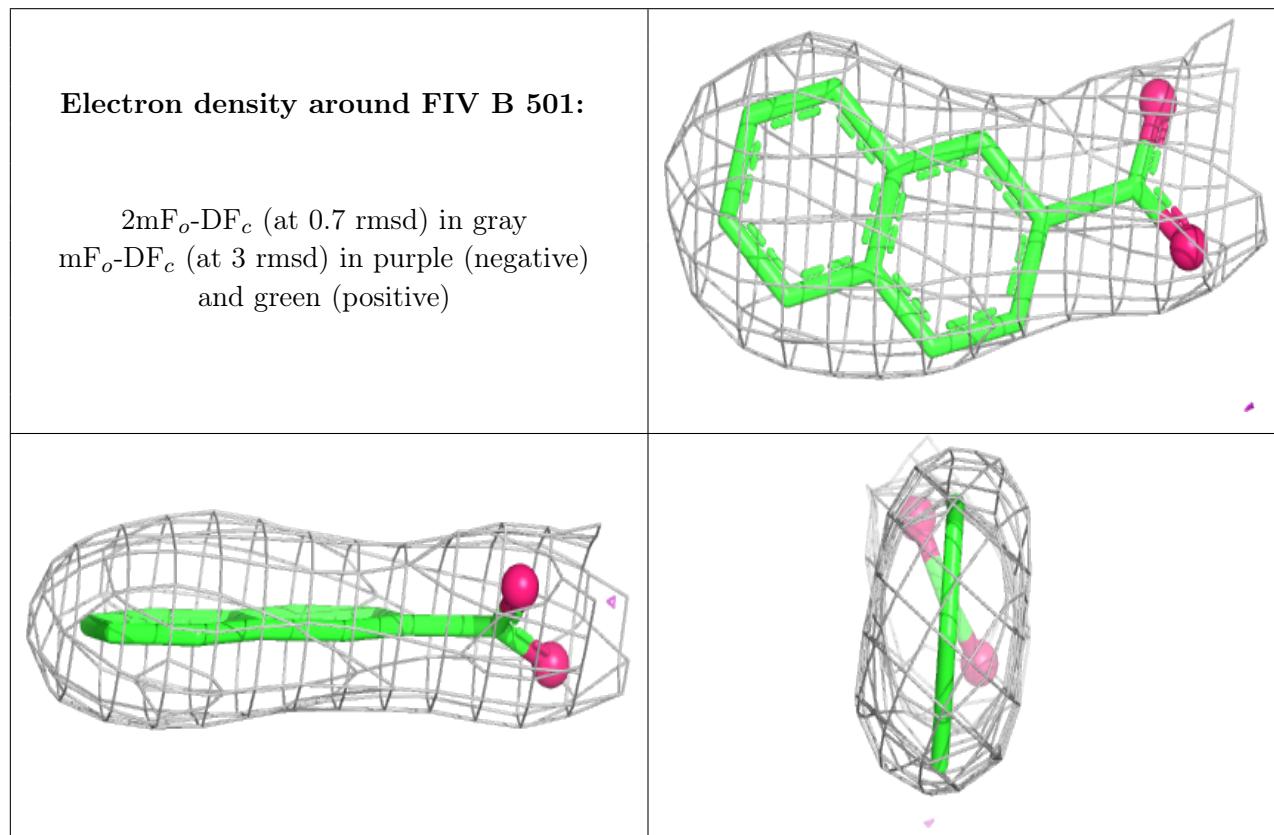
There are no monosaccharides in this entry.

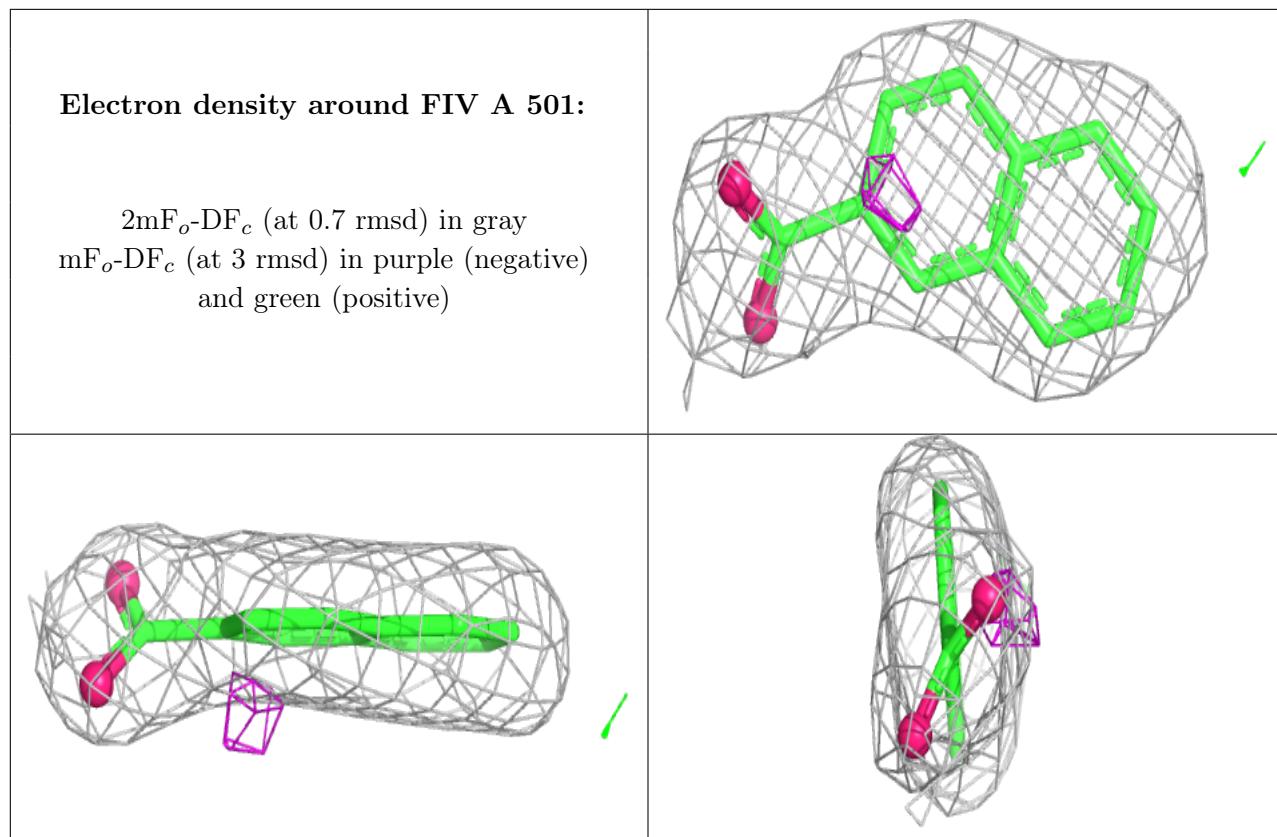
6.4 Ligands [\(i\)](#)

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
2	FIV	B	501	13/13	0.93	0.14	69,84,90,90	0
2	FIV	A	501	13/13	0.95	0.13	55,57,65,68	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.