

Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 05:27 PM JST

PDB ID	:	6LPQ
Title	:	Crystal structure of human D-2-hydroxyglutarate dehydrogenase in complex
		with D-malate (D-MAL)
Authors	:	Yang, J.; Zhu, H.; Ding, J.
Deposited on	:	2020-01-12
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 (i) 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:

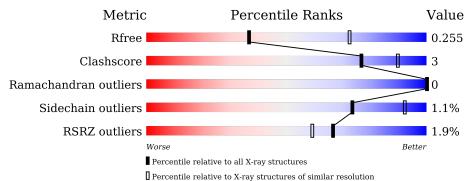
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	А	481	^{2%} 89%	7%	·
1	В	481	% 90%	6%	•



6LPQ

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7153 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 1	400	Total	С	Ν	0	\mathbf{S}	0	0	0
	466	3511	2228	618	646	19	0	0	0	
1	В	467	Total	С	Ν	0	S	0	0	0
	I B	467	3516	2230	613	654	19		0	0

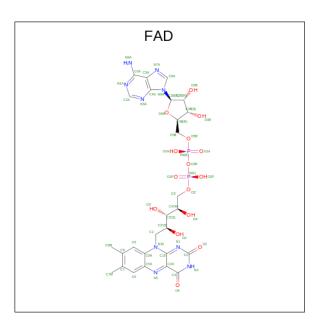
• Molecule 1 is a protein called D-2-hydroxyglutarate dehydrogenase, mitochondrial.

Chain	Residue	Modelled	Actual	Comment	Reference
А	47	GLY	-	expression tag	UNP Q8N465
А	48	PRO	-	expression tag	UNP Q8N465
А	49	GLY	-	expression tag	UNP Q8N465
А	50	SER	-	expression tag	UNP $Q8N465$
А	522	HIS	-	expression tag	UNP Q8N465
А	523	HIS	-	expression tag	UNP Q8N465
А	524	HIS	-	expression tag	UNP Q8N465
А	525	HIS	-	expression tag	UNP Q8N465
А	526	HIS	-	expression tag	UNP Q8N465
А	527	HIS	-	expression tag	UNP Q8N465
В	47	GLY	-	expression tag	UNP Q8N465
В	48	PRO	-	expression tag	UNP Q8N465
В	49	GLY	-	expression tag	UNP Q8N465
В	50	SER	-	expression tag	UNP Q8N465
В	522	HIS	-	expression tag	UNP Q8N465
В	523	HIS	-	expression tag	UNP Q8N465
В	524	HIS	-	expression tag	UNP Q8N465
В	525	HIS	-	expression tag	UNP Q8N465
В	526	HIS	-	expression tag	UNP Q8N465
В	527	HIS	-	expression tag	UNP Q8N465

There are 20 discrepancies between the modelled and reference sequences:

• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).





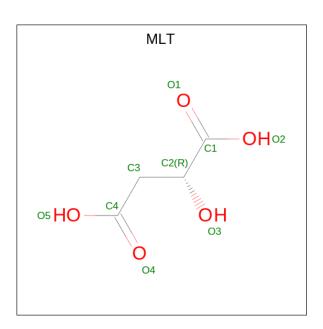
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	2 1	1	Total	С	Ν	Ο	Р	0	0
	1	53	27	9	15	2	0	0	
0	2 B	D 1	Total	С	Ν	Ο	Р	0	0
		1	53	27	9	15	2	U	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0

