



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:19 AM UTC

PDB ID : 8GKY / pdb_00008gky
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

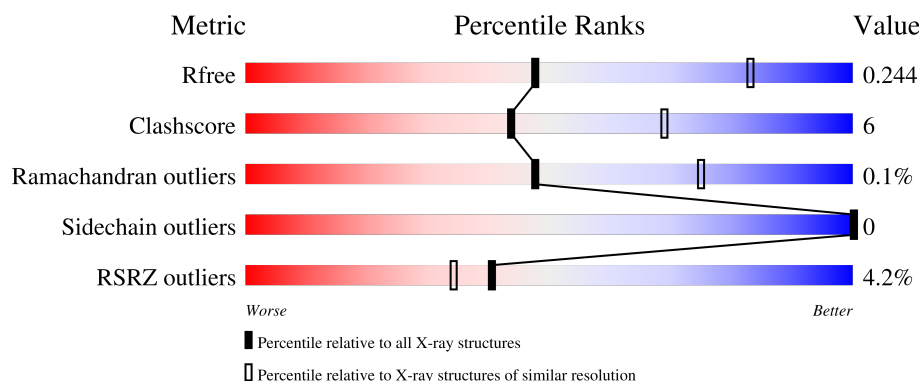
1 Overall quality at a glance

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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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	3% 80% 13% 7%
1	B	493	4% 77% 16% 6%

2 Entry composition

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
1	A	459	Total	C	N	O	S	0	1	0
			3578	2255	644	663	16			
1	B	461	Total	C	N	O	S	0	1	0
			3573	2249	638	670	16			

There are 36 discrepancies between the modelled and reference sequences:

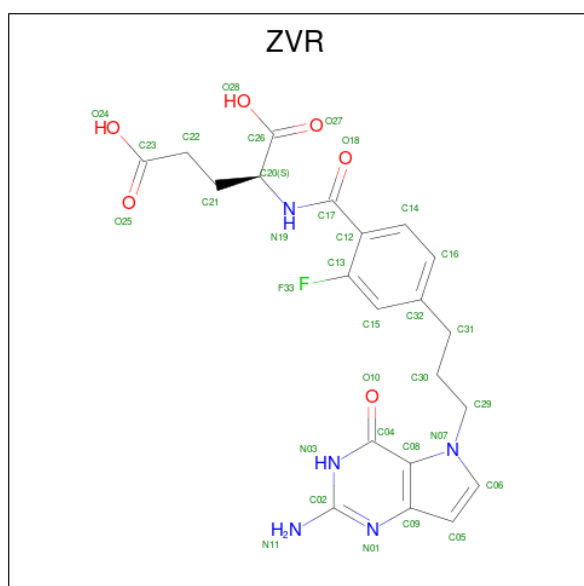
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	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 (CCD ID: ZVR) (formula: $C_{21}H_{22}FN_5O_6$) (labeled as "Ligand of Interest" by depositor).



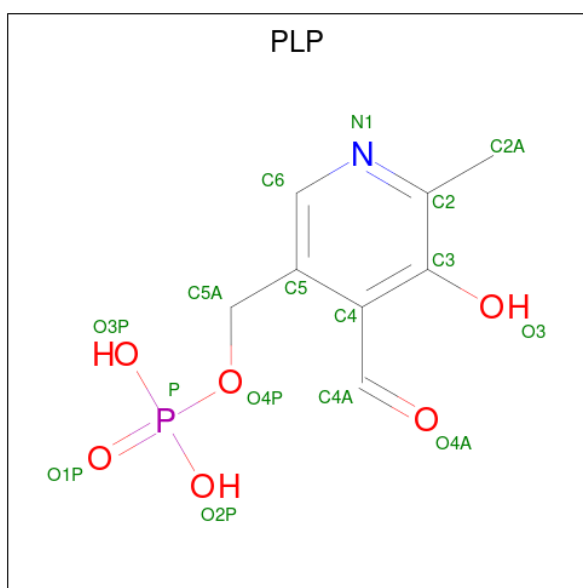
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	21	1	5	6		
2	B	1	Total	C	F	N	O	0	0
			33	21	1	5	6		

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



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

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 5 is water.

