



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 04:32 PM EDT

PDB ID : 8GKY
Title : Human mitochondrial serine hydroxymethyltransferase (SHMT2) Y105F in complex with PLP, glycine and AGF359 inhibitor
Authors : Katinas, J.M.; Dann III, C.E.
Deposited on : 2023-03-20
Resolution : 2.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

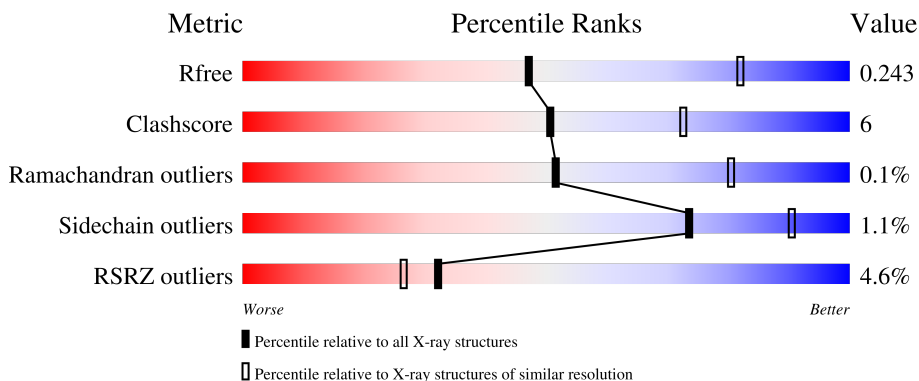
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


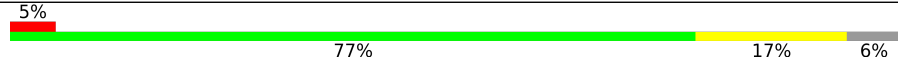
The reported resolution of this entry is 2.77 Å.

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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	493	
1	B	493	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7258 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
			Total	C	N	O	S			
1	A	459	3578	2255	644	663	16	0	1	0
1	B	461	3573	2249	638	670	16	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

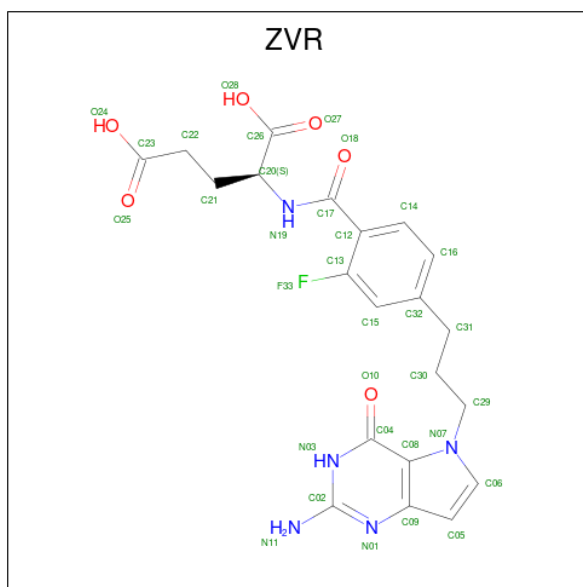
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	UNP P34897
A	19	HIS	-	expression tag	UNP P34897
A	20	HIS	-	expression tag	UNP P34897
A	21	HIS	-	expression tag	UNP P34897
A	22	SER	-	expression tag	UNP P34897
A	23	SER	-	expression tag	UNP P34897
A	24	GLY	-	expression tag	UNP P34897
A	25	LEU	-	expression tag	UNP P34897
A	26	VAL	-	expression tag	UNP P34897
A	27	PRO	-	expression tag	UNP P34897
A	28	ARG	-	expression tag	UNP P34897
A	105	PHE	TYR	engineered mutation	UNP P34897
B	12	MET	-	initiating methionine	UNP P34897
B	13	GLY	-	expression tag	UNP P34897
B	14	SER	-	expression tag	UNP P34897
B	15	SER	-	expression tag	UNP P34897
B	16	HIS	-	expression tag	UNP P34897
B	17	HIS	-	expression tag	UNP P34897
B	18	HIS	-	expression tag	UNP P34897

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P34897
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897
B	27	PRO	-	expression tag	UNP P34897
B	28	ARG	-	expression tag	UNP P34897
B	105	PHE	TYR	engineered mutation	UNP P34897

- Molecule 2 is N-{4-[3-(2-amino-4-oxo-3,4-dihydro-5H-pyrrolo[3,2-d]pyrimidin-5-yl)propyl]-2-fluorobenzoyl}-L-glutamic acid (three-letter code: ZVR) (formula: C₂₁H₂₂FN₅O₆) (labeled as "Ligand of Interest" by depositor).



