



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 04:22 PM EST

PDB ID : 7LUB  
Title : Crystal structure of recombinant human fumarase in complex with D-2-amin  
o-3-phosphono-propionic acid  
Authors : Cardoso, I.A.; Nonato, M.C.  
Deposited on : 2021-02-21  
Resolution : 2.15 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](mailto: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.

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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 : 2.26  
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) : 2.26

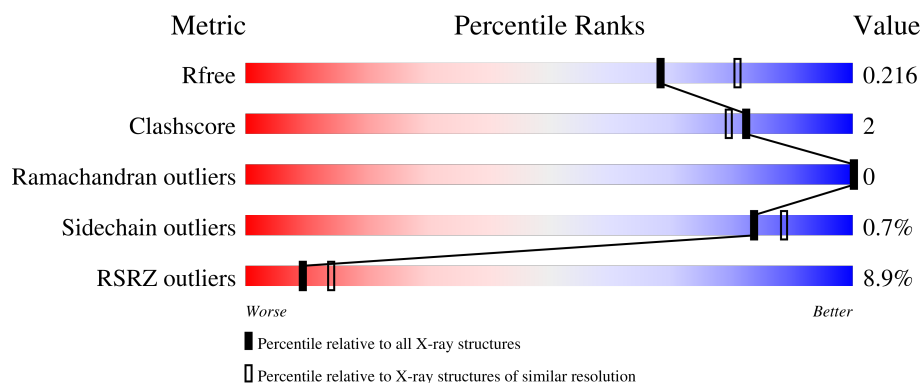
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	466	<div> <div>10%</div> <div>92%</div> <div>6%</div> </div>
1	B	466	<div> <div>8%</div> <div>93%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

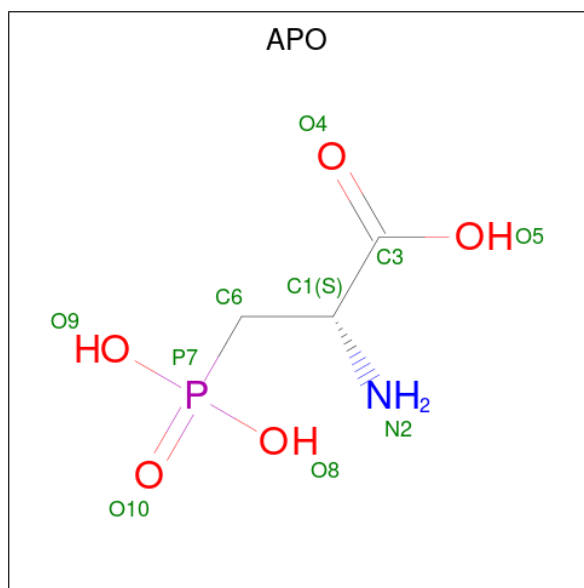
There are 4 unique types of molecules in this entry. The entry contains 7191 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fumarate hydratase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	2	0
			3422	2154	597	649	22			
1	B	462	Total	C	N	O	S	0	1	0
			3425	2155	595	653	22			

- Molecule 2 is D-2-AMINO-3-PHOSPHONO-PROPIONIC ACID (three-letter code: APO) (formula:  $C_3H_8NO_5P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	3	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



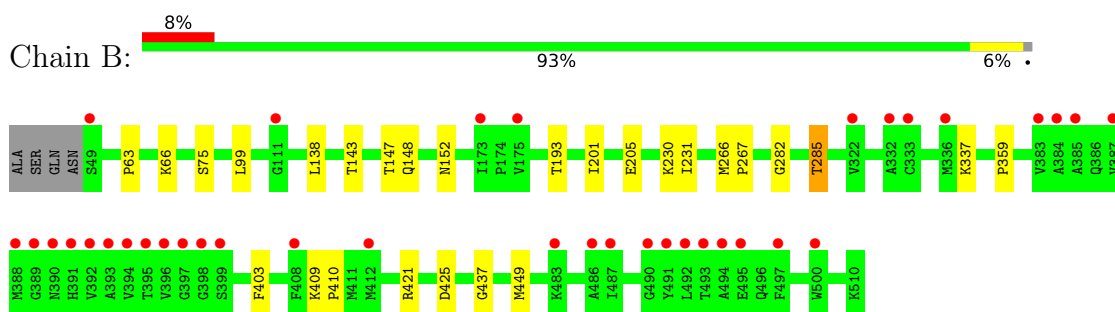
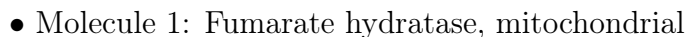
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	1
			158	158		
4	B	141	Total	O	0	1
			142	142		



