



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:57 AM UTC

PDB ID : 8SVL / pdb_00008svl
Title : Plasmodium falciparum M1 aminopeptidase bound to MMV1557817
Authors : McGowan, S.; Drinkwater, N.
Deposited on : 2023-05-17
Resolution : 1.50 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

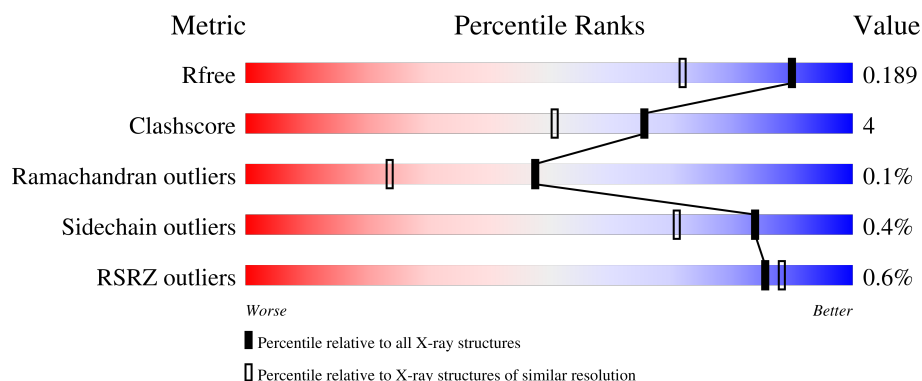
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	1091	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8676 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 M1 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	889	Total	C	N	O	S	0	18	0
			7310	4706	1178	1398	28			

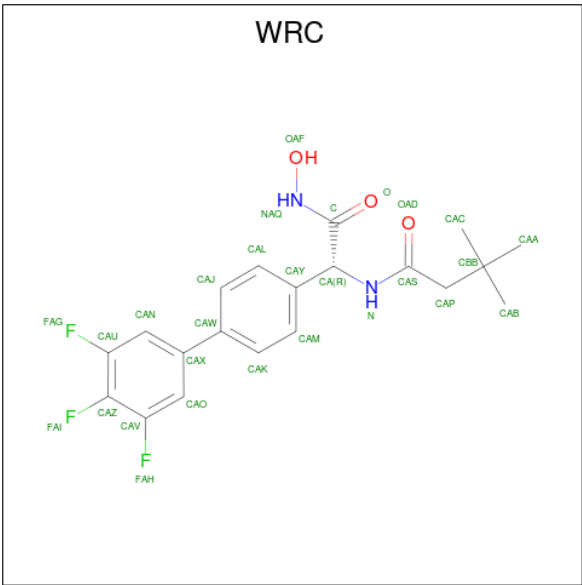
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLN	ASN	conflict	UNP O96935
A	223	GLN	ASN	conflict	UNP O96935
A	378	PRO	HIS	conflict	UNP O96935
A	501	GLN	ASN	conflict	UNP O96935
A	745	GLN	ASN	conflict	UNP O96935
A	795	GLN	ASN	conflict	UNP O96935
A	1069	GLN	ASN	conflict	UNP O96935
A	1086	HIS	-	expression tag	UNP O96935
A	1087	HIS	-	expression tag	UNP O96935
A	1088	HIS	-	expression tag	UNP O96935
A	1089	HIS	-	expression tag	UNP O96935
A	1090	HIS	-	expression tag	UNP O96935
A	1091	HIS	-	expression tag	UNP O96935

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]-3,3-dimethylbutanamide (CCD ID: WRC) (formula: C₂₀H₂₁F₃N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Mg	0	0
			5	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1284	Total	O	0	0
			1284	1284		