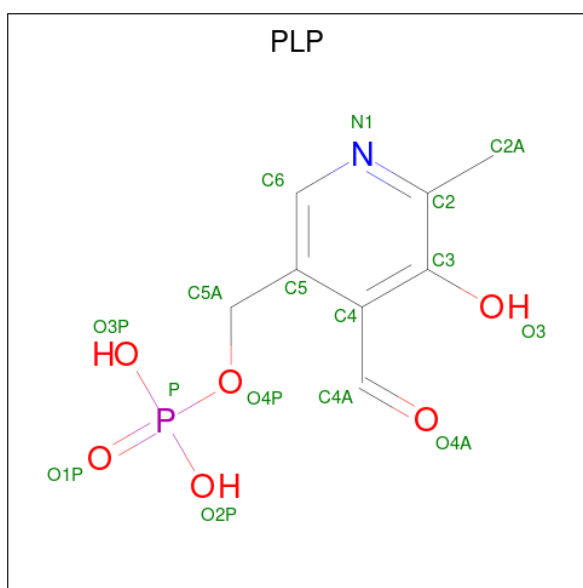
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	21	1	5	6		
2	B	1	Total	C	F	N	O	0	0
			33	21	1	5	6		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

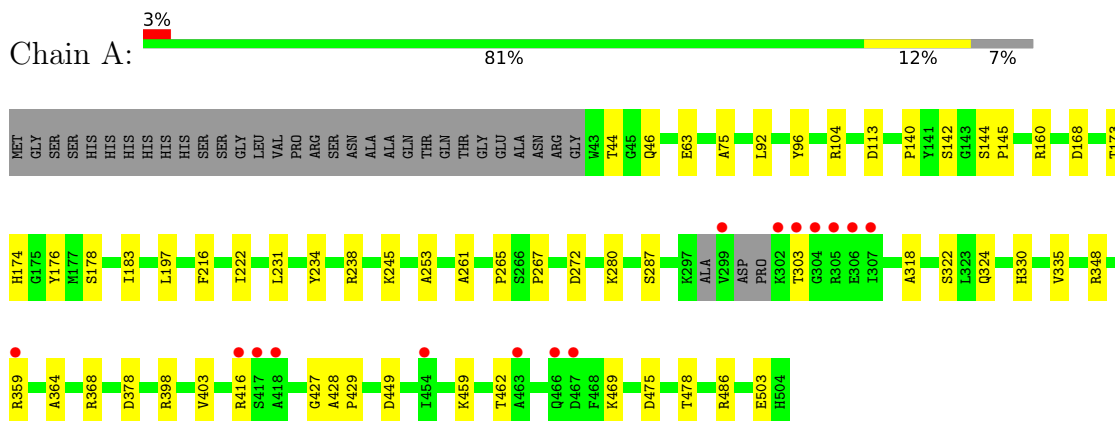
- Molecule 5 is water.