- Molecule 1: Fumarate hydratase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.90Å 190.90Å 116.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.15 49.80 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.85-2.15) 100.0 (49.80-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.186 , 0.209 0.193 , 0.216	Depositor DCC
$R_{free}$ test set	3399 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, APO

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	0.66	0/3481	0.72	0/4721
1	B	0.67	0/3487	0.72	0/4738
All	All	0.66	0/6968	0.72	0/9459

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

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	3422	0	3386	21	0
1	B	3425	0	3388	15	0
2	A	10	0	5	1	0
2	B	10	0	5	0	0
3	A	24	0	32	0	0
4	A	158	0	0	0	0
4	B	142	0	0	0	0
All	All	7191	0	6816	34	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 (34) 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:230:LYS:HE2	1:A:355:GLU:OE1	1.91	0.70
1:B:75:SER:OG	1:B:148:GLN:HG3	1.95	0.66
1:A:456:VAL:CG2	1:A:482:LEU:HD22	2.26	0.65
1:B:138:LEU:HD13	1:B:148:GLN:HB3	1.80	0.63
1:B:409:LYS:HB2	1:B:410:PRO:HD3	1.87	0.57
1:A:409:LYS:HB2	1:A:410:PRO:HD3	1.86	0.57
1:A:456:VAL:HG13	1:A:459:LEU:HD12	1.88	0.56
1:B:143[A]:THR:HG21	1:B:147:THR:HB	1.89	0.54
1:B:421:ARG:NH1	1:B:425:ASP:OD2	2.40	0.53
1:A:188:ASN:OD1	2:A:601:APO:HC1	2.12	0.50
1:A:403:PHE:O	1:B:337:LYS:NZ	2.38	0.50
1:A:230:LYS:CE	1:A:355:GLU:OE1	2.59	0.50
1:B:99:LEU:HD13	1:B:193:THR:HG21	1.93	0.50
1:A:397:GLY:HA3	1:A:411:MET:HE1	1.95	0.49
1:B:266:MET:N	1:B:267:PRO:CD	2.76	0.48
1:A:266:MET:N	1:A:267:PRO:CD	2.77	0.47
1:A:337:LYS:NZ	1:B:403:PHE:O	2.42	0.47
1:A:484:GLU:O	1:A:488:GLU:HG2	2.15	0.46
1:A:99:LEU:HD13	1:A:193:THR:HG21	1.97	0.46
1:A:456:VAL:HG21	1:A:482:LEU:HD22	1.97	0.45
1:B:282:GLY:O	1:B:285:THR:HG22	2.16	0.45
1:A:282:GLY:O	1:A:285:THR:HG22	2.16	0.45
1:B:231:ILE:HB	1:B:449:MET:HA	1.98	0.45
1:A:453:LEU:O	1:A:456:VAL:HG23	2.17	0.44
1:A:140:VAL:HG21	1:A:414[A]:LYS:HD2	1.99	0.44
1:B:143[A]:THR:HG22	1:B:148:GLN:OE1	2.18	0.44
1:B:201:ILE:HG23	1:B:205:GLU:HG3	2.00	0.43
1:A:456:VAL:HG22	1:A:482:LEU:HD13	2.01	0.42
1:A:63:PRO:HB2	1:A:66:LYS:HG2	2.01	0.42
1:B:359:PRO:HG3	1:B:437:GLY:HA3	2.01	0.42
1:A:82:GLY:HA3	1:A:86:GLU:HG3	2.01	0.42
1:B:63:PRO:HB2	1:B:66:LYS:HG2	2.02	0.41
1:A:456:VAL:CG2	1:A:482:LEU:HD13	2.51	0.40
1:A:191:PHE:HB3	1:A:192:PRO:HD3	2.02	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	454/466 (97%)	441 (97%)	13 (3%)	0	100	100
1	B	461/466 (99%)	445 (96%)	16 (4%)	0	100	100
All	All	915/932 (98%)	886 (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	355/374 (95%)	353 (99%)	2 (1%)	86	90
1	B	356/374 (95%)	353 (99%)	3 (1%)	81	86
All	All	711/748 (95%)	706 (99%)	5 (1%)	84	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	285	THR
1	B	152	ASN
1	B	230	LYS
1	B	285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	APO	B	601	-	5,9,9	2.09	3 (60%)	6,13,13	1.10	0
3	GOL	A	604[B]	-	5,5,5	0.09	0	5,5,5	0.22	0
3	GOL	A	604[A]	-	5,5,5	0.09	0	5,5,5	0.25	0
3	GOL	A	602	-	5,5,5	0.14	0	5,5,5	0.38	0
3	GOL	A	603	-	5,5,5	0.08	0	5,5,5	0.24	0
2	APO	A	601	-	5,9,9	3.48	4 (80%)	6,13,13	2.49	2 (33%)

