



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 12:33 PM EDT

PDB ID : 6XHT
Title : Crystal structure of S. aureus TarI in complex with CDP-ribitol (space group P1211)
Authors : Li, F.K.K.; Strynadka, N.C.J.
Deposited on : 2020-06-19
Resolution : 1.80 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 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 : 2.18
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) : 2.18

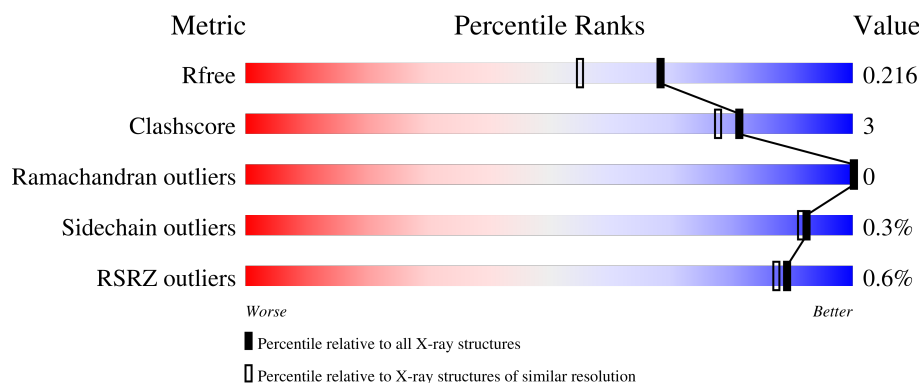
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	261	 83%7%10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12400 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 Ribitol-5-phosphate cytidyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1812	1149	307	350	6			
1	B	236	Total	C	N	O	S	0	0	0
			1811	1148	308	350	5			
1	C	236	Total	C	N	O	S	0	0	0
			1822	1157	309	350	6			
1	D	236	Total	C	N	O	S	0	0	0
			1808	1149	308	345	6			
1	E	230	Total	C	N	O	S	0	0	0
			1776	1130	298	343	5			
1	F	236	Total	C	N	O	S	0	0	0
			1843	1169	317	351	6			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	expression tag	UNP Q2G1C0
A	240	GLY	-	expression tag	UNP Q2G1C0
A	241	SER	-	expression tag	UNP Q2G1C0
A	242	LEU	-	expression tag	UNP Q2G1C0
A	243	VAL	-	expression tag	UNP Q2G1C0
A	244	PRO	-	expression tag	UNP Q2G1C0
A	245	ARG	-	expression tag	UNP Q2G1C0
A	246	GLY	-	expression tag	UNP Q2G1C0
A	247	SER	-	expression tag	UNP Q2G1C0
A	248	ALA	-	expression tag	UNP Q2G1C0
A	249	ALA	-	expression tag	UNP Q2G1C0
A	250	ALA	-	expression tag	UNP Q2G1C0
A	251	ALA	-	expression tag	UNP Q2G1C0
A	252	LEU	-	expression tag	UNP Q2G1C0
A	253	GLU	-	expression tag	UNP Q2G1C0
A	254	HIS	-	expression tag	UNP Q2G1C0
A	255	HIS	-	expression tag	UNP Q2G1C0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	HIS	-	expression tag	UNP Q2G1C0
A	257	HIS	-	expression tag	UNP Q2G1C0
A	258	HIS	-	expression tag	UNP Q2G1C0
A	259	HIS	-	expression tag	UNP Q2G1C0
A	260	HIS	-	expression tag	UNP Q2G1C0
A	261	HIS	-	expression tag	UNP Q2G1C0
B	239	GLY	-	expression tag	UNP Q2G1C0
B	240	GLY	-	expression tag	UNP Q2G1C0
B	241	SER	-	expression tag	UNP Q2G1C0
B	242	LEU	-	expression tag	UNP Q2G1C0
B	243	VAL	-	expression tag	UNP Q2G1C0
B	244	PRO	-	expression tag	UNP Q2G1C0
B	245	ARG	-	expression tag	UNP Q2G1C0
B	246	GLY	-	expression tag	UNP Q2G1C0
B	247	SER	-	expression tag	UNP Q2G1C0
B	248	ALA	-	expression tag	UNP Q2G1C0
B	249	ALA	-	expression tag	UNP Q2G1C0
B	250	ALA	-	expression tag	UNP Q2G1C0
B	251	ALA	-	expression tag	UNP Q2G1C0
B	252	LEU	-	expression tag	UNP Q2G1C0
B	253	GLU	-	expression tag	UNP Q2G1C0
B	254	HIS	-	expression tag	UNP Q2G1C0
B	255	HIS	-	expression tag	UNP Q2G1C0
B	256	HIS	-	expression tag	UNP Q2G1C0
B	257	HIS	-	expression tag	UNP Q2G1C0
B	258	HIS	-	expression tag	UNP Q2G1C0
B	259	HIS	-	expression tag	UNP Q2G1C0
B	260	HIS	-	expression tag	UNP Q2G1C0
B	261	HIS	-	expression tag	UNP Q2G1C0
C	239	GLY	-	expression tag	UNP Q2G1C0
C	240	GLY	-	expression tag	UNP Q2G1C0
C	241	SER	-	expression tag	UNP Q2G1C0
C	242	LEU	-	expression tag	UNP Q2G1C0
C	243	VAL	-	expression tag	UNP Q2G1C0
C	244	PRO	-	expression tag	UNP Q2G1C0
C	245	ARG	-	expression tag	UNP Q2G1C0
C	246	GLY	-	expression tag	UNP Q2G1C0
C	247	SER	-	expression tag	UNP Q2G1C0
C	248	ALA	-	expression tag	UNP Q2G1C0
C	249	ALA	-	expression tag	UNP Q2G1C0
C	250	ALA	-	expression tag	UNP Q2G1C0
C	251	ALA	-	expression tag	UNP Q2G1C0

Continued on next page...

Continued from previous page...

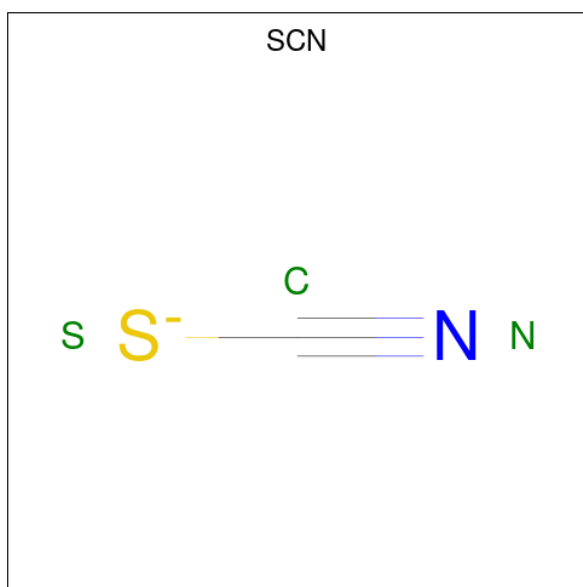
Chain	Residue	Modelled	Actual	Comment	Reference
C	252	LEU	-	expression tag	UNP Q2G1C0
C	253	GLU	-	expression tag	UNP Q2G1C0
C	254	HIS	-	