



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 02:26 am BST

PDB ID : 6QVG / pdb\_00006qvg  
Title : Human SHMT2 in complex with lometrexol  
Authors : Scaletti, E.; Jemth, A.S.; Helleday, T.; Stenmark, P.  
Deposited on : 2019-03-01  
Resolution : 2.32 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

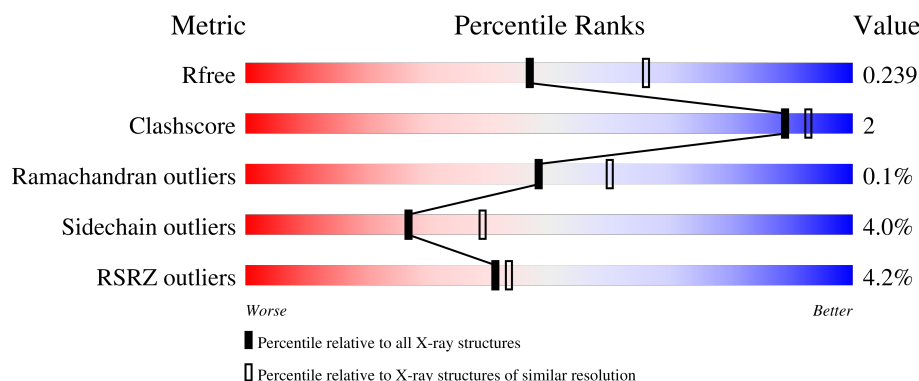
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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))
$R_{free}$	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	504	<div> <div>3%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>
1	B	504	<div> <div>5%</div> <div>84%</div> <div>6%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLY	A	601	-	X	-	-

## 2 Entry composition [i](#)

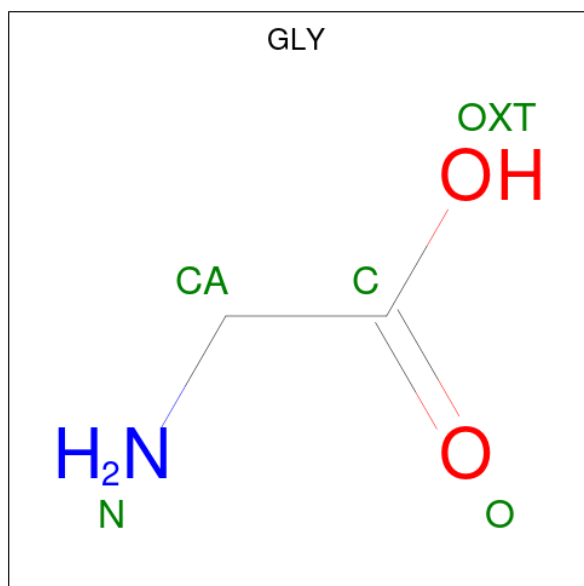
There are 9 unique types of molecules in this entry. The entry contains 7607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	2	0
			3563	2245	643	659	16			
1	B	454	Total	C	N	O	S	0	0	0
			3546	2236	636	658	16			

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula:  $C_2H_5NO_2$ ).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).

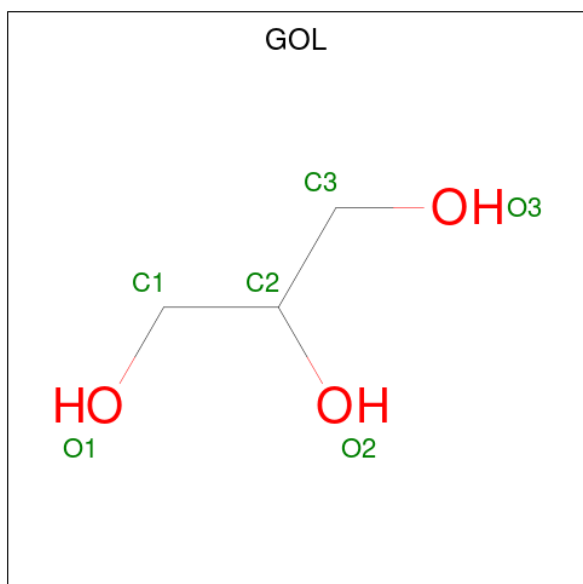


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

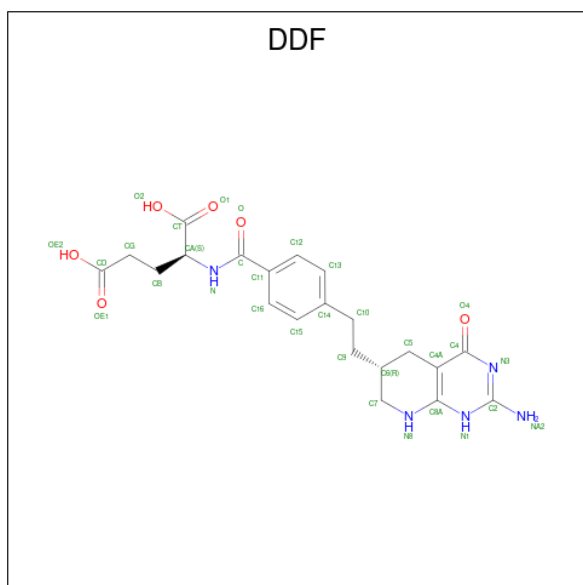
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