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	APO	B	601	-	-	2/4/9/9	-
3	GOL	A	604[B]	-	-	2/4/4/4	-
3	GOL	A	604[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	602	-	-	2/4/4/4	-
3	GOL	A	603	-	-	2/4/4/4	-
2	APO	A	601	-	-	3/4/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	APO	P7-O10	6.04	1.62	1.50
2	A	601	APO	P7-C6	3.16	1.82	1.78
2	B	601	APO	P7-O8	2.70	1.61	1.54
2	A	601	APO	P7-O8	2.69	1.61	1.54
2	B	601	APO	P7-C6	2.66	1.81	1.78
2	B	601	APO	P7-O9	2.54	1.60	1.54
2	A	601	APO	P7-O9	-2.49	1.49	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	APO	O10-P7-C6	-4.51	103.18	111.54
2	A	601	APO	O9-P7-C6	2.88	113.79	106.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

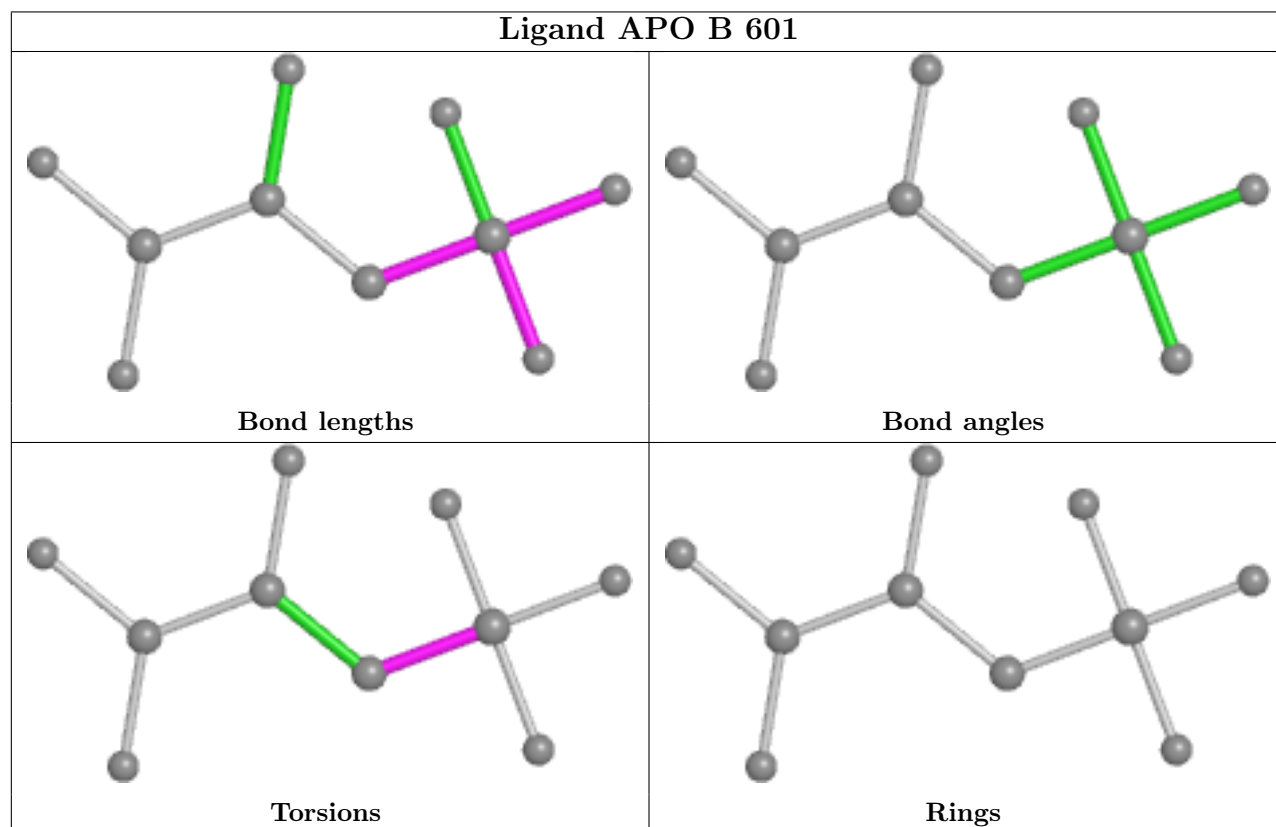
Mol	Chain	Res	Type	Atoms
2	A	601	APO	C1-C6-P7-O8
2	A	601	APO	C1-C6-P7-O9
2	A	601	APO	C1-C6-P7-O10
3	A	602	GOL	O1-C1-C2-C3
3	A	603	GOL	O1-C1-C2-O2
3	A	604[B]	GOL	O1-C1-C2-C3
3	A	603	GOL	O1-C1-C2-C3
3	A	602	GOL	O1-C1-C2-O2
3	A	604[B]	GOL	O1-C1-C2-O2
3	A	604[A]	GOL	O1-C1-C2-O2
2	B	601	APO	C1-C6-P7-O8
2	B	601	APO	C1-C6-P7-O10
3	A	604[A]	GOL	C1-C2-C3-O3