- Molecule 1: M1 family aminopeptidase

E872	N527	GLU	ASN	THR	MET
D890	T636	ASN	ASN	ASN	LYS
N912	V637	ASN	ASN	THR	THR
R969	T638	ASN	ASN	ALA	GLY
E977	E566	ASN	ARG	SER	CYS
L982	V569	VAL	VAL	GLU	TYR
R1008	N573	LYS	VAL	PHE	ILE
R1009	F574	LYS	VAL	SER	ILE
T1037	Y575	ASN	ASN	ASN	PHE
E1041	M689	GLU	GLU	TRP	VAL
L1045	K629	Q223	ASN	ASN	LEU
W1046	K632	R228	THR	ASP	LEU
Q1054	A637	L256	SER	GLN	ALA
N1059	W645	S257	LYS	LYS	LEU
E1076	D661	K261	ARG	ASP	TYR
R1080	K664	V264	LYS	ILE	ASP
N1083	N672	Y269	PRO	PHE	ASN
K1084	E679	T270	PHE	ASN	LYS
LEU	D772	Y271	GLU	ASN	LYS
HIS	F688	D272	GLY	ASN	ILE
HIS	N723	M273	THR	LYS	LYS
HIS	V726	S291	GLN	PRO	ASN
HIS	T769	S292	VAL	GLN	LEU
HIS	L777	E293	ASP	ARG	ARG
HIS	M778	K309	LYS	ILE	ILE
HIS	N781	R332	MET	SER	SER
HIS	T797	K335	ASN	THR	THR
HIS	H815	H370	ASN	ILE	SER
HIS	G819	P377	ASN	GLY	CYS
HIS	I834	Y403	ASN	LYS	ILE
HIS	N835	Q423	SER	ARG	ILE
HIS	F836	L442	ASP	LEU	SER
HIS	V837	V459	HIS	SER	ARG
HIS	S838	K465	LEU	GLU	SER
HIS	D847	Y502	ASN	LYS	LEU
HIS			VAL	ASN	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.90Å 109.01Å 118.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.66 – 1.50 42.66 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.66-1.50) 100.0 (42.66-1.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.155 , 0.189 0.157 , 0.189	Depositor DCC
R_{free} test set	7575 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.7	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	0.97	EDS
Total number of atoms	8676	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: WRC, GOL, MG, ZN

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	1.01	0/7528	0.99	2/10193 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	377	PRO	N-CA-C	6.20	118.26	110.70
1	A	265	GLU	N-CA-C	5.07	117.58	110.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	370	HIS	Sidechain
1	A	527	ASN	Sidechain

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	7310	0	7180	53	0
2	A	1	0	0	0	0
3	A	28	0	0	0	0
4	A	48	0	64	6	0
5	A	5	0	0	0	0
6	A	1284	0	0	34	0
All	All	8676	0	7244	56	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 4.