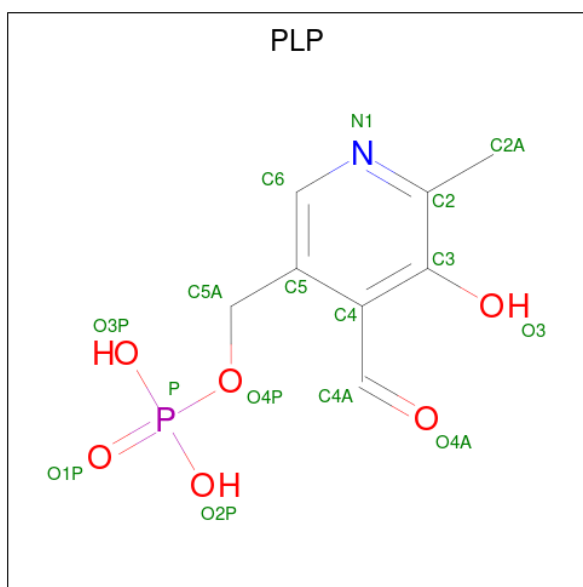
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 5,10-DIDEAZATETRAHYDROFOLIC ACID (CCD ID: DDF) (formula:  $C_{21}H_{25}N_5O_6$ ) (labeled as "Ligand of Interest" by depositor).



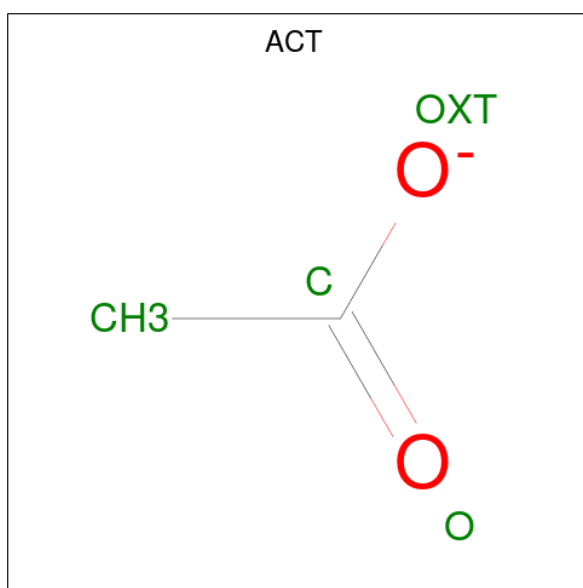
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			32	21	5	6		
6	B	1	Total	C	N	O	0	0
			32	21	5	6		

- Molecule 7 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
7	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

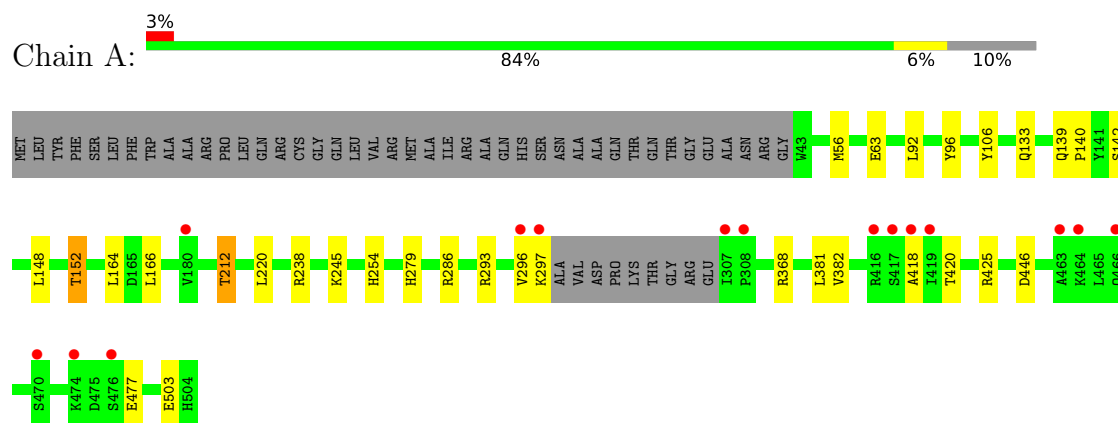
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	212	Total 212	O 212	0	0
9	B	156	Total 156	O 156	0	0