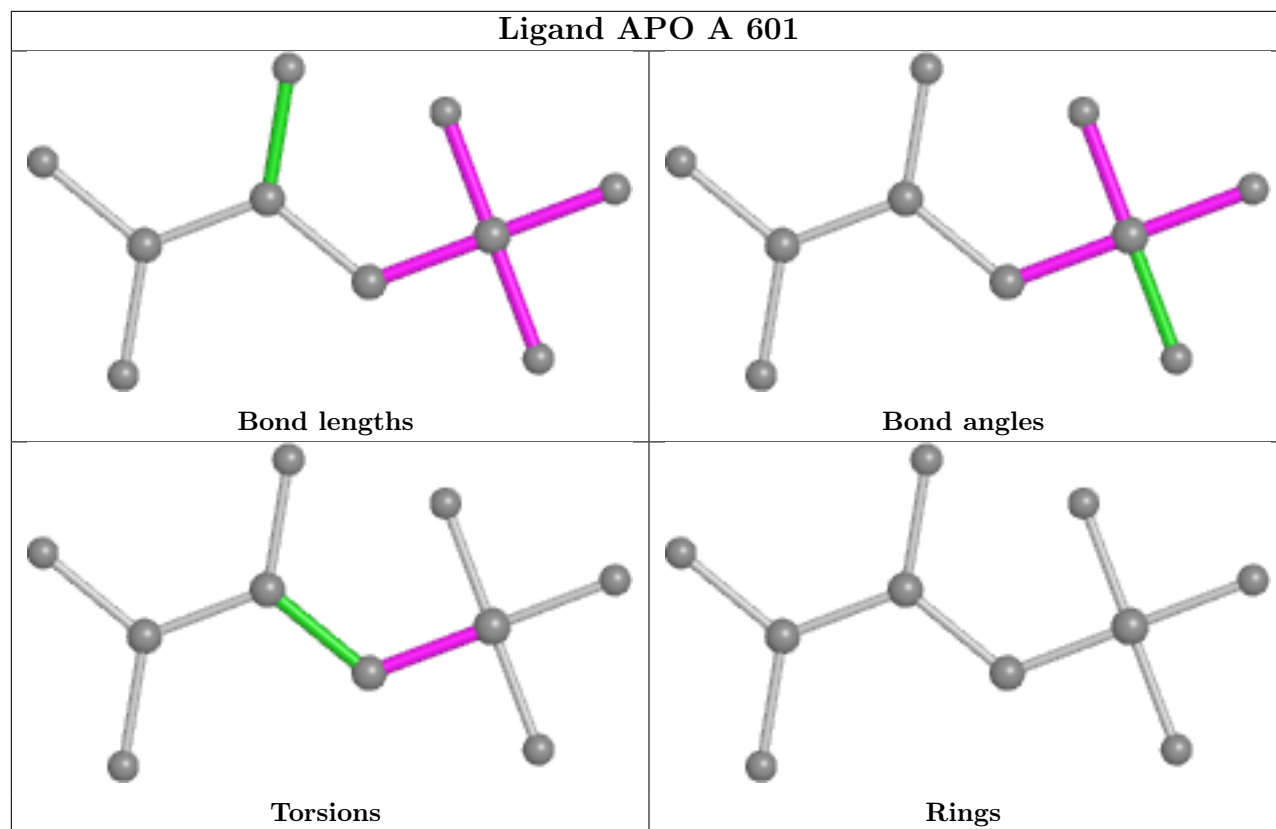
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	APO	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/466 (98%)	0.30	45 (9%) <b>7</b> <b>11</b>	30, 47, 93, 111	0
1	B	462/466 (99%)	0.27	37 (8%) <b>12</b> <b>17</b>	33, 50, 75, 86	0
All	All	922/932 (98%)	0.28	82 (8%) <b>9</b> <b>14</b>	30, 49, 82, 111	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	5.6
1	A	500	TRP	5.6
1	B	392	VAL	5.1
1	A	490	GLY	5.0
1	A	497	PHE	4.9
1	B	497	PHE	4.3
1	A	396	VAL	4.3
1	A	394	VAL	4.3
1	B	396	VAL	4.2
1	A	493	THR	4.1
1	A	392	VAL	4.1
1	A	491	TYR	3.9
1	A	480	SER	3.9
1	A	393	ALA	3.8
1	A	462	HIS	3.8
1	B	394	VAL	3.8
1	B	487	ILE	3.7
1	A	395	THR	3.6
1	B	491	TYR	3.6
1	B	494	ALA	3.5
1	B	500	TRP	3.5
1	B	492	LEU	3.5
1	B	393	ALA	3.5
1	A	472	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	387	VAL	3.3
1	A	397	GLY	3.3
1	B	395	THR	3.2
1	A	492	LEU	3.2
1	B	486	ALA	3.2
1	B	388	MET	3.1