All (56) 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:847:ASP:OD1	1:A:1008[A]:ARG:NH2	1.90	1.03
1:A:781[A]:ASN:OD1	6:A:1201:HOH:O	1.87	0.91
1:A:890[B]:ASP:OD1	6:A:1202:HOH:O	1.91	0.88
1:A:228:ARG:NH1	1:A:293:GLU:OE2	2.10	0.84
1:A:1037[A]:THR:OG1	6:A:1203:HOH:O	1.99	0.80
1:A:769:THR:OG1	4:A:1109:GOL:H11	1.86	0.74
1:A:573:ASN:OD1	6:A:1205:HOH:O	2.06	0.73
1:A:969:ARG:NH1	6:A:1210:HOH:O	2.17	0.72
1:A:403:TYR:OH	6:A:1206:HOH:O	2.10	0.70
1:A:1059[B]:ASN:OD1	6:A:1207:HOH:O	2.11	0.69
1:A:912:ASN:ND2	6:A:1224:HOH:O	2.28	0.66
1:A:566:GLU:OE2	6:A:1208:HOH:O	2.14	0.65
1:A:257[B]:SER:OG	1:A:291:SER:OG	2.16	0.63
1:A:536:THR:OG1	6:A:1204:HOH:O	2.06	0.61
1:A:969:ARG:NH2	6:A:1227:HOH:O	2.31	0.59
1:A:977:GLU:OE2	6:A:1212:HOH:O	2.18	0.57
1:A:256:ILE:HD11	1:A:269:TYR:CD2	2.39	0.57
1:A:223:GLN:HG3	6:A:2185:HOH:O	2.05	0.56
1:A:672:ASN:ND2	6:A:1223:HOH:O	2.27	0.56
1:A:778[B]:MET:HE2	6:A:2289:HOH:O	2.07	0.55
1:A:834:ILE:HD13	1:A:1045:LEU:HD22	1.88	0.55
1:A:538:THR:HG21	1:A:819:GLY:HA3	1.88	0.55
1:A:1083:ASN:ND2	6:A:1217:HOH:O	2.23	0.54
1:A:723:ASN:ND2	6:A:1213:HOH:O	2.18	0.54
1:A:872:GLU:OE1	6:A:1214:HOH:O	2.19	0.53
1:A:1076:GLU:OE2	1:A:1080:ARG:NE	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:PHE:CD1	4:A:1104:GOL:H2	2.46	0.51
1:A:778[B]:MET:SD	1:A:797:THR:HG21	2.51	0.50
4:A:1105:GOL:H32	6:A:1203:HOH:O	2.11	0.50
1:A:442:LEU:HB3	1:A:502:TYR:CE1	2.47	0.50
1:A:332:ARG:HG3	1:A:335:MET:HG2	1.94	0.49
1:A:1041:GLU:OE1	6:A:1216:HOH:O	2.20	0.49
1:A:271:TYR:CZ	1:A:273:ASN:HA	2.49	0.48
4:A:1107:GOL:H32	6:A:2224:HOH:O	2.14	0.47
1:A:632:LYS:NZ	6:A:1244:HOH:O	2.44	0.47
1:A:679:GLU:HG3	6:A:1981:HOH:O	2.15	0.47
1:A:538:THR:HG23	6:A:1204:HOH:O	2.14	0.46
1:A:1037[B]:THR:HG22	4:A:1105:GOL:H31	1.96	0.46
1:A:1046:TRP:O	1:A:1054:GLN:HG2	2.16	0.45
1:A:661:ASP:CG	1:A:664:LYS:HD2	2.42	0.45
1:A:465:LYS:NZ	6:A:1262:HOH:O	2.51	0.44
1:A:569:VAL:HB	1:A:1076:GLU:HG3	1.99	0.44
1:A:575:TYR:HB2	6:A:1318:HOH:O	2.18	0.44
1:A:629:LYS:NZ	1:A:637:ALA:O	2.34	0.43
1:A:726:VAL:HG22	6:A:1411:HOH:O	2.17	0.43
1:A:589:MET:HE1	1:A:645:TRP:CE2	2.54	0.43
1:A:423:GLN:NE2	6:A:1215:HOH:O	2.19	0.42
1:A:777:LEU:HD23	1:A:777:LEU:HA	1.88	0.42
1:A:536:THR:HG21	6:A:2128:HOH:O	2.18	0.42
1:A:838:SER:HA	6:A:1233:HOH:O	2.20	0.42
1:A:309:LYS:NZ	6:A:1268:HOH:O	2.52	0.41
1:A:261:LYS:HE3	6:A:1998:HOH:O	2.19	0.41
1:A:688:PHE:CD2	1:A:688:PHE:C	2.99	0.41
1:A:982:LEU:HD23	1:A:982:LEU:HA	1.87	0.41
1:A:1009:ARG:NH1	6:A:1272:HOH:O	2.53	0.40
4:A:1104:GOL:H31	6:A:1327:HOH:O	2.21	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	905/1091 (83%)	889 (98%)	15 (2%)	1 (0%)	48 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	VAL

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	815/1012 (80%)	811 (100%)	4 (0%)	81 66