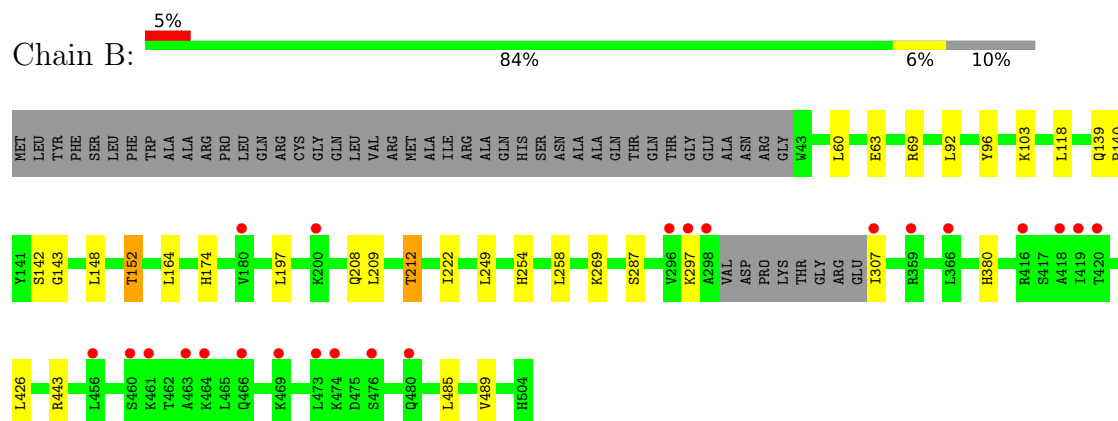
### 3 Residue-property plots [i](#)

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: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.81Å 158.81Å 208.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	208.26 – 2.32 137.53 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.7 (208.26-2.32) 99.7 (137.53-2.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.199 , 0.236 0.206 , 0.239	Depositor DCC
$R_{free}$ test set	3369 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, GOL, PEG, NA, ACT, DDF

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	0.48	0/3634	0.73	1/4911 (0.0%)
1	B	0.46	0/3617	0.73	0/4890
All	All	0.47	0/7251	0.73	1/9801 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	LEU	CA-CB-CG	5.79	128.61	115.30

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	3563	0	3559	17	0
1	B	3546	0	3540	12	0
2	A	5	0	2	0	0
3	A	14	0	20	0	0
4	A	1	0	0	0	0
5	A	12	0	16	1	0
6	A	32	0	23	0	0
6	B	32	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	15	0	6	0	0
7	B	15	0	6	1	0
8	B	4	0	3	0	0
9	A	212	0	0	2	0
9	B	156	0	0	1	0
All	All	7607	0	7198	26	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 (26) 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:212:THR:HG21	9:A:824:HOH:O	1.82	0.77
1:A:293[B]:ARG:HH11	1:A:293[B]:ARG:HB3	1.57	0.69
1:B:212:THR:HG21	9:B:784:HOH:O	1.93	0.68
1:A:148:LEU:O	1:A:152:THR:HG23	2.01	0.61
1:A:368:ARG:NH1	1:A:446:ASP:OD1	2.42	0.53
1:B:143:GLY:HA3	7:B:603:PLP:H5A2	1.92	0.51
1:A:279:HIS:CD2	1:A:286:ARG:HA	2.46	0.51
1:A:92:LEU:HD23	1:B:63:GLU:HG2	1.93	0.50
1:A:56:MET:HE2	1:B:118:LEU:HD23	1.95	0.48
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.94	0.48
1:A:293[A]:ARG:HG3	1:A:293[A]:ARG:HH11	1.78	0.48
1:A:420:THR:HA	5:A:605:GOL:H2	1.95	0.48
1:A:296:VAL:HG22	1:A:297:LYS:HG2	1.96	0.48
1:A:133:GLN:HE21	1:A:293[B]:ARG:NH2	2.12	0.47
1:A:293[B]:ARG:HH11	1:A:293[B]:ARG:CB	2.23	0.47
1:B:148:LEU:O	1:B:152:THR:HG23	2.15	0.47
1:B:258:LEU:HD11	1:B:380:HIS:HB3	1.99	0.45
1:B:208:GLN:O	1:B:212:THR:HB	2.17	0.44
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.52	0.44
1:B:485:LEU:O	1:B:489:VAL:HG23	2.18	0.44
1:A:381:LEU:C	1:A:381:LEU:HD12	2.38	0.43
1:B:222:ILE:HG12	1:B:249:LEU:HD23	2.02	0.42
1:A:279:HIS:CD2	1:A:279:HIS:H	2.38	0.41
1:B:139:GLN:N	1:B:140:PRO:CD	2.84	0.40
1:A:139:GLN:N	1:A:140:PRO:CD	2.84	0.40
1:A:425[B]:ARG:NH2	9:A:702:HOH:O	2.53	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	451/504 (90%)	438 (97%)	12 (3%)	1 (0%)	44	54
1	B	450/504 (89%)	434 (96%)	16 (4%)	0	100	100
All	All	901/1008 (89%)	872 (97%)	28 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	418	ALA