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

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)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.199 , 0.243 0.200 , 0.244	Depositor DCC
R_{free} test set	1918 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.19	0/3648	0.39	0/4931
1	B	0.19	0/3644	0.38	0/4932
All	All	0.19	0/7292	0.39	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

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	37	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	1	0
5	A	1	0	0	0	0
All	All	7258	0	7089	87	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 (87) 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:A:193:MET:HE1	1:A:212:THR:HB	1.82	0.59
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:177:MET:HE2	1:A:187:SER:HB2	1.92	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:A:238:ARG:HH22	1:A:272:ASP:CG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HB2	1:A:237:MET:HE2	1.95	0.47
1:A:390:GLY:O	1:A:459:LYS:NZ	2.46	0.47
1:A:43:TRP:CD1	1:B:346:MET:HE2	2.49	0.47
1:B:142:SER:C	1:B:145:PRO:HD2	2.39	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
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: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:142:SER:C	1:A:145:PRO:HD2	2.41	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:65:ASP:CG	1:A:494:ARG:HH12	2.27	0.42
1:A:359:ARG:HH22	1:A:378:ASP:HA	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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	455/493 (92%)	437 (96%)	17 (4%)	1 (0%)	43	70
1	B	458/493 (93%)	434 (95%)	24 (5%)	0	100	100
All	All	913/986 (93%)	871 (95%)	41 (4%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	THR

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	375/405 (93%)	375 (100%)	0	100	100
1	B	372/405 (92%)	372 (100%)	0	100	100
All	All	747/810 (92%)	747 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
1	A	330	HIS
1	A	466	GLN
1	A	487	GLN
1	A	491	GLN
1	B	61	GLN
1	B	133	GLN
1	B	353	GLN