1	B	483	LYS	3.1
1	A	48	ASN	3.1
1	A	487	ILE	3.0
1	B	391	HIS	3.0
1	B	385	ALA	3.0
1	B	333	CYS	3.0
1	B	397	GLY	2.9
1	A	465	TYR	2.9
1	B	49	SER	2.8
1	A	408	PHE	2.8
1	A	399	SER	2.8
1	A	389	GLY	2.8
1	B	389	GLY	2.8
1	A	387	VAL	2.8
1	A	385	ALA	2.8
1	A	388	MET	2.8
1	A	322	VAL	2.8
1	B	336	MET	2.7
1	A	49	SER	2.7
1	A	407	VAL	2.7
1	B	495	GLU	2.7
1	B	383	VAL	2.6
1	A	495	GLU	2.6
1	A	458	ALA	2.6
1	A	468	ALA	2.6
1	B	493	THR	2.6
1	B	173	ILE	2.5
1	A	412	MET	2.5
1	B	384	ALA	2.5
1	A	460	ASN	2.5
1	A	50	PHE	2.5
1	A	461	PRO	2.4
1	A	400	ASN	2.3
1	A	414[A]	LYS	2.3
1	A	390	ASN	2.3
1	B	399	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	490	GLY	2.2
1	B	111	GLY	2.2
1	A	383	VAL	2.2
1	B	322	VAL	2.2
1	A	485	THR	2.2
1	A	398	GLY	2.2
1	B	408	PHE	2.2
1	A	405	LEU	2.1
1	B	390	ASN	2.1
1	B	332	ALA	2.1
1	A	411	MET	2.1
1	B	175	VAL	2.1
1	B	398	GLY	2.1
1	B	412	MET	2.0
1	A	54	TYR	2.0
1	A	391	HIS	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.