### 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	376/413 (91%)	363 (96%)	13 (4%)	31	44
1	B	374/413 (91%)	357 (96%)	17 (4%)	23	34
All	All	750/826 (91%)	720 (96%)	30 (4%)	27	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	A	106	TYR
1	A	142	SER
1	A	152	THR
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	166	LEU
1	A	212	THR
1	A	238	ARG
1	A	245	LYS
1	A	254	HIS
1	A	382	VAL
1	A	477	GLU
1	A	503	GLU
1	B	60	LEU
1	B	69	ARG
1	B	96	TYR
1	B	103	LYS
1	B	142	SER
1	B	152	THR
1	B	164	LEU
1	B	197	LEU
1	B	209	LEU
1	B	212	THR
1	B	254	HIS
1	B	269	LYS
1	B	287	SER
1	B	297	LYS
1	B	307	ILE
1	B	426	LEU
1	B	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	279	HIS
1	B	487	GLN
1	B	491	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
6	DDF	B	602	-	33,34,34	2.82	14 (42%)	34,47,47	2.45	13 (38%)
3	PEG	A	603	-	6,6,6	0.48	0	5,5,5	0.45	0
2	GLY	A	601	-	4,4,4	1.16	1 (25%)	3,4,4	1.87	1 (33%)
6	DDF	A	607	-	33,34,34	3.11	18 (54%)	34,47,47	2.51	11 (32%)
8	ACT	B	601	-	3,3,3	0.78	0	3,3,3	0.70	0
5	GOL	A	606	-	5,5,5	0.38	0	5,5,5	0.34	0
7	PLP	A	608	1	15,15,16	2.70	3 (20%)	20,22,23	2.10	4 (20%)
5	GOL	A	605	-	5,5,5	0.44	0	5,5,5	0.67	0
7	PLP	B	603	1	15,15,16	2.77	3 (20%)	20,22,23	2.26	6 (30%)
3	PEG	A	602	-	6,6,6	0.49	0	5,5,5	0.49	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
6	DDF	B	602	-	-	8/22/31/31	0/3/3/3
3	PEG	A	603	-	-	1/4/4/4	-
2	GLY	A	601	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DDF	A	607	-	-	13/22/31/31	0/3/3/3
5	GOL	A	606	-	-	4/4/4/4	-
7	PLP	A	608	1	-	2/6/6/8	0/1/1/1
5	GOL	A	605	-	-	2/4/4/4	-
7	PLP	B	603	1	-	2/6/6/8	0/1/1/1
3	PEG	A	602	-	-	1/4/4/4	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	607	DDF	C2-N1	8.17	1.49	1.35
6	B	602	DDF	C2-N1	7.96	1.49	1.35
7	B	603	PLP	C5-C4	7.62	1.48	1.40
7	A	608	PLP	C5-C4	7.17	1.48	1.40
7	A	608	PLP	C3-C2	6.26	1.47	1.40
7	B	603	PLP	C3-C2	6.19	1.47	1.40
6	B	602	DDF	C8A-N1	5.76	1.45	1.34
6	B	602	DDF	O4-C4	5.36	1.38	1.24
6	A	607	DDF	CA-CT	5.28	1.66	1.52
6	A	607	DDF	O4-C4	5.22	1.37	1.24
6	A	607	DDF	C8A-N1	5.04	1.44	1.34
6	B	602	DDF	C7-N8	5.01	1.53	1.44
6	A	607	DDF	C2-N3	4.83	1.44	1.35
6	A	607	DDF	CA-N	4.74	1.55	1.45
6	B	602	DDF	C2-N3	4.15	1.42	1.35
6	A	607	DDF	C7-N8	4.12	1.51	1.44
6	B	602	DDF	C11-C	3.98	1.58	1.50
6	A	607	DDF	C11-C	3.98	1.58	1.50
6	A	607	DDF	CB-CA	3.94	1.62	1.53
7	B	603	PLP	C3-C4	3.69	1.47	1.40
7	A	608	PLP	C3-C4	3.63	1.47	1.40
6	A	607	DDF	C7-C6	-3.10	1.50	1.53
6	B	602	DDF	CA-N	3.03	1.52	1.45
6	B	602	DDF	C7-C6	-2.92	1.50	1.53
6	B	602	DDF	C4A-C4	2.82	1.47	1.41
6	A	607	DDF	C4A-C4	2.67	1.47	1.41
6	B	602	DDF	CA-CT	2.44	1.59	1.52
6	A	607	DDF	CG-CD	2.38	1.56	1.50
6	A	607	DDF	O-C	2.35	1.28	1.23
6	A	607	DDF	C16-C11	2.29	1.43	1.39
6	A	607	DDF	C-N	2.25	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	602	DDF	O-C	2.24	1.27	1.23
6	B	602	DDF	C5-C6	2.23	1.58	1.52
2	A	601	GLY	OXT-C	-2.20	1.23	1.30
6	A	607	DDF	C16-C15	2.19	1.42	1.38
6	A	607	DDF	OE1-CD	2.16	1.29	1.22
6	B	602	DDF	CG-CD	2.11	1.55	1.50
6	A	607	DDF	CB-CG	2.10	1.59	1.52
6	B	602	DDF	OE1-CD	2.02	1.28	1.22