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 oligosaccharides 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	$\# Z > 2$
3	GLY	A	602	-	4,4,4	1.16	1 (25%)	3,4,4	1.57	0
2	ZVR	B	601	-	34,35,35	1.77	6 (17%)	45,49,49	1.85	9 (20%)
4	PLP	A	603	1	15,15,16	2.27	5 (33%)	21,22,23	1.57	4 (19%)
2	ZVR	A	601	-	34,35,35	1.79	6 (17%)	45,49,49	1.93	12 (26%)
4	PLP	B	603	1	15,15,16	2.34	5 (33%)	21,22,23	1.49	2 (9%)
3	GLY	B	602	-	4,4,4	1.12	1 (25%)	3,4,4	1.63	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
3	GLY	A	602	-	-	0/2/2/2	-
2	ZVR	B	601	-	-	10/23/23/23	0/3/3/3
4	PLP	A	603	1	-	2/6/6/8	0/1/1/1
2	ZVR	A	601	-	-	10/23/23/23	0/3/3/3
4	PLP	B	603	1	-	3/6/6/8	0/1/1/1
3	GLY	B	602	-	-	0/2/2/2	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	PLP	C4A-C4	5.39	1.62	1.51
2	A	601	ZVR	C17-N19	5.34	1.46	1.34
4	B	603	PLP	C4A-C4	5.15	1.61	1.51
2	B	601	ZVR	C17-N19	5.14	1.46	1.34
2	B	601	ZVR	C02-N11	5.08	1.46	1.34
2	A	601	ZVR	C02-N11	5.05	1.46	1.34
4	A	603	PLP	C2A-C2	3.87	1.56	1.50
4	B	603	PLP	C2A-C2	3.62	1.56	1.50
2	B	601	ZVR	C04-N03	-3.31	1.32	1.38
2	A	601	ZVR	C04-N03	-3.28	1.32	1.38
4	B	603	PLP	C6-N1	3.12	1.40	1.34
4	A	603	PLP	C6-N1	3.04	1.40	1.34
4	B	603	PLP	C5-C4	-2.96	1.37	1.40
4	A	603	PLP	C5A-C5	2.55	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ZVR	C06-N07	-2.52	1.32	1.38
2	A	601	ZVR	C12-C17	2.49	1.55	1.50
2	A	601	ZVR	C06-N07	-2.49	1.32	1.38
2	B	601	ZVR	C12-C17	2.40	1.55	1.50
4	B	603	PLP	C5A-C5	2.31	1.56	1.50
2	A	601	ZVR	O10-C04	-2.28	1.19	1.23
2	B	601	ZVR	O10-C04	-2.25	1.19	1.23
3	A	602	GLY	OXT-C	-2.20	1.23	1.30
3	B	602	GLY	OXT-C	-2.14	1.23	1.30
4	A	603	PLP	C5-C4	-2.12	1.38	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ZVR	C09-C08-C04	-5.56	116.93	121.36
2	A	601	ZVR	C09-C08-C04	-5.36	117.08	121.36
2	A	601	ZVR	C08-C04-N03	4.97	119.69	110.94
2	B	601	ZVR	C08-C04-N03	4.91	119.58	110.94
2	A	601	ZVR	C08-C09-N01	-4.74	120.27	124.81
2	B	601	ZVR	C08-C09-N01	-4.58	120.42	124.81
4	B	603	PLP	O4P-C5A-C5	4.41	117.63	109.36
4	A	603	PLP	O4P-C5A-C5	3.97	116.80	109.36
2	A	601	ZVR	C20-N19-C17	3.53	130.02	121.56
2	B	601	ZVR	C05-C09-N01	3.09	133.54	123.36
2	B	601	ZVR	C15-C13-C12	-3.07	120.08	123.48
2	A	601	ZVR	C05-C09-N01	3.00	133.25	123.36
4	A	603	PLP	C4A-C4-C5	2.96	123.99	120.94
2	B	601	ZVR	C14-C12-C13	2.82	119.83	116.70
2	B	601	ZVR	O10-C04-C08	-2.68	121.03	127.62
2	A	601	ZVR	O10-C04-C08	-2.66	121.09	127.62
2	A	601	ZVR	C14-C12-C13	2.64	119.64	116.70
2	A	601	ZVR	C02-N03-C04	-2.47	120.64	125.11
4	A	603	PLP	C4A-C4-C3	-2.28	116.71	120.52
2	A	601	ZVR	C09-N01-C02	2.27	120.19	116.63
2	A	601	ZVR	C13-C12-C17	-2.24	118.23	124.32
2	B	601	ZVR	C09-N01-C02	2.22	120.11	116.63
4	A	603	PLP	C5A-C5-C6	-2.18	115.81	119.36
2	B	601	ZVR	C02-N03-C04	-2.15	121.20	125.11
2	A	601	ZVR	O24-C23-C22	2.11	120.68	114.00
2	A	601	ZVR	O28-C26-C20	2.07	120.51	113.51
3	B	602	GLY	OXT-C-O	-2.02	118.13	123.33
4	B	603	PLP	C5-C6-N1	-2.01	120.57	123.83

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
4	A	603	PLP	C4-C5-C5A-O4P
4	A	603	PLP	C6-C5-C5A-O4P
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	C13-C12-C17-O18
2	B	601	ZVR	N19-C20-C21-C22
2	B	601	ZVR	C26-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	A	601	ZVR	C21-C20-C26-O28
2	A	601	ZVR	C21-C20-C26-O27
2	B	601	ZVR	C21-C20-C26-O27
2	B	601	ZVR	C21-C20-C26-O28
2	B	601	ZVR	C20-C21-C22-C23
2	A	601	ZVR	C21-C22-C23-O25
2	A	601	ZVR	C21-C22-C23-O24