• Molecule 4 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



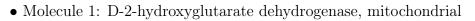


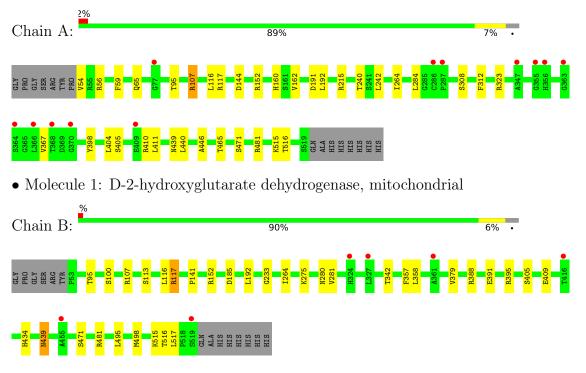
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 4 5 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 4 5 \end{array}$	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	72.61Å 94.57 Å 73.67 Å	Depositor
a, b, c, α , β , γ	90.00° 111.55° 90.00°	Depositor
Resolution (Å)	41.14 - 2.80	Depositor
Resolution (A)	41.14 - 2.80	EDS
% Data completeness	94.4 (41.14-2.80)	Depositor
(in resolution range)	95.0(41.14-2.80)	EDS
R _{merge}	0.30	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.71 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15rc1_3420	Depositor
P. P.	0.215 , 0.255	Depositor
R, R_{free}	0.215 , 0.255	DCC
R_{free} test set	1084 reflections $(4.97%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.9	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 42.2	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.041 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7153	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: ZN, MLT, FAD

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/3584	0.53	1/4869~(0.0%)	
1	В	0.27	0/3589	0.53	1/4877~(0.0%)	
All	All	0.27	0/7173	0.53	2/9746~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	117	ARG	CG-CD-NE	-6.19	98.80	111.80
1	А	410	ARG	CG-CD-NE	-5.24	100.79	111.80

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	А	3511	0	3511	19	0
1	В	3516	0	3504	17	0
2	А	53	0	31	3	0
2	В	53	0	31	4	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	9	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	9	0	4	2	0
All	All	7153	0	7084	42	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 3.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:95:THR:OG1	1:B:481:ARG:NH2	2.11	0.82
1:B:116:LEU:HD11	1:B:264:ILE:HD12	1.79	0.65
1:B:495:LEU:HA	1:B:498:MET:HE2	1.79	0.65
2:A:601:FAD:N5	4:A:603:MLT:H2	2.13	0.63
2:B:601:FAD:N5	4:B:603:MLT:H2	2.14	0.62
1:A:116:LEU:HD11	1:A:264:ILE:HD12	1.80	0.62
1:B:515:LYS:HB3	1:B:516:THR:HG22	1.81	0.61
1:B:100:SER:HB2	1:B:141:PRO:HG2	1.83	0.59
1:B:113:SER:O	1:B:117:ARG:HG3	2.03	0.58
1:A:515:LYS:HB3	1:A:516:THR:HG22	1.85	0.58
1:A:215:ARG:HB2	1:A:308:SER:HA	1.85	0.58
1:A:56:ARG:NH2	1:A:59:PHE:O	2.37	0.58
1:B:498:MET:HE3	1:B:517:LEU:HD22	1.87	0.56
1:A:56:ARG:NH1	1:A:144:ASP:OD1	2.39	0.55
1:A:160:HIS:CE1	1:A:162:VAL:HG22	2.44	0.53
1:B:405:SER:HB2	1:B:471:SER:HB3	1.90	0.52
1:B:357:PHE:CD2	1:B:358:LEU:HD12	2.47	0.50
2:B:601:FAD:H2'	2:B:601:FAD:N1	2.27	0.49
1:A:107:ARG:HG3	1:A:152:ARG:CZ	2.43	0.48
1:A:162:VAL:HG21	1:B:409:GLU:OE2	2.14	0.47
1:A:65:GLN:N	1:A:65:GLN:OE1	2.48	0.47
1:A:160:HIS:ND1	1:A:162:VAL:HG22	2.31	0.46
1:A:404:LEU:HD22	1:A:465:THR:HG21	1.97	0.46
1:B:107:ARG:HH12	1:B:152:ARG:NH1	2.14	0.46
1:A:240:THR:HG22	1:A:242:LEU:H	1.82	0.44
1:B:185:ASP:HA	1:B:275:LYS:HD3	1.99	0.43
1:A:398:TYR:N	1:A:446:ALA:O	2.49	0.43
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.68	0.43
2:B:601:FAD:H9	2:B:601:FAD:H1'2	1.80	0.43
1:B:117:ARG:HG2	1:B:233:GLY:HA3	2.01	0.43
1:A:411:LEU:HG	1:A:440:LEU:HB2	2.00	0.43
1:B:434:HIS:HB2	1:B:439:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:C	1:A:192:LEU:HD12	2.40	0.42
2:A:601:FAD:C4X	4:A:603:MLT:H2	2.49	0.42
2:B:601:FAD:C4X	4:B:603:MLT:H2	2.49	0.42
1:A:405:SER:HB2	1:A:471:SER:HB3	2.00	0.42
2:A:601:FAD:N1	2:A:601:FAD:H2'	2.35	0.42
1:B:281:VAL:HG21	1:B:379:VAL:HG13	2.02	0.41
1:A:284:LEU:HD13	1:A:367:VAL:HG21	2.02	0.41
1:A:95:THR:OG1	1:A:481:ARG:NH2	2.52	0.41
1:B:388:ARG:HA	1:B:391:GLU:OE2	2.21	0.41
1:B:280:ASN:HB2	1:B:342:THR:OG1	2.21	0.40