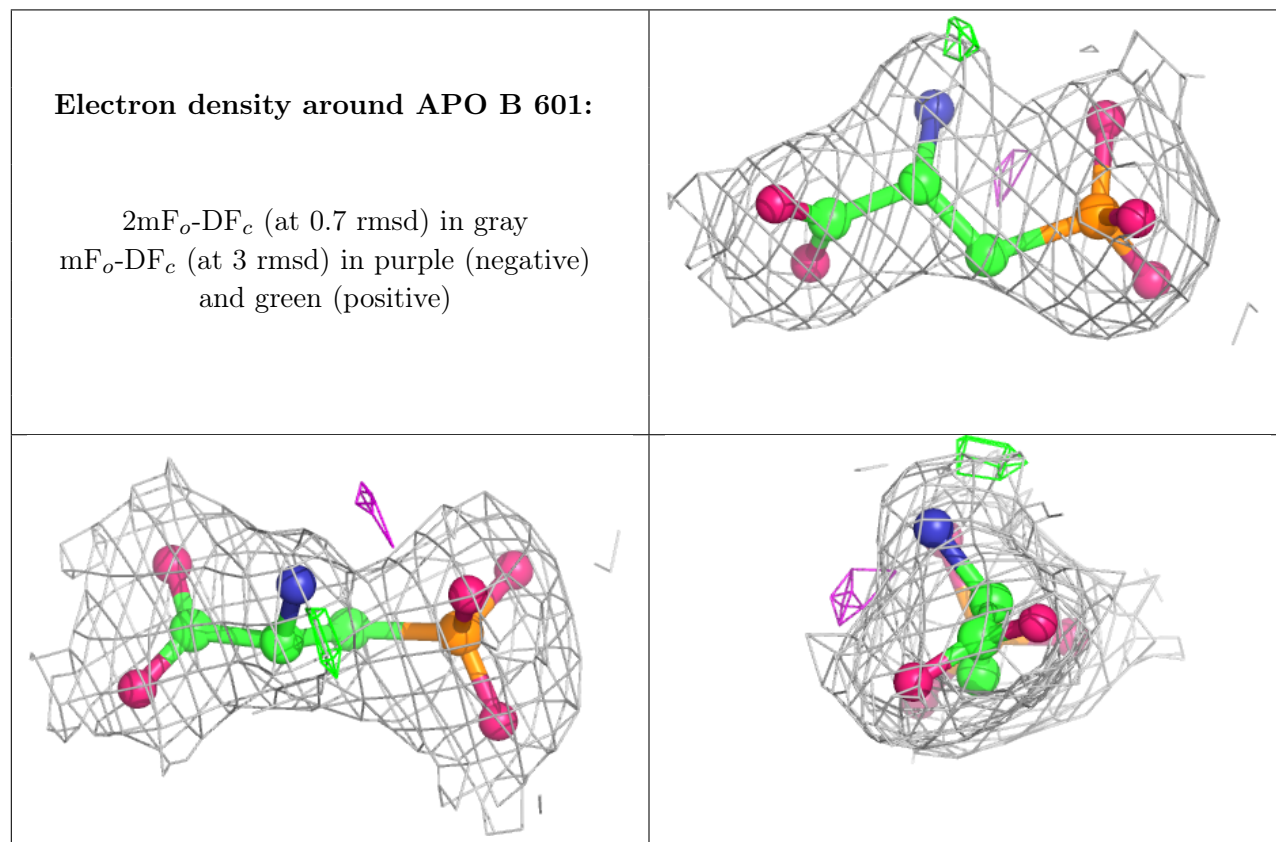
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	604[A]	6/6	0.83	0.24	71,77,77,77	6
3	GOL	A	604[B]	6/6	0.83	0.24	51,55,55,55	6
3	GOL	A	603	6/6	0.93	0.14	48,50,51,52	0
3	GOL	A	602	6/6	0.94	0.11	51,55,62,62	0
2	APO	B	601	10/10	0.96	0.11	52,55,57,61	0
2	APO	A	601	10/10	0.98	0.10	43,47,49,49	0