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

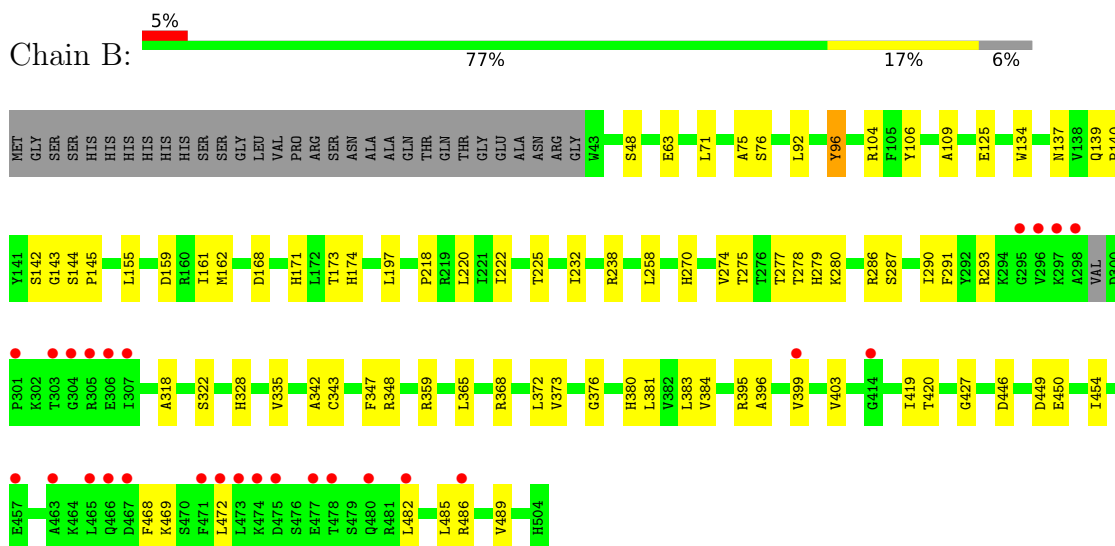
3 Residue-property plots i

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: 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, α , β , γ	157.97Å 157.97Å 206.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 2.77 48.52 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.52-2.77) 99.6 (48.52-2.77)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.199 , 0.243 0.199 , 0.243	Depositor DCC
R_{free} test set	1917 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7258	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: PLP, ZVR

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	0.29	0/3648	0.46	0/4931
1	B	0.29	0/3644	0.47	0/4932
All	All	0.29	0/7292	0.46	0/9863