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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	А	464/481~(96%)	457 (98%)	7~(2%)	0	100 100
1	В	465/481 (97%)	454 (98%)	11 (2%)	0	100 100
All	All	929/962~(97%)	911 (98%)	18 (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	А	375/397~(94%)	370~(99%)	5 (1%)	69 91
1	В	377/397~(95%)	374 (99%)	3 (1%)	81 94
All	All	752/794~(95%)	744 (99%)	8 (1%)	73 92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	54	VAL
1	А	107	ARG
1	А	117	ARG
1	А	312	PHE
1	А	439	ASN
1	В	192	LEU
1	В	395	ARG
1	В	439	ASN

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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



Mol	Type	Chain	Res	es Link Bond lengths				Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	FAD	А	601	-	$53,\!58,\!58$	0.48	0	68,89,89	0.52	2 (2%)
2	FAD	В	601	-	53,58,58	0.49	0	68,89,89	0.51	1 (1%)
4	MLT	В	603	3	8,8,8	1.45	1 (12%)	10,10,10	1.97	3 (30%)
4	MLT	А	603	3	8,8,8	1.15	1 (12%)	10,10,10	1.96	3 (30%)

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).

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	FAD	А	601	-	-	9/30/50/50	0/6/6/6
2	FAD	В	601	-	-	9/30/50/50	0/6/6/6
4	MLT	В	603	3	-	4/8/8/8	-
4	MLT	А	603	3	-	5/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	В	603	MLT	C2-C1	2.34	1.55	1.52
4	А	603	MLT	C2-C1	2.04	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	603	MLT	O2-C1-C2	3.79	121.05	112.72
4	В	603	MLT	O2-C1-C2	3.78	121.01	112.72
4	В	603	MLT	C2-C3-C4	3.26	120.21	112.13
4	А	603	MLT	C2-C3-C4	3.15	119.93	112.13
4	В	603	MLT	O2-C1-O1	-2.96	117.36	124.09
4	А	603	MLT	O2-C1-O1	-2.76	117.83	124.09
2	А	601	FAD	C5A-C6A-N6A	2.29	123.84	120.35
2	В	601	FAD	C5A-C6A-N6A	2.27	123.81	120.35
2	А	601	FAD	P-O3P-PA	-2.08	125.69	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	А	601	FAD	N10-C1'-C2'-O2'
2	А	601	FAD	N10-C1'-C2'-C3'
2	А	601	FAD	C2'-C3'-C4'-O4'
2	А	601	FAD	O3'-C3'-C4'-O4'
2	А	601	FAD	C3'-C4'-C5'-O5'
2	А	601	FAD	O4'-C4'-C5'-O5'
2	В	601	FAD	N10-C1'-C2'-O2'
2	В	601	FAD	N10-C1'-C2'-C3'
2	В	601	FAD	C2'-C3'-C4'-O4'
2	В	601	FAD	C2'-C3'-C4'-C5'
2	В	601	FAD	O3'-C3'-C4'-O4'
2	В	601	FAD	C3'-C4'-C5'-O5'
2	В	601	FAD	O4'-C4'-C5'-O5'
2	А	601	FAD	O3'-C3'-C4'-C5'
2	В	601	FAD	O3'-C3'-C4'-C5'
2	А	601	FAD	C2'-C3'-C4'-C5'
2	А	601	FAD	C2'-C1'-N10-C10
2	В	601	FAD	C2'-C1'-N10-C10
4	В	603	MLT	C2-C3-C4-O5
4	А	603	MLT	O2-C1-C2-C3
4	А	603	MLT	C2-C3-C4-O4
4	А	603	MLT	C2-C3-C4-O5
4	В	603	MLT	C2-C3-C4-O4
4	А	603	MLT	O2-C1-C2-O3
4	А	603	MLT	O1-C1-C2-C3
4	В	603	MLT	O1-C1-C2-C3
4	В	603	MLT	O2-C1-C2-C3