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	688	PHE
1	A	838	SER
1	A	1008[A]	ARG
1	A	1008[B]	ARG

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	219	ASN
1	A	464	ASN
1	A	468	ASN
1	A	621	ASN
1	A	626	GLN
1	A	723	ASN
1	A	775	GLN
1	A	779	ASN

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](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	$\# Z > 2$
4	GOL	A	1108	-	5,5,5	0.44	0	5,5,5	0.54	0
4	GOL	A	1110	-	5,5,5	0.36	0	5,5,5	0.58	0
4	GOL	A	1105	-	5,5,5	0.81	0	5,5,5	1.28	0
4	GOL	A	1107	-	5,5,5	0.54	0	5,5,5	0.53	0
4	GOL	A	1103	-	5,5,5	0.49	0	5,5,5	1.26	1 (20%)
4	GOL	A	1106	-	5,5,5	0.48	0	5,5,5	1.25	1 (20%)
3	WRC	A	1102	2	28,29,29	1.93	8 (28%)	38,42,42	1.97	11 (28%)
4	GOL	A	1109	-	5,5,5	0.61	0	5,5,5	1.13	0
4	GOL	A	1104	-	5,5,5	0.35	0	5,5,5	0.81	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
4	GOL	A	1108	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1110	-	-	2/4/4/4	-
4	GOL	A	1105	-	-	2/4/4/4	-
4	GOL	A	1107	-	-	2/4/4/4	-
4	GOL	A	1103	-	-	2/4/4/4	-
4	GOL	A	1106	-	-	3/4/4/4	-
3	WRC	A	1102	2	-	5/23/23/23	0/2/2/2
4	GOL	A	1109	-	-	1/4/4/4	-
4	GOL	A	1104	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	WRC	CAY-CA	-6.38	1.42	1.52
3	A	1102	WRC	CAP-CAS	2.98	1.55	1.51
3	A	1102	WRC	CAK-CAM	2.74	1.43	1.38
3	A	1102	WRC	FAI-CAZ	2.59	1.38	1.34
3	A	1102	WRC	CAX-CAW	-2.58	1.42	1.49
3	A	1102	WRC	CAJ-CAW	2.39	1.44	1.39
3	A	1102	WRC	CAO-CAX	2.14	1.43	1.39
3	A	1102	WRC	CA-N	2.10	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	WRC	CAM-CAY-CA	-5.15	112.53	120.78
3	A	1102	WRC	CAK-CAM-CAY	-4.58	116.61	121.18
3	A	1102	WRC	CAY-CA-C	3.36	116.34	108.42
3	A	1102	WRC	CAL-CAY-CAM	3.21	122.28	118.30
3	A	1102	WRC	CAO-CAX-CAW	-3.18	115.51	120.84
3	A	1102	WRC	CAL-CAJ-CAW	-2.75	117.59	121.12
3	A	1102	WRC	CAL-CAY-CA	2.67	125.07	120.78
3	A	1102	WRC	CAX-CAO-CAV	-2.59	117.56	119.61
3	A	1102	WRC	O-C-CA	2.55	124.84	120.58
4	A	1106	GOL	O1-C1-C2	-2.30	100.00	110.38
3	A	1102	WRC	FAH-CAV-CAZ	-2.30	115.21	118.32
4	A	1103	GOL	C3-C2-C1	-2.25	103.54	111.80
3	A	1102	WRC	CAY-CA-N	2.02	117.84	112.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