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	3578	0	3556	31	0
1	B	3573	0	3515	52	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
3	A	5	0	2	0	0
3	B	5	0	2	0	0
4	A	15	0	7	1	0
4	B	15	0	7	2	0
5	A	1	0	0	0	0
All	All	7258	0	7089	82	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 (82) 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:278:THR:HG21	1:B:335:VAL:HG12	1.39	1.01
1:B:278:THR:HG21	1:B:335:VAL:CG1	2.03	0.87
1:B:71:LEU:CD1	1:B:489:VAL:HG13	2.26	0.65
1:B:485:LEU:O	1:B:489:VAL:HG23	1.97	0.63
1:A:44:THR:HG23	1:A:46:GLN:H	1.62	0.63
1:B:71:LEU:HD11	1:B:489:VAL:HG13	1.81	0.63
1:B:472:LEU:HD23	1:B:482:LEU:HD11	1.82	0.61
1:B:143:GLY:HA3	4:B:603:PLP:H5A1	1.83	0.59
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.84	0.59
1:B:275:THR:HG22	1:B:290:ILE:HG12	1.85	0.58
1:B:168:ASP:HB3	1:B:197:LEU:HG	1.87	0.55
1:B:368:ARG:NH1	1:B:446:ASP:OD1	2.40	0.55
1:B:373:VAL:HG22	1:B:383:LEU:HB2	1.89	0.55
1:B:372:LEU:HD12	1:B:376:GLY:HA2	1.88	0.54
1:B:450:GLU:HG2	1:B:485:LEU:HD22	1.90	0.54
1:A:142:SER:OG	4:A:603:PLP:O2P	2.25	0.54
1:B:368:ARG:NH2	1:B:449:ASP:OD1	2.30	0.53
1:A:459:LYS:HA	1:A:462:THR:HG22	1.90	0.53
1:A:287:SER:HB3	1:A:335:VAL:HG11	1.91	0.53
1:B:96:TYR:HB3	1:B:106:TYR:HE2	1.74	0.53
1:A:398:ARG:HG2	1:A:469:LYS:HG2	1.91	0.52
1:B:395:ARG:HB3	1:B:468:PHE:CZ	2.45	0.52
1:B:450:GLU:O	1:B:454:ILE:HG13	2.11	0.51
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.26	0.51
1:B:395:ARG:HD3	1:B:468:PHE:CD1	2.45	0.51
1:A:475:ASP:HB3	1:A:478:THR:HB	1.93	0.51
1:A:364:ALA:O	1:A:368[B]:ARG:HG2	2.11	0.50
1:A:144:SER:HA	1:A:173:THR:HG21	1.93	0.50
1:B:162:MET:HG3	1:B:218:PRO:HB3	1.93	0.50
1:B:274:VAL:HB	1:B:291:PHE:HB2	1.95	0.49
1:B:75:ALA:HA	1:B:427:GLY:HA3	1.96	0.48
1:B:419:ILE:HG23	1:B:420:THR:HG23	1.95	0.48
1:A:176:TYR:CE2	1:A:183:ILE:HD12	2.49	0.48
1:B:125:GLU:HG2	1:B:343:CYS:SG	2.54	0.48
1:B:318:ALA:HA	1:B:322:SER:HB2	1.94	0.48
1:B:171:HIS:HB2	4:B:603:PLP:H2A3	1.95	0.47
1:B:238:ARG:NH1	1:B:270:HIS:O	2.39	0.47
2:A:601:ZVR:F33	2:A:601:ZVR:N19	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LEU:HD13	1:B:384:VAL:HG11	1.97	0.47
1:B:403:VAL:HA	1:B:486:ARG:HB2	1.98	0.46
1:A:168:ASP:HB3	1:A:197:LEU:HG	1.98	0.46
1:A:238:ARG:HH22	1:A:272:ASP:CG	2.19	0.46
1:B:469:LYS:HA	1:B:472:LEU:HD12	1.98	0.46
1:B:174:HIS:CD2	1:B:222:ILE:HG21	2.51	0.46
1:B:277:THR:HG23	1:B:279:HIS:CE1	2.50	0.46
1:A:174:HIS:CD2	1:A:222:ILE:HG21	2.51	0.46
1:B:342:ALA:HA	1:B:347:PHE:CG	2.51	0.46
1:B:258:LEU:HD11	1:B:380:HIS:HB3	1.98	0.45
1:B:76:SER:HB2	1:B:280:LYS:HE3	1.98	0.45
1:A:104:ARG:NE	1:A:113:ASP:OD1	2.46	0.45
1:A:253:ALA:HB1	1:A:280:LYS:HE3	1.99	0.45
1:B:395:ARG:HB3	1:B:468:PHE:CE2	2.51	0.45
1:A:503:GLU:OE1	1:A:503:GLU:N	2.39	0.45
1:B:134:TRP:CZ2	1:B:293:ARG:HD3	2.52	0.44
1:B:287:SER:HB3	1:B:335:VAL:HG11	1.99	0.44
1:A:63:GLU:HG2	1:B:92:LEU:HD23	2.00	0.44
1:A:234:TYR:CZ	1:A:267:PRO:HB3	2.52	0.44
1:A:261:ALA:HB1	1:A:348:ARG:HA	1.99	0.43
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.52	0.43
1:B:137:ASN:OD1	1:B:140:PRO:HD3	2.18	0.43
1:B:225:THR:HG23	1:B:232:ILE:HD11	2.00	0.43
1:A:330:HIS:CD2	1:A:330:HIS:H	2.37	0.43
1:B:144:SER:HA	1:B:173:THR:HG21	2.01	0.43
1:A:140:PRO:HA	1:A:324:GLN:OE1	2.19	0.43
1:B:96:TYR:HB3	1:B:106:TYR:CE2	2.54	0.43
1:A:92:LEU:HD23	1:B:63:GLU:HG2	2.00	0.42
1:B:380:HIS:CE1	1:B:381:LEU:HD23	2.54	0.42
1:A:359:ARG:HH22	1:A:378:ASP:HA	1.84	0.42
1:B:142:SER:C	1:B:145:PRO:HD2	2.39	0.42
1:A:368[A]:ARG:NH1	1:A:449:ASP:OD2	2.53	0.42
1:B:161:ILE:HD13	1:B:220:LEU:HB3	2.00	0.42
1:B:396:ALA:HA	1:B:399:VAL:HG12	2.02	0.42
1:A:403:VAL:HA	1:A:486:ARG:HB2	2.02	0.42
1:B:71:LEU:HD12	1:B:489:VAL:HG13	2.02	0.41
1:A:428:ALA:N	1:A:429:PRO:CD	2.83	0.41
1:A:231:LEU:HD13	1:A:265:PRO:HD2	2.03	0.41
1:A:142:SER:C	1:A:145:PRO:HD2	2.41	0.41
1:A:178:SER:HB2	1:A:183:ILE:HD11	2.01	0.41
1:B:155:LEU:HB3	1:B:159:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:GLN:N	1:B:140:PRO:CD	2.84	0.40
1:B:104:ARG:HD2	1:B:109:ALA:CB	2.51	0.40
1:A:318:ALA:HA	1:A:322:SER:HB2	2.03	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	455/493 (92%)	437 (96%)	17 (4%)	1 (0%)	47 76
1	B	458/493 (93%)	434 (95%)	24 (5%)	0	100 100
All	All	913/986 (93%)	871 (95%)	41 (4%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	THR

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	375/405 (93%)	372 (99%)	3 (1%)	81 93
1	B	372/405 (92%)	367 (99%)	5 (1%)	69 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	747/810 (92%)	739 (99%)	8 (1%)	73 90

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

Mol	Chain	Res	Type
1	A	96	TYR
1	A	245	LYS
1	A	416	ARG
1	B	48	SER
1	B	96	TYR
1	B	328	HIS
1	B	348	ARG
1	B	359	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS

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](#)