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	607	DDF	C11-C-N	6.63	129.78	117.06
6	B	602	DDF	C11-C-N	6.30	129.14	117.06
7	B	603	PLP	O4P-C5A-C5	6.26	121.28	109.35
6	A	607	DDF	NA2-C2-N3	6.19	126.88	117.25
6	B	602	DDF	NA2-C2-N3	5.90	126.42	117.25
7	A	608	PLP	O4P-C5A-C5	5.86	120.53	109.35
6	A	607	DDF	O-C-C11	-5.47	111.19	120.94
6	B	602	DDF	O-C-C11	-4.82	112.34	120.94
7	B	603	PLP	C4A-C4-C5	4.61	125.68	120.94
6	A	607	DDF	N1-C2-N3	-4.16	118.90	125.42
7	A	608	PLP	C4A-C4-C5	3.90	124.95	120.94
6	B	602	DDF	N1-C2-N3	-3.88	119.33	125.42
6	A	607	DDF	C2-N3-C4	3.18	120.98	115.93
6	A	607	DDF	CA-N-C	3.13	129.27	121.60
6	B	602	DDF	C6-C7-N8	3.08	116.98	111.50
6	B	602	DDF	CA-N-C	3.04	129.04	121.60
6	B	602	DDF	C2-N3-C4	2.97	120.65	115.93
7	A	608	PLP	C6-N1-C2	2.92	124.58	119.17
6	A	607	DDF	C10-C9-C6	2.88	118.16	114.47
6	B	602	DDF	CB-CA-N	2.86	116.65	110.88
2	A	601	GLY	OXT-C-O	-2.67	116.66	123.30
6	B	602	DDF	C10-C9-C6	2.63	117.84	114.47
6	B	602	DDF	C16-C11-C12	-2.62	114.86	118.59
7	B	603	PLP	C6-N1-C2	2.58	123.94	119.17
6	A	607	DDF	C16-C11-C12	-2.58	114.92	118.59
7	B	603	PLP	C2A-C2-N1	2.44	122.43	117.67
6	B	602	DDF	CG-CB-CA	2.39	117.62	113.16
7	B	603	PLP	O2P-P-O4P	-2.29	100.63	106.73
6	B	602	DDF	O-C-N	-2.17	118.46	122.45
6	A	607	DDF	CB-CA-N	2.15	115.23	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	607	DDF	CG-CB-CA	2.10	117.09	113.16
7	A	608	PLP	O3-C3-C2	2.07	122.01	117.49
6	B	602	DDF	OE2-CD-CG	2.06	120.66	114.03
7	B	603	PLP	C4A-C4-C3	-2.05	117.02	120.50
6	A	607	DDF	OE2-CD-CG	2.03	120.56	114.03

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLY	O-C-CA-N
2	A	601	GLY	OXT-C-CA-N
5	A	606	GOL	O1-C1-C2-C3
6	A	607	DDF	N-CA-CB-CG
7	B	603	PLP	C4-C5-C5A-O4P
7	B	603	PLP	C6-C5-C5A-O4P
6	B	602	DDF	CB-CA-N-C
3	A	603	PEG	O2-C3-C4-O4
6	A	607	DDF	CT-CA-N-C
5	A	605	GOL	O1-C1-C2-C3
5	A	606	GOL	C1-C2-C3-O3
6	A	607	DDF	CB-CA-N-C
6	A	607	DDF	CT-CA-CB-CG
6	B	602	DDF	C5-C6-C9-C10
5	A	605	GOL	O1-C1-C2-O2
3	A	602	PEG	O2-C3-C4-O4
6	B	602	DDF	N-CA-CT-O2
6	B	602	DDF	CT-CA-N-C
6	A	607	DDF	N-CA-CT-O1
6	A	607	DDF	N-CA-CT-O2
7	A	608	PLP	C6-C5-C5A-O4P
5	A	606	GOL	O2-C2-C3-O3
5	A	606	GOL	O1-C1-C2-O2
6	B	602	DDF	N-CA-CT-O1
6	A	607	DDF	CB-CA-CT-O2
7	A	608	PLP	C5A-O4P-P-O1P
6	B	602	DDF	CT-CA-CB-CG
6	A	607	DDF	CB-CA-CT-O1
6	A	607	DDF	CA-CB-CG-CD
6	A	607	DDF	C9-C10-C14-C15
6	A	607	DDF	C9-C10-C14-C13
6	A	607	DDF	OE1-CD-CG-CB