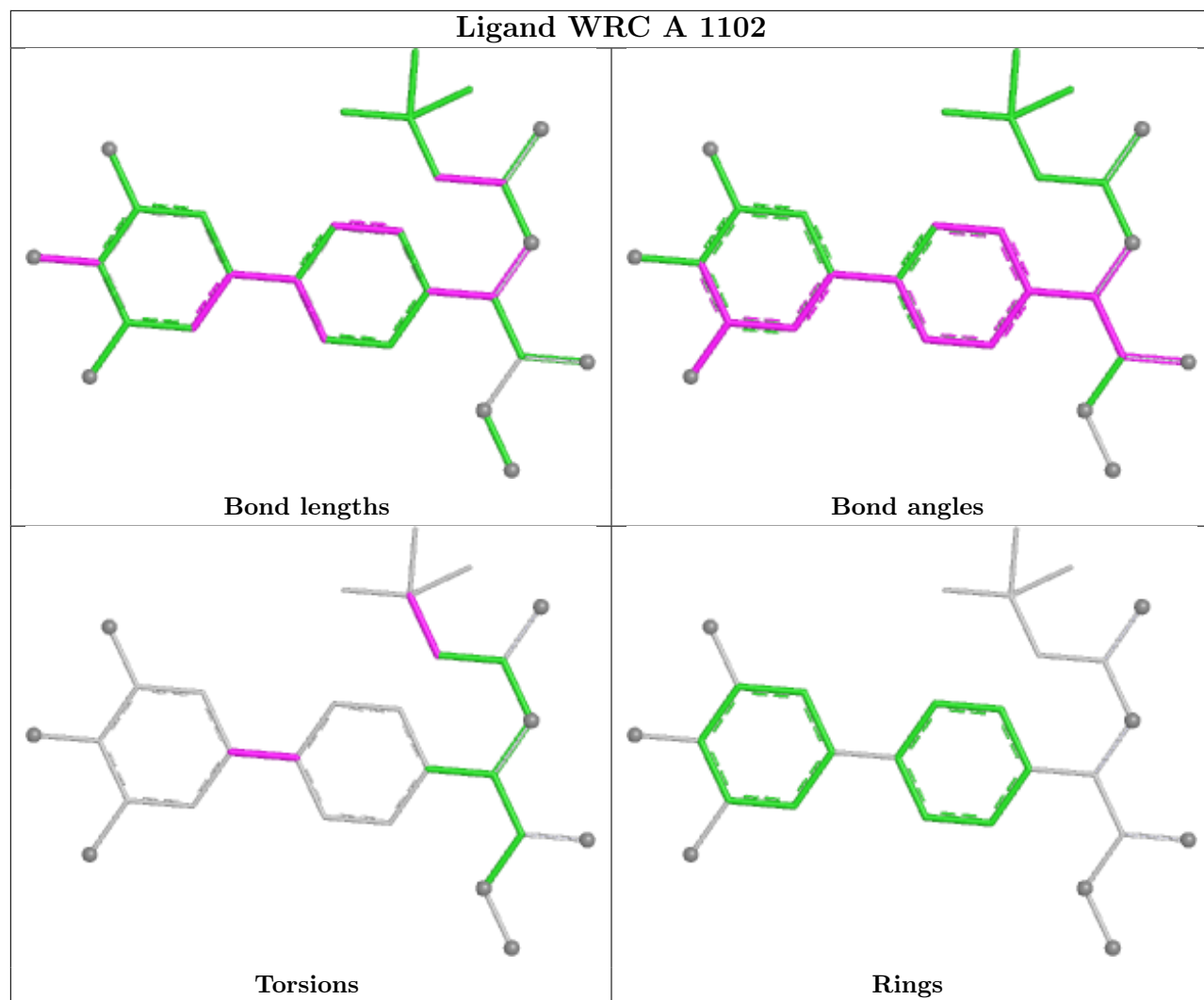
Mol	Chain	Res	Type	Atoms
4	A	1104	GOL	O1-C1-C2-C3
4	A	1105	GOL	O1-C1-C2-O2
4	A	1105	GOL	O1-C1-C2-C3
4	A	1106	GOL	C1-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-C3
3	A	1102	WRC	CAJ-CAW-CAX-CAO
4	A	1103	GOL	C1-C2-C3-O3
4	A	1108	GOL	C1-C2-C3-O3
4	A	1110	GOL	O1-C1-C2-C3
3	A	1102	WRC	CAK-CAW-CAX-CAO
4	A	1106	GOL	O2-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-O2
3	A	1102	WRC	CAJ-CAW-CAX-CAN
4	A	1104	GOL	O1-C1-C2-O2
4	A	1110	GOL	O1-C1-C2-O2
3	A	1102	WRC	CAK-CAW-CAX-CAN
4	A	1106	GOL	O1-C1-C2-O2
4	A	1103	GOL	O2-C2-C3-O3
4	A	1109	GOL	O1-C1-C2-O2
3	A	1102	WRC	CAS-CAP-CBB-CAA