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
4	PLP	B	603	1	15,15,16	2.26	5 (33%)	20,22,23	1.49	1 (5%)
2	ZVR	B	601	-	32,35,35	1.94	5 (15%)	40,49,49	1.26	4 (10%)
2	ZVR	A	601	-	32,35,35	1.96	5 (15%)	40,49,49	1.41	8 (20%)
4	PLP	A	603	1	15,15,16	2.18	5 (33%)	20,22,23	1.54	4 (20%)
3	GLY	B	602	-	4,4,4	1.10	1 (25%)	3,4,4	1.64	1 (33%)
3	GLY	A	602	-	4,4,4	1.14	1 (25%)	3,4,4	1.59	1 (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
4	PLP	B	603	1	-	3/6/6/8	0/1/1/1
2	ZVR	B	601	-	-	10/23/23/23	0/3/3/3
2	ZVR	A	601	-	-	10/23/23/23	0/3/3/3
4	PLP	A	603	1	-	2/6/6/8	0/1/1/1
3	GLY	B	602	-	-	0/2/2/2	-
3	GLY	A	602	-	-	0/2/2/2	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ZVR	C17-N19	5.70	1.46	1.34
2	B	601	ZVR	C17-N19	5.49	1.46	1.34
4	A	603	PLP	C4A-C4	5.16	1.62	1.51
2	B	601	ZVR	C02-N11	5.00	1.46	1.34
2	A	601	ZVR	C02-N11	4.97	1.46	1.34
4	B	603	PLP	C4A-C4	4.93	1.61	1.51
2	B	601	ZVR	C06-N07	-3.82	1.32	1.38
2	A	601	ZVR	C06-N07	-3.77	1.32	1.38
4	A	603	PLP	C2A-C2	3.62	1.56	1.50
2	B	601	ZVR	C04-N03	-3.50	1.32	1.37
2	A	601	ZVR	C04-N03	-3.47	1.32	1.37
4	B	603	PLP	C2A-C2	3.39	1.56	1.50
4	B	603	PLP	C6-N1	3.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	PLP	C5-C4	-2.98	1.37	1.40
4	A	603	PLP	C6-N1	2.93	1.40	1.34
4	A	603	PLP	C5A-C5	2.45	1.57	1.50
2	A	601	ZVR	C12-C17	2.44	1.55	1.50
2	B	601	ZVR	C12-C17	2.35	1.55	1.50
4	B	603	PLP	C5A-C5	2.22	1.56	1.50
3	A	602	GLY	OXT-C	-2.14	1.23	1.30
4	A	603	PLP	C5-C4	-2.12	1.38	1.40
3	B	602	GLY	OXT-C	-2.08	1.23	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	PLP	O4P-C5A-C5	4.34	117.63	109.35
4	A	603	PLP	O4P-C5A-C5	3.91	116.80	109.35
2	A	601	ZVR	C20-N19-C17	3.44	130.02	121.60
2	B	601	ZVR	C15-C13-C12	-3.23	120.08	123.53
4	A	603	PLP	C4A-C4-C5	2.97	123.99	120.94
2	A	601	ZVR	C13-C12-C17	-2.96	118.23	125.09
2	B	601	ZVR	C14-C12-C13	2.78	119.83	116.67
2	A	601	ZVR	C14-C12-C13	2.61	119.64	116.67
2	A	601	ZVR	C02-N03-C04	-2.42	120.64	125.10
2	A	601	ZVR	C09-N01-C02	2.31	120.19	117.93
4	A	603	PLP	C4A-C4-C3	-2.23	116.71	120.50
2	B	601	ZVR	C09-N01-C02	2.23	120.11	117.93
4	A	603	PLP	C5A-C5-C6	-2.17	115.81	119.37
2	A	601	ZVR	O28-C26-C20	2.14	120.51	113.40
2	B	601	ZVR	C02-N03-C04	-2.11	121.20	125.10
2	A	601	ZVR	C15-C13-C12	-2.11	121.28	123.53
3	B	602	GLY	OXT-C-O	-2.07	118.13	123.30
2	A	601	ZVR	O24-C23-C22	2.07	120.68	114.03
3	A	602	GLY	OXT-C-O	-2.03	118.23	123.30

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ZVR	C21-C20-N19-C17
2	B	601	ZVR	C13-C12-C17-N19
2	B	601	ZVR	C13-C12-C17-O18
4	A	603	PLP	C4-C5-C5A-O4P
4	A	603	PLP	C6-C5-C5A-O4P