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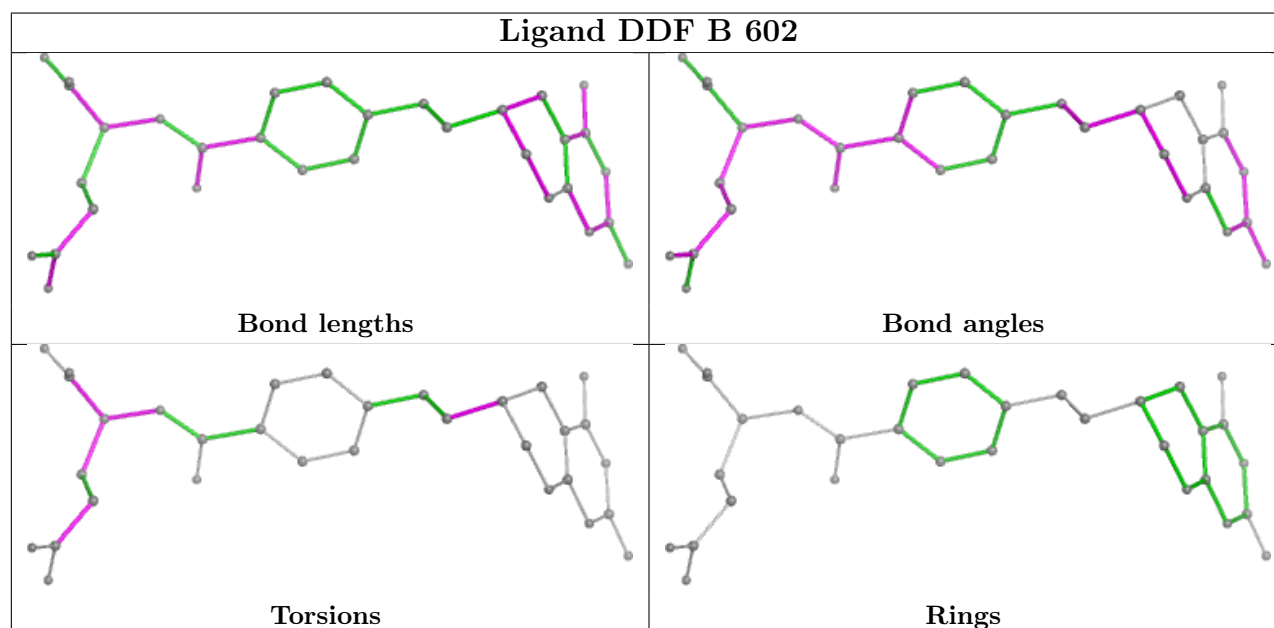
Mol	Chain	Res	Type	Atoms
6	B	602	DDF	OE2-CD-CG-CB
6	B	602	DDF	OE1-CD-CG-CB
6	A	607	DDF	OE2-CD-CG-CB

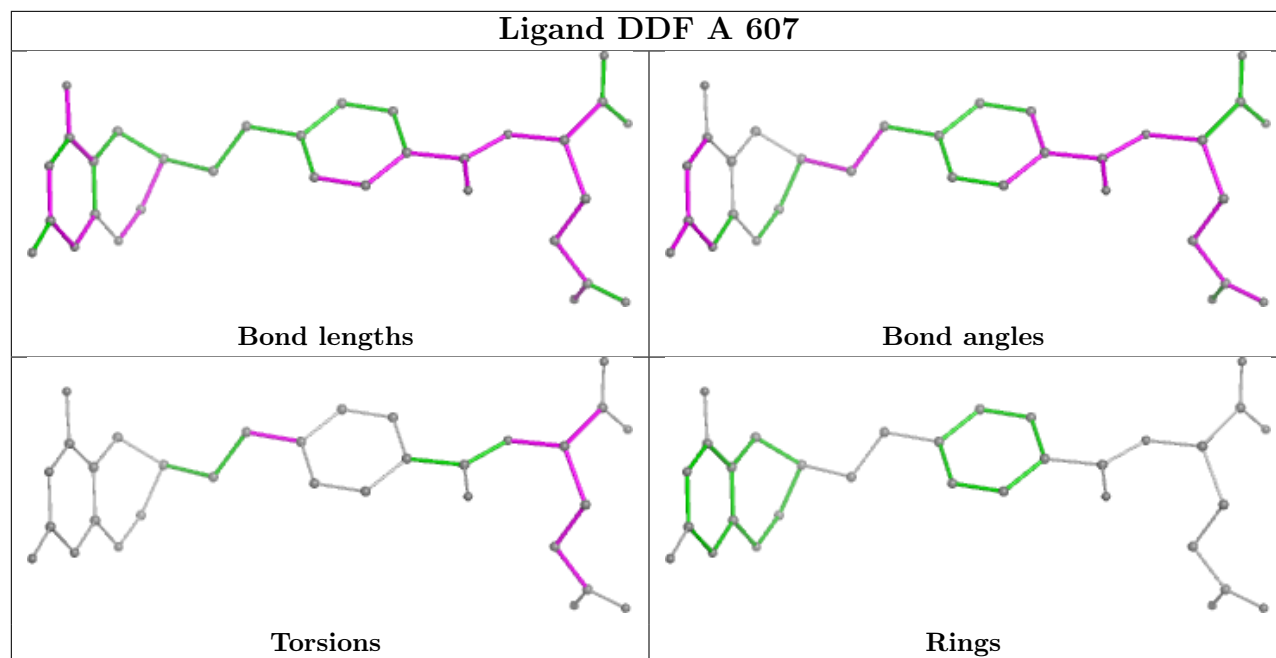
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	GOL	1	0
7	B	603	PLP	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	453/504 (89%)	-0.23	15 (3%)	49	52	14, 28, 60, 93	2 (0%)
1	B	454/504 (90%)	0.32	23 (5%)	34	37	20, 39, 73, 94	0
All	All	907/1008 (89%)	0.05	38 (4%)	41	43	14, 34, 65, 94	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ALA	8.8
1	A	307	ILE	7.5
1	B	307	ILE	6.2
1	B	416	ARG	5.9
1	A	417	SER	4.6
1	A	297	LYS	4.6
1	B	464	LYS	3.9
1	A	418	ALA	3.8
1	B	180	VAL	3.6
1	A	296	VAL	3.5
1	A	416	ARG	3.1
1	B	476	SER	3.0
1	B	474	LYS	3.0
1	B	359	ARG	2.9
1	A	474	LYS	2.9
1	A	419	ILE	2.9
1	A	180	VAL	2.8
1	B	473	LEU	2.8
1	B	463	ALA	2.7
1	B	466	GLN	2.7
1	B	460	SER	2.6
1	A	463	ALA	2.5
1	B	200	LYS	2.5
1	B	296	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	469	LYS	2.4
1	A	476	SER	2.4
1	B	297	LYS	2.4
1	A	470	SER	2.3
1	A	464	LYS	2.3
1	B	418	ALA	2.2
1	A	308	PRO	2.2
1	B	420	THR	2.2
1	B	461	LYS	2.2
1	B	456	LEU	2.1
1	B	419	ILE	2.1
1	A	466	GLN	2.1
1	B	480	GLN	2.0
1	B	366	LEU	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.