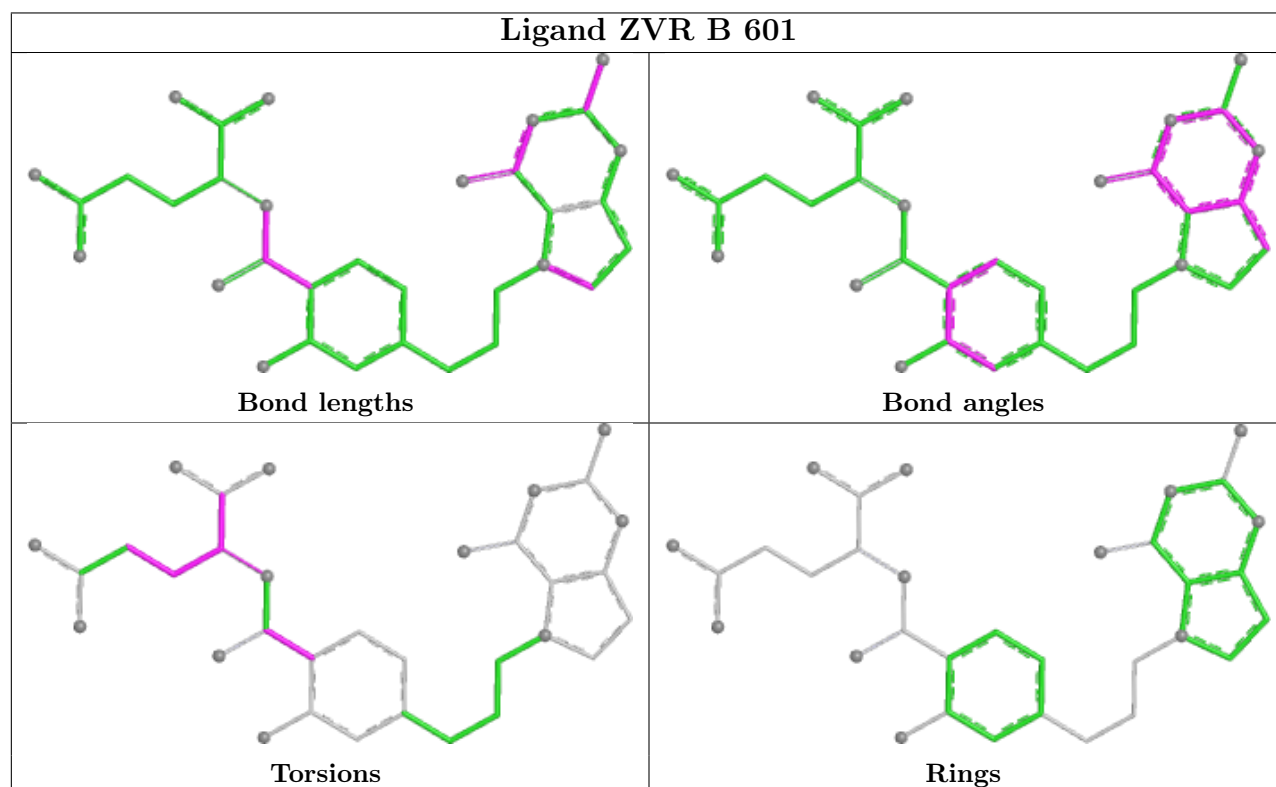
There are no ring outliers.