There are no ring outliers.

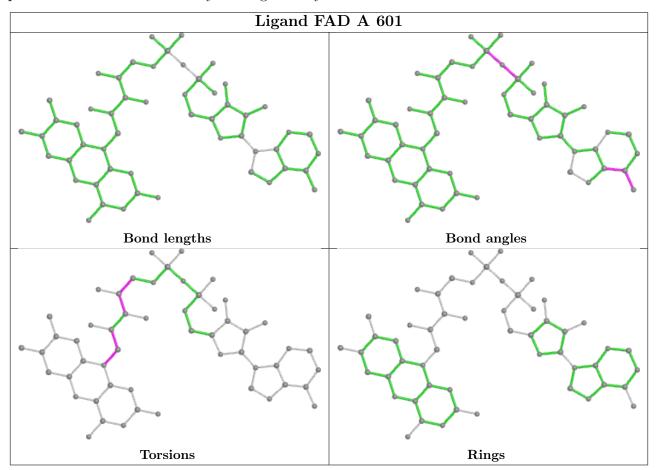
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	601	FAD	3	0
2	В	601	FAD	4	0
4	В	603	MLT	2	0
4	А	603	MLT	2	0

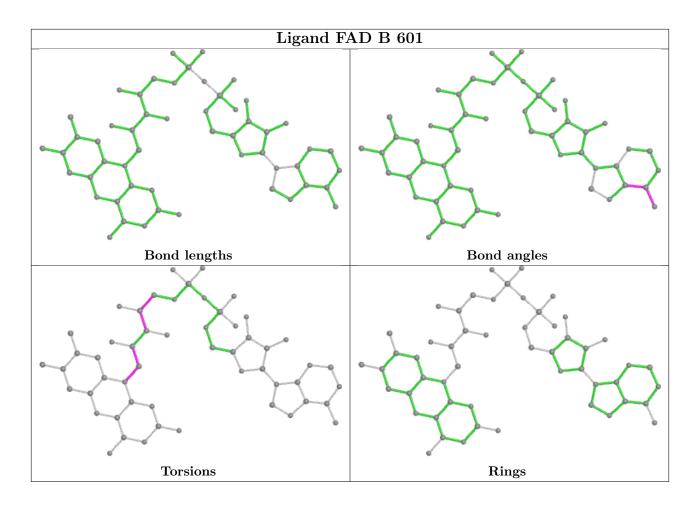
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be