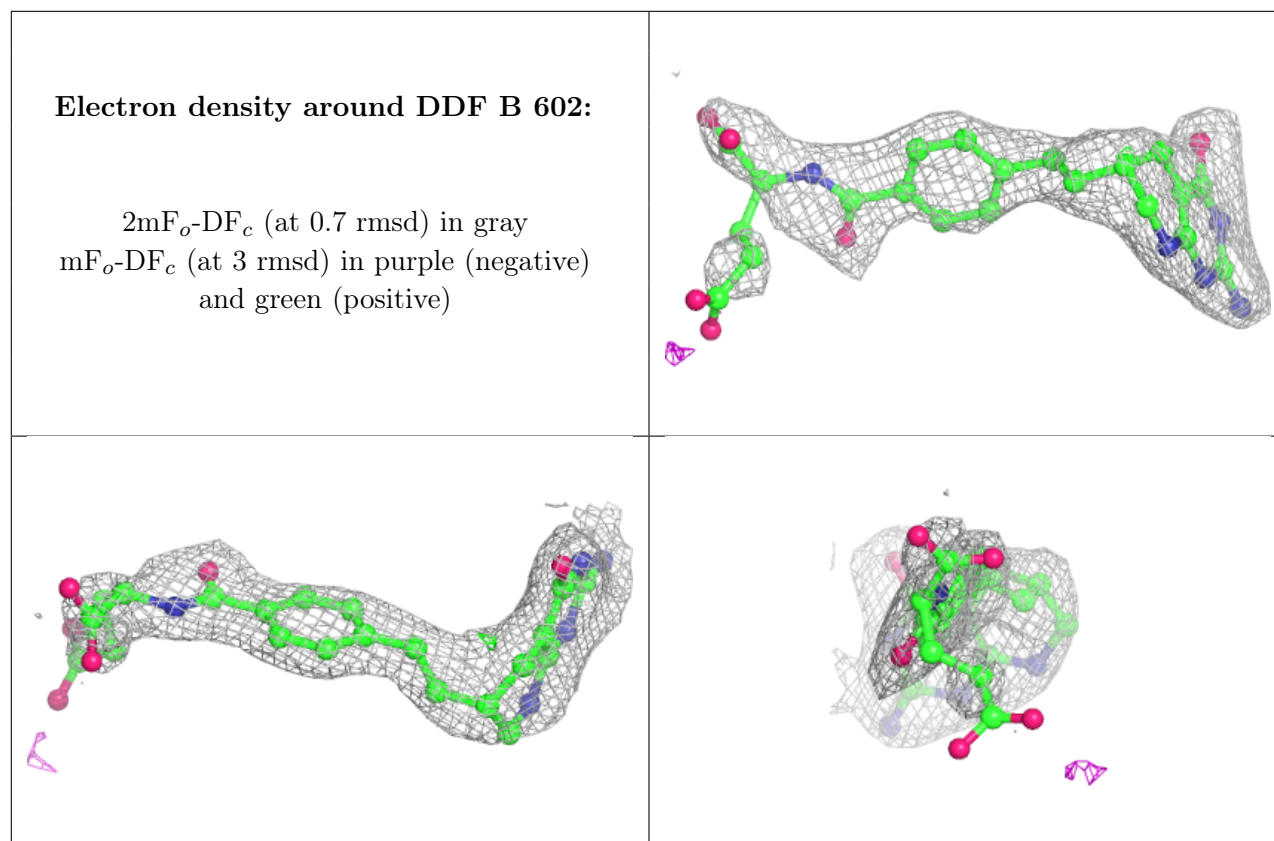
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	A	602	7/7	0.76	0.30	58,63,71,71	0
3	PEG	A	603	7/7	0.76	0.32	68,72,73,75	0
5	GOL	A	605	6/6	0.76	0.21	53,55,57,58	0
8	ACT	B	601	4/4	0.79	0.20	51,53,55,57	0
2	GLY	A	601	5/5	0.84	0.35	57,58,61,69	0
6	DDF	B	602	32/32	0.88	0.16	48,63,91,92	0
5	GOL	A	606	6/6	0.88	0.20	56,60,64,65	0
6	DDF	A	607	32/32	0.89	0.15	44,50,83,85	0
4	NA	A	604	1/1	0.90	0.22	56,56,56,56	0