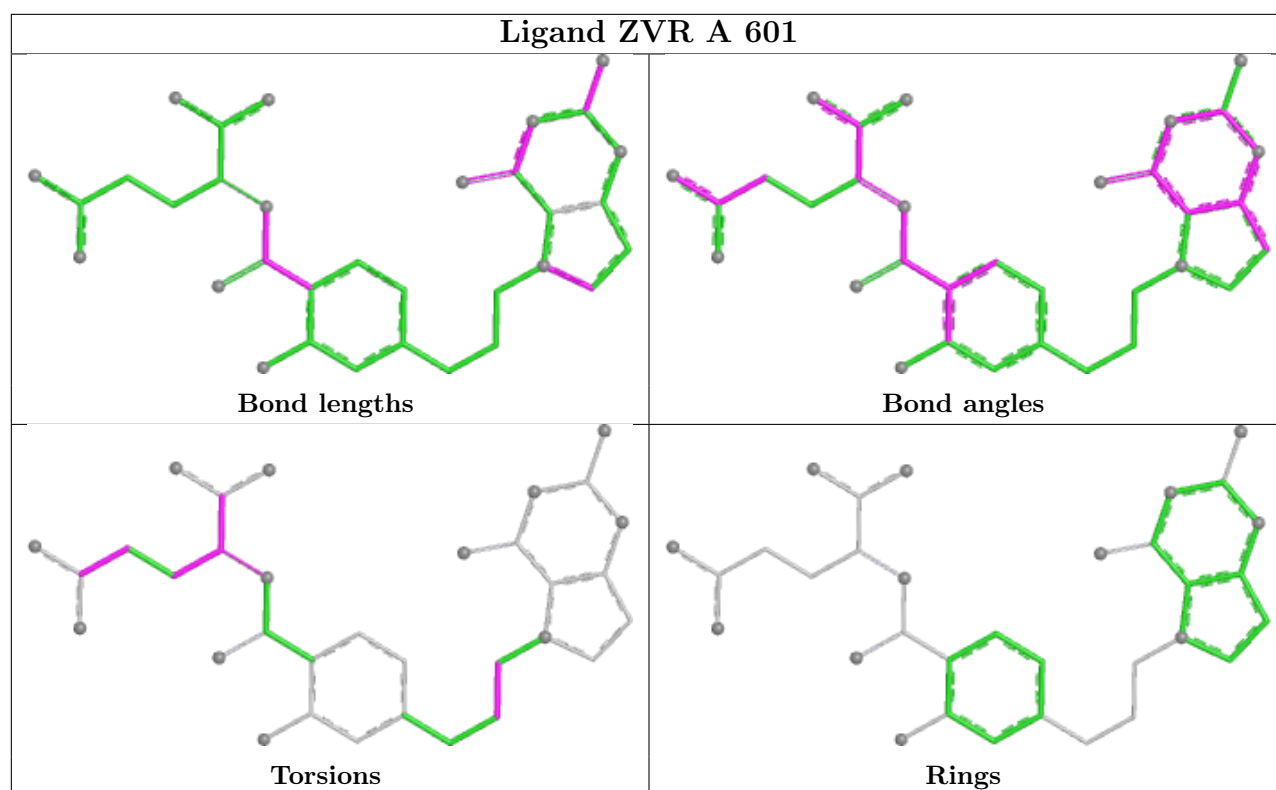
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	PLP	1	0
2	A	601	ZVR	1	0
4	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, 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%)	-0.10	17 (3%) 45 38	23, 40, 76, 121	1 (0%)
1	B	461/493 (93%)	0.19	22 (4%) 35 30	27, 56, 93, 126	1 (0%)
All	All	920/986 (93%)	0.05	39 (4%) 40 34	23, 48, 87, 126	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ALA	6.8
1	A	418	ALA	5.1
1	A	419	ILE	4.9
1	A	415	ASP	4.7
1	B	105	PHE	4.6
1	A	299	VAL	4.4
1	A	297	LYS	4.2
1	B	305	ARG	4.2
1	B	301	PRO	3.9
1	B	303	THR	3.8
1	A	417	SER	3.8
1	A	416	ARG	3.8
1	B	416	ARG	3.6
1	B	304	GLY	3.6
1	A	420	THR	3.6
1	A	305	ARG	3.5
1	A	105	PHE	3.4
1	B	300	ASP	3.4
1	A	306	GLU	3.3
1	B	418	ALA	3.1
1	A	303	THR	3.0
1	B	106	TYR	3.0
1	A	302	LYS	2.8
1	B	414	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	106	TYR	2.8
1	B	417	SER	2.7
1	B	467	ASP	2.7
1	B	387	ARG	2.6
1	B	419	ILE	2.6
1	B	302	LYS	2.6
1	B	307	ILE	2.5
1	B	395	ARG	2.4
1	B	503	GLU	2.4
1	A	414	GLY	2.4
1	B	110	GLU	2.3
1	A	304	GLY	2.2
1	B	415	ASP	2.1
1	B	463	ALA	2.1
1	A	453	ASN	2.1

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 oligosaccharides in this entry.