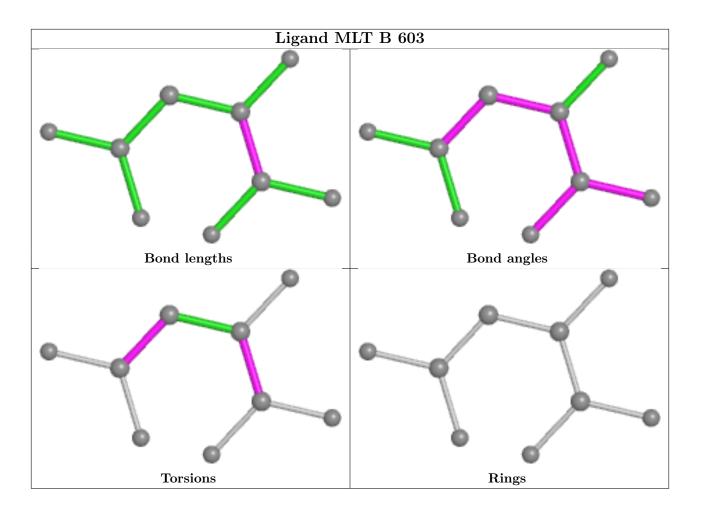
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



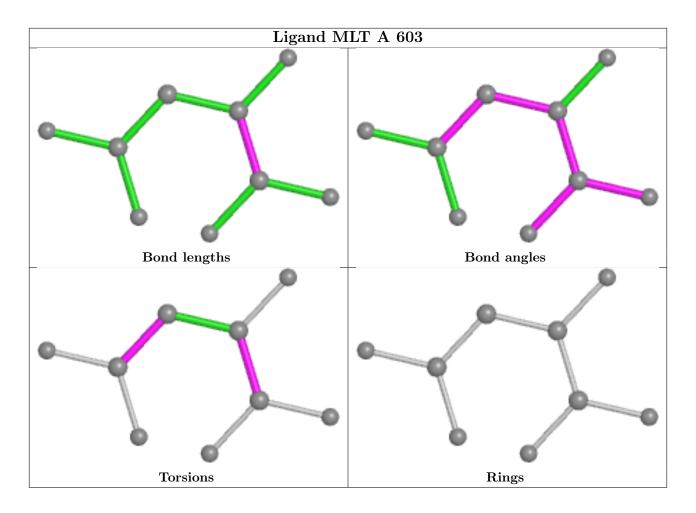












5.7 Other polymers (i)

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 (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	466/481~(96%)	0.05	12 (2%) 56 46	20, 32, 51, 68	0
1	В	$467/481 \ (97\%)$	-0.12	6 (1%) 77 72	18, 28, 47, 61	0
All	All	933/962~(96%)	-0.03	18 (1%) 66 59	18, 30, 49, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	366	LEU	2.9
1	А	370	GLY	2.9
1	В	327	LEU	2.8
1	А	287	PRO	2.8
1	А	363	GLY	2.6
1	В	416	THR	2.5
1	А	286	CYS	2.5
1	В	361	ALA	2.5
1	А	356	HIS	2.4
1	А	364	SER	2.4
1	А	77	GLY	2.3
1	А	368	THR	2.2
1	В	324	HIS	2.2
1	А	355	GLY	2.2
1	А	347	ALA	2.2
1	В	519	SER	2.1
1	В	455	ALA	2.1
1	А	409	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 monosaccharides in this entry.

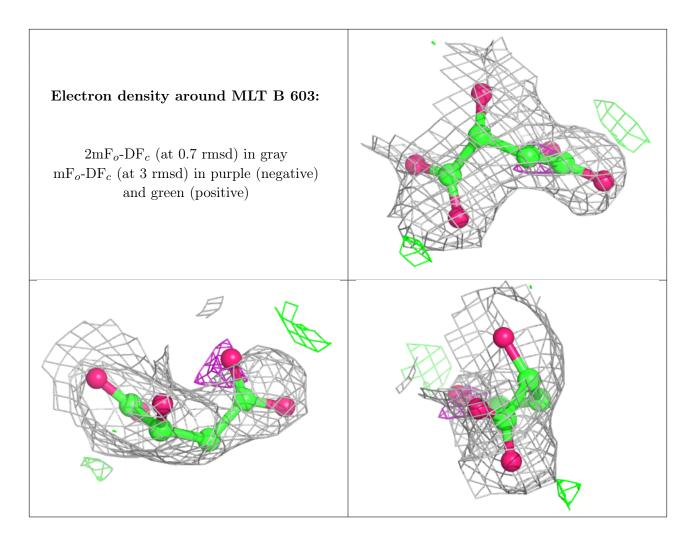
6.4 Ligands (i)