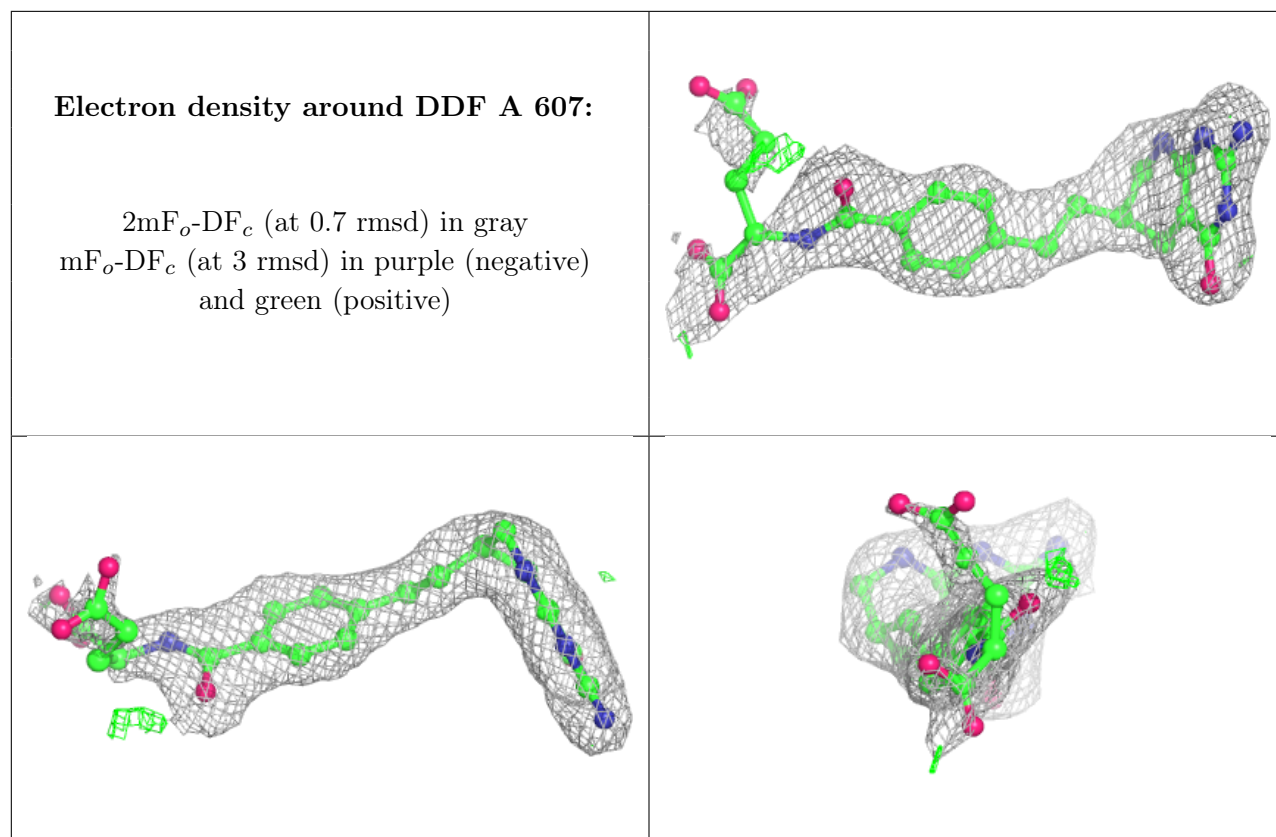
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	PLP	B	603	15/16	0.96	0.08	32,36,38,38	0
7	PLP	A	608	15/16	0.98	0.05	23,24,25,25	0

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.