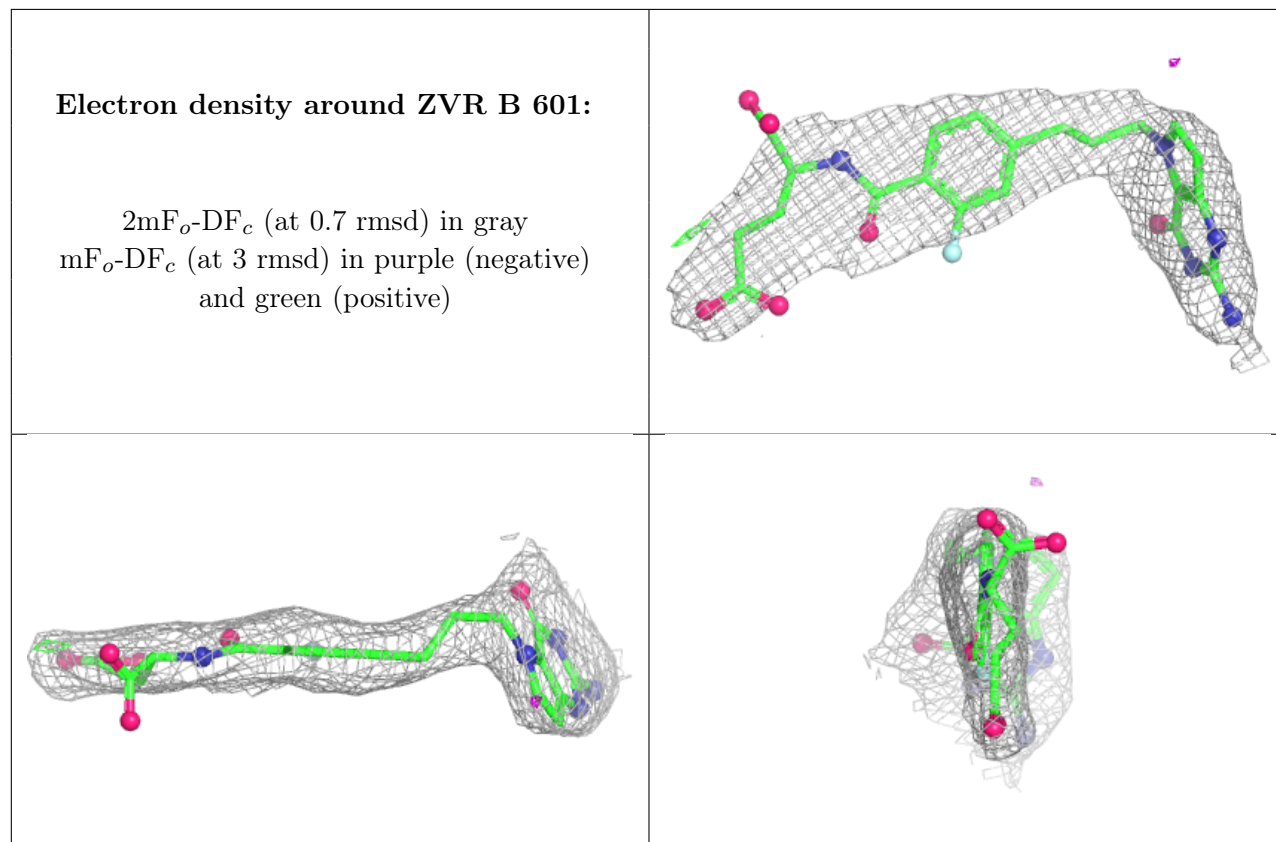
6.4 Ligands [i](#)