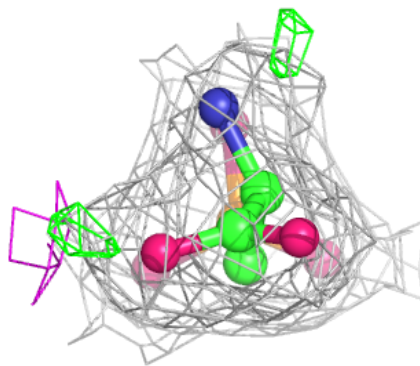
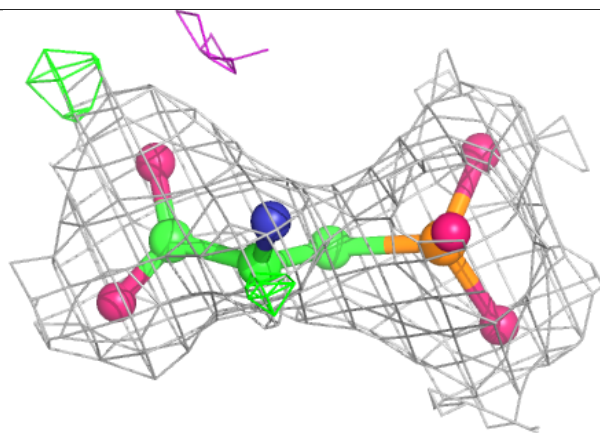
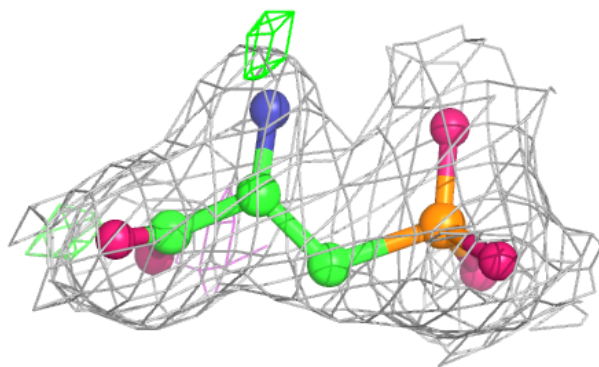


The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around APO A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.