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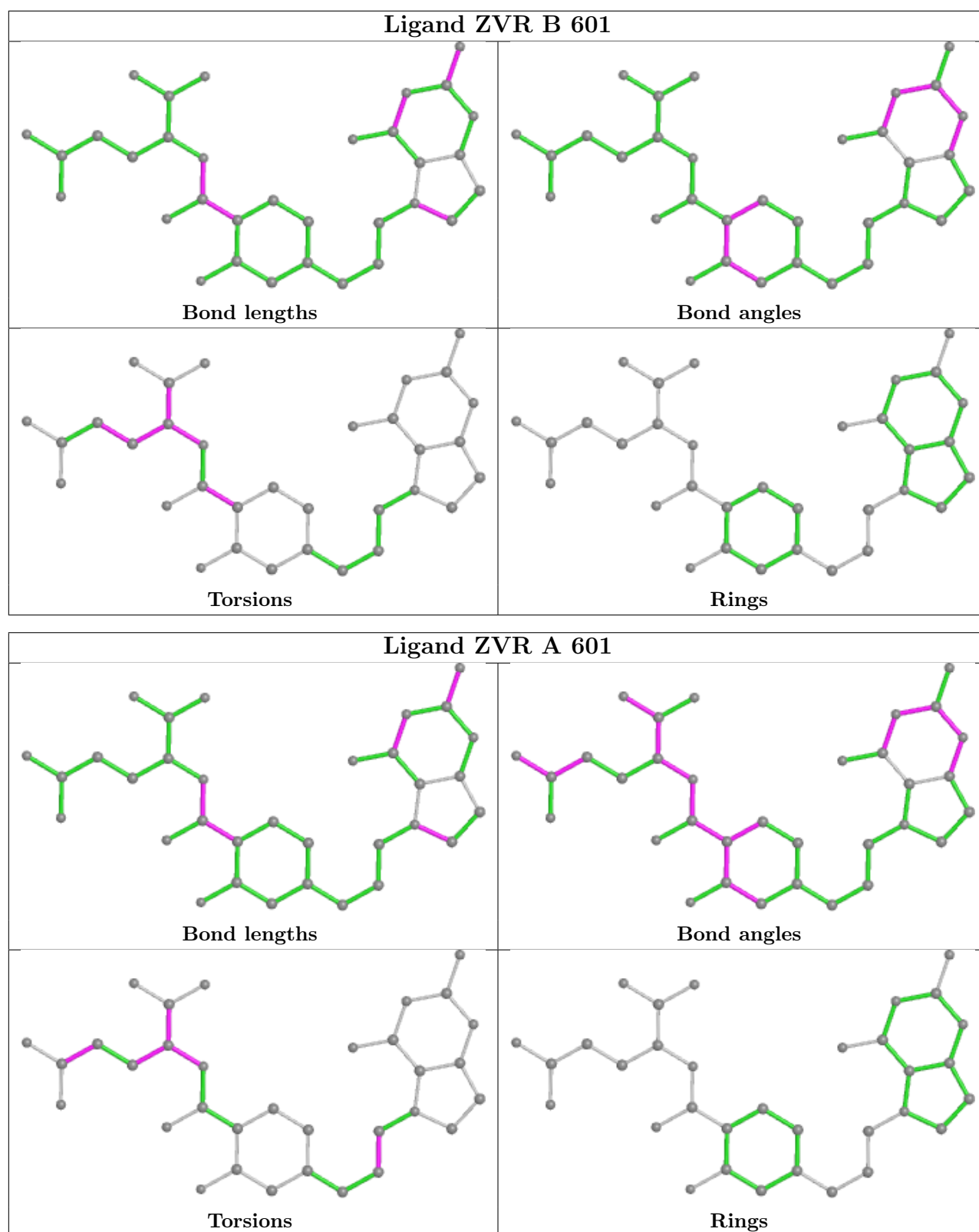
Mol	Chain	Res	Type	Atoms
4	B	603	PLP	C5A-O4P-P-O2P
4	B	603	PLP	C5A-O4P-P-O3P
2	A	601	ZVR	N19-C20-C21-C22
2	A	601	ZVR	N07-C29-C30-C31
2	B	601	ZVR	C21-C20-N19-C17
2	A	601	ZVR	C26-C20-C21-C22
2	B	601	ZVR	C26-C20-C21-C22
2	B	601	ZVR	N19-C20-C21-C22
2	A	601	ZVR	N19-C20-C26-O27
2	A	601	ZVR	N19-C20-C26-O28
4	B	603	PLP	C5A-O4P-P-O1P
2	B	601	ZVR	N19-C20-C26-O27
2	B	601	ZVR	N19-C20-C26-O28
2	B	601	ZVR	C21-C20-C26-O28
2	B	601	ZVR	C20-C21-C22-C23
2	A	601	ZVR	C21-C20-C26-O27
2	A	601	ZVR	C21-C20-C26-O28
2	B	601	ZVR	C21-C20-C26-O27
2	A	601	ZVR	C21-C22-C23-O25
2	A	601	ZVR	C21-C22-C23-O24