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1105	GOL	2	0
4	A	1107	GOL	1	0
4	A	1109	GOL	1	0
4	A	1104	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	889/1091 (81%)	-0.37	5 (0%) 85 88	7, 19, 33, 51	49 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	VAL	3.3
1	A	196	PRO	2.9
1	A	527	ASN	2.5
1	A	574	PHE	2.2
1	A	815	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 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(Å ²)	Q<0.9
4	GOL	A	1106	6/6	0.74	0.20	25,32,33,36	6
4	GOL	A	1107	6/6	0.76	0.20	58,62,64,65	0

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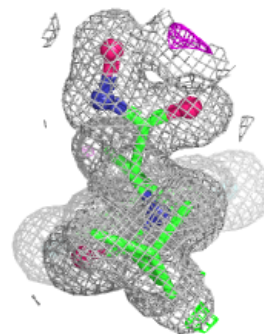
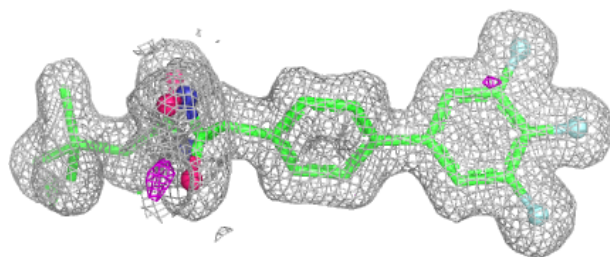
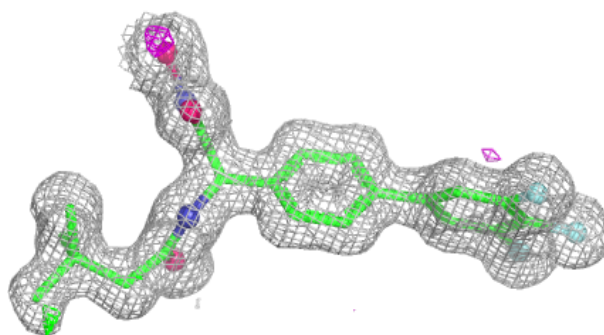
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	1110	6/6	0.81	0.15	52,53,54,57	1
4	GOL	A	1105	6/6	0.83	0.19	39,43,46,51	0
4	GOL	A	1109	6/6	0.83	0.14	24,31,41,42	0
4	GOL	A	1104	6/6	0.83	0.19	57,58,59,59	1
4	GOL	A	1108	6/6	0.90	0.12	22,26,27,28	1
4	GOL	A	1103	6/6	0.93	0.09	24,27,28,28	0
5	MG	A	1112	1/1	0.95	0.16	37,37,37,37	0
5	MG	A	1113	1/1	0.95	0.15	37,37,37,37	0
5	MG	A	1114	1/1	0.96	0.17	32,32,32,32	0
3	WRC	A	1102	28/28	0.98	0.04	9,11,16,23	0
5	MG	A	1115	1/1	0.98	0.16	19,19,19,19	1
5	MG	A	1111	1/1	0.99	0.20	27,27,27,27	0
2	ZN	A	1101	1/1	1.00	0.03	14,14,14,14	1

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 WRC A 1102:

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.