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

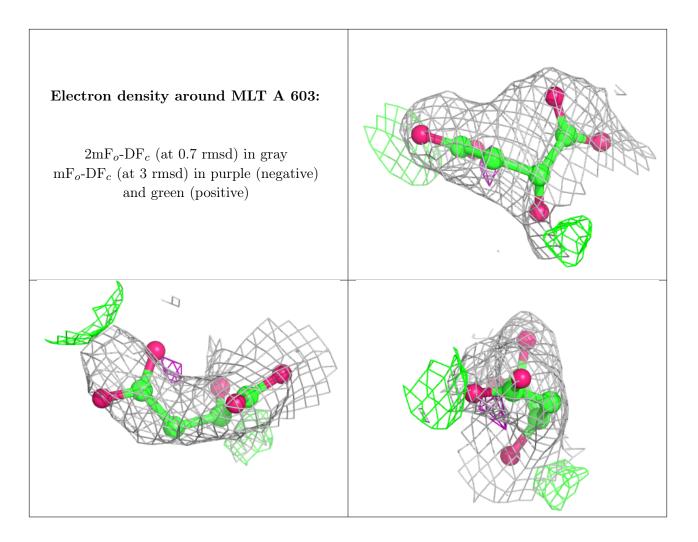
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MLT	В	603	9/9	0.93	0.20	$26,\!31,\!33,\!35$	0
4	MLT	А	603	9/9	0.95	0.21	31,33,41,43	0
2	FAD	А	601	53/53	0.95	0.17	20,27,34,38	0
2	FAD	В	601	53/53	0.97	0.16	18,24,32,33	0
3	ZN	А	602	1/1	0.99	0.14	27,27,27,27	0
3	ZN	В	602	1/1	0.99	0.09	28,28,28,28	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.

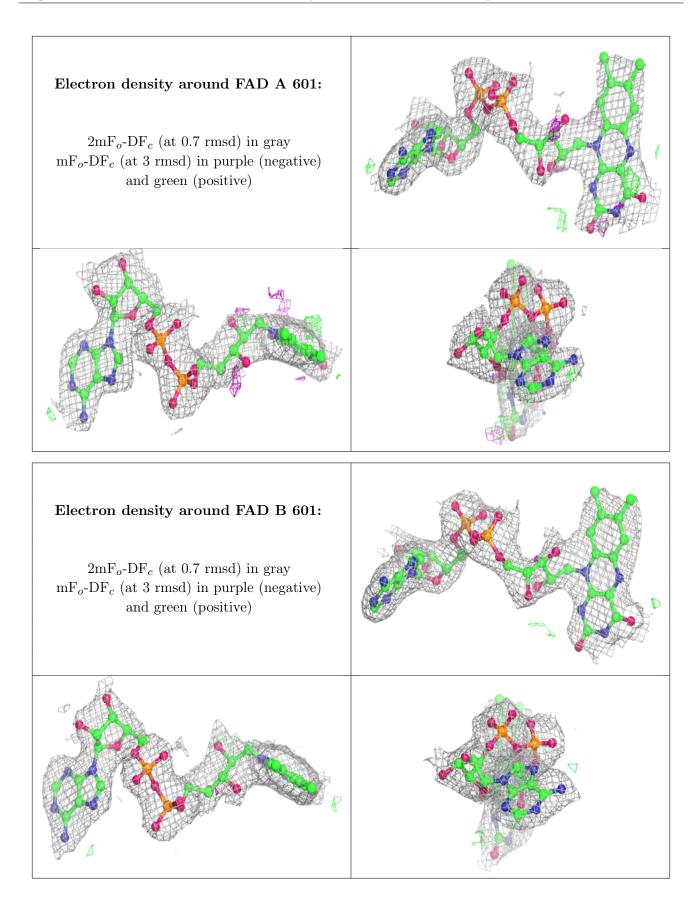




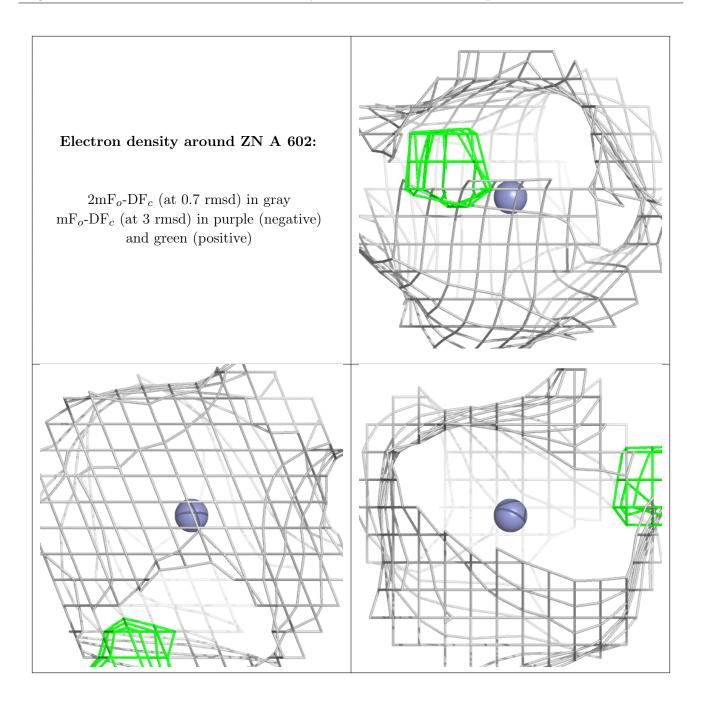




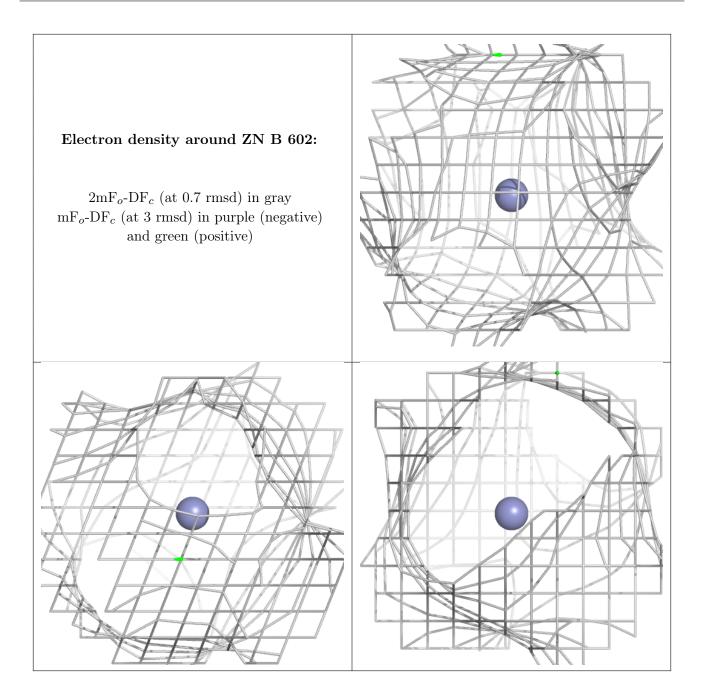












6.5 Other polymers (i)

There are no such residues in this entry.