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	PLP	2	0
2	A	601	ZVR	1	0
4	A	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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/493 (93%)	-0.03	15 (3%) 46 41	23, 40, 76, 121	0
1	B	461/493 (93%)	0.20	27 (5%) 22 17	27, 56, 93, 126	0
All	All	920/986 (93%)	0.09	42 (4%) 32 26	23, 48, 87, 126	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ILE	5.1
1	B	301	PRO	4.9
1	B	471	PHE	4.8
1	B	304	GLY	4.4
1	B	306	GLU	4.2
1	A	303	THR	4.2
1	A	299	VAL	3.9
1	B	473	LEU	3.8
1	A	304	GLY	3.8
1	B	303	THR	3.6
1	A	305	ARG	3.5
1	B	474	LYS	3.1
1	A	418	ALA	3.1
1	B	305	ARG	3.0
1	B	482	LEU	2.9
1	B	414	GLY	2.9
1	B	467	ASP	2.9
1	A	467	ASP	2.8
1	B	296	VAL	2.7
1	A	417	SER	2.7
1	A	302	LYS	2.7
1	B	463	ALA	2.7
1	B	399	VAL	2.7
1	B	477	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	472	LEU	2.6
1	B	478	THR	2.6
1	B	298	ALA	2.5
1	B	480	GLN	2.5
1	A	466	GLN	2.5
1	B	466	GLN	2.5
1	A	416	ARG	2.5
1	B	475	ASP	2.5
1	A	306	GLU	2.3
1	A	454	ILE	2.3
1	B	465	LEU	2.3
1	B	457	GLU	2.3
1	B	297	LYS	2.2
1	A	463	ALA	2.2
1	B	486	ARG	2.1
1	B	307	ILE	2.1
1	A	359	ARG	2.1
1	B	295	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.

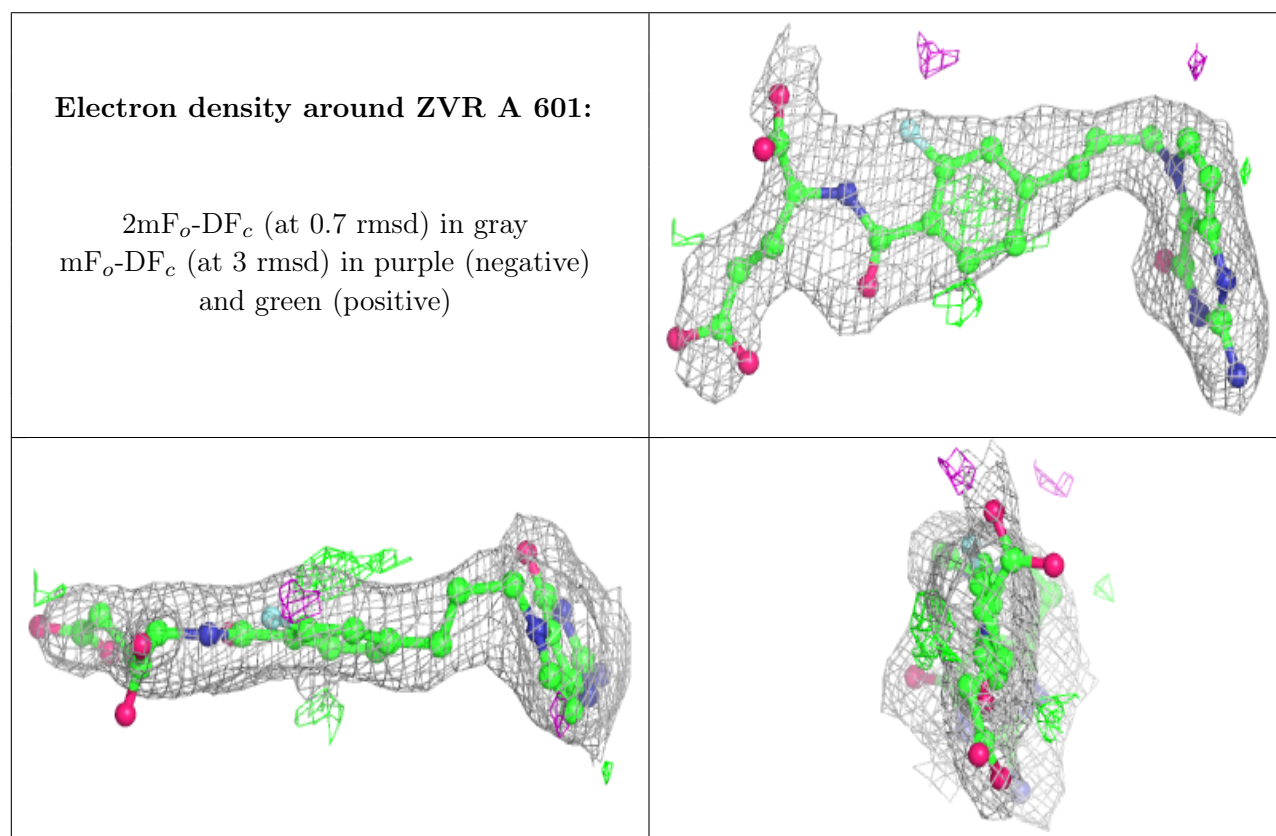
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZVR	A	601	33/33	0.91	0.20	26,49,89,97	0
2	ZVR	B	601	33/33	0.91	0.19	49,63,114,117	0
3	GLY	B	602	5/5	0.93	0.25	59,69,75,75	0
3	GLY	A	602	5/5	0.97	0.25	46,59,64,71	5
4	PLP	B	603	15/16	0.97	0.21	43,47,59,66	0