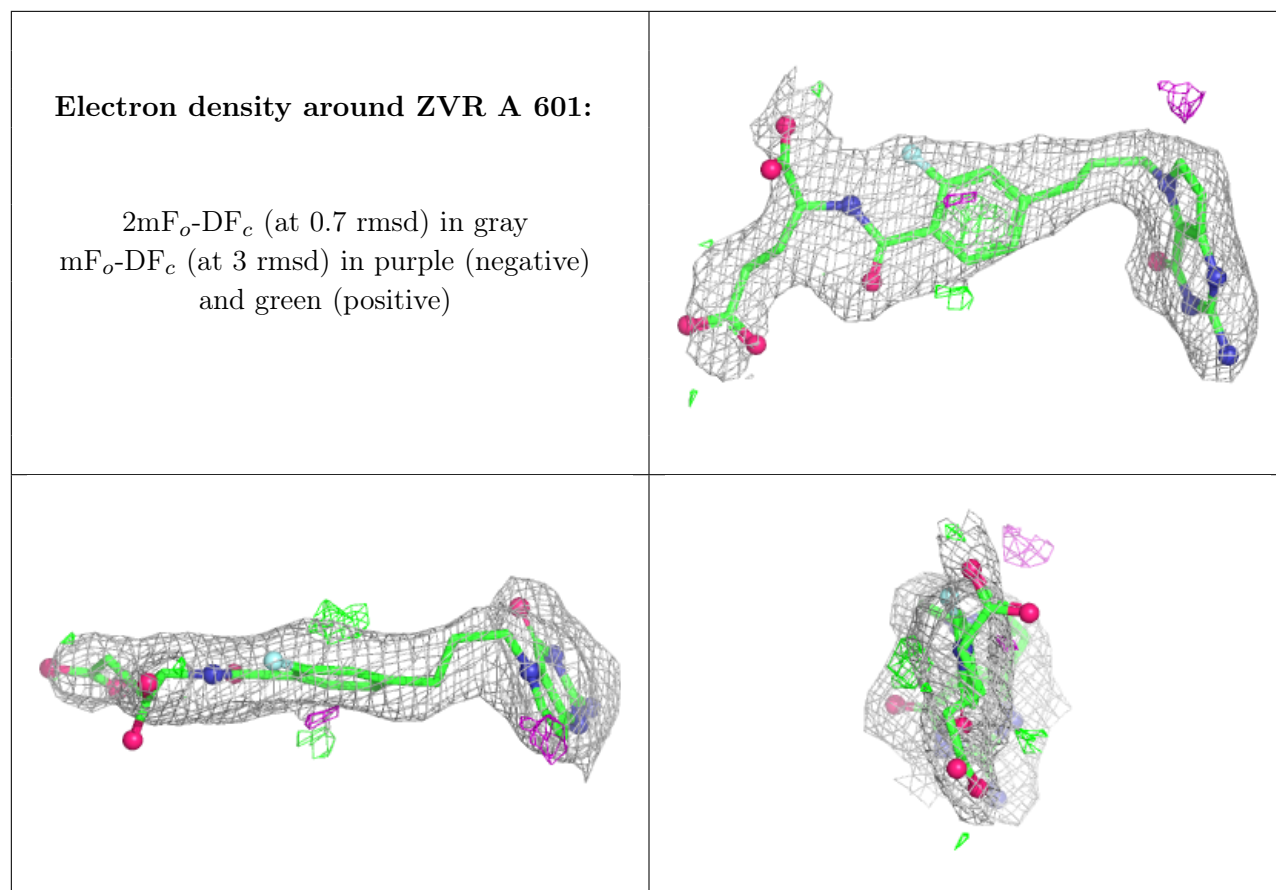
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZVR	B	601	33/33	0.89	0.15	49,63,114,117	0
2	ZVR	A	601	33/33	0.90	0.13	26,49,89,97	0
3	GLY	B	602	5/5	0.91	0.15	59,69,75,75	0
3	GLY	A	602	5/5	0.93	0.16	46,59,64,71	5
4	PLP	B	603	15/16	0.96	0.09	43,47,59,66	0
4	PLP	A	603	15/16	0.98	0.06	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 ⓘ

There are no such residues in this entry.