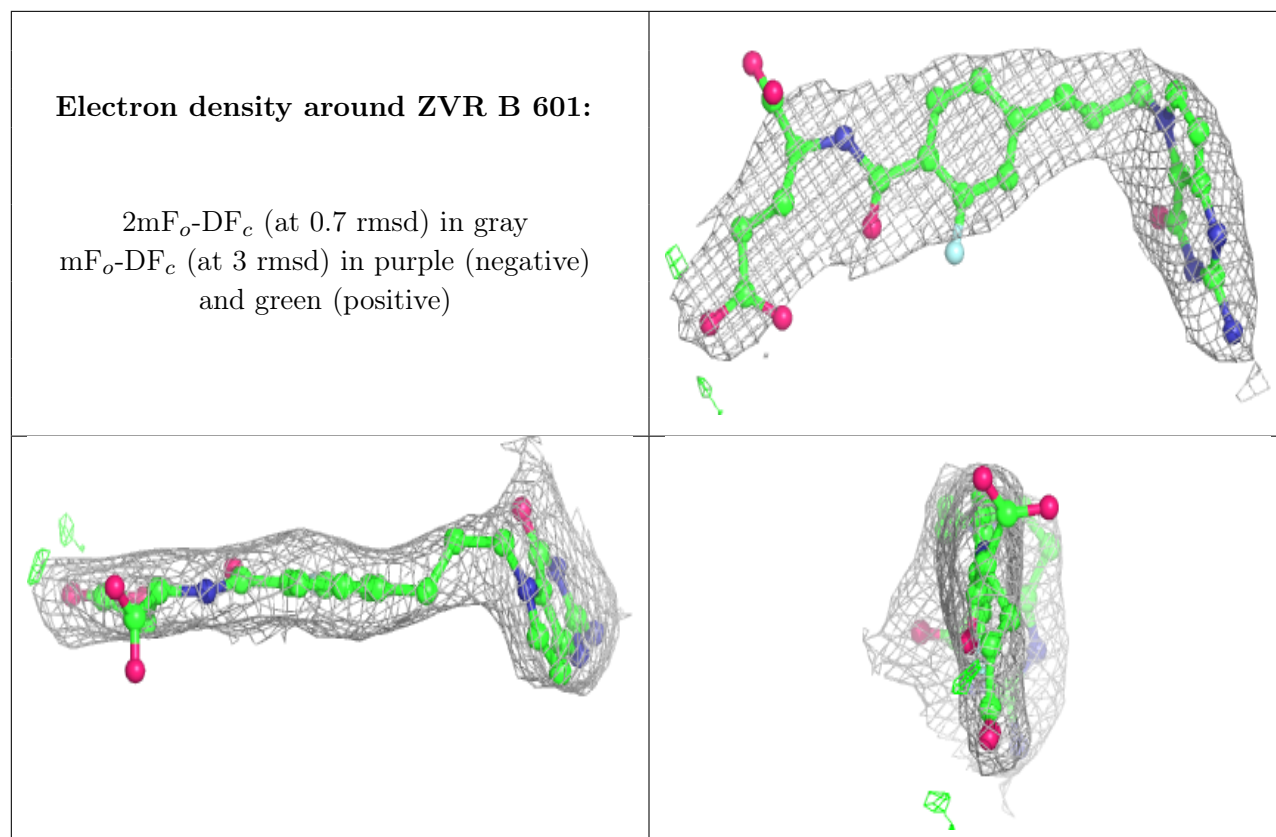
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PLP	A	603	15/16	0.98	0.17	27,33,43,44	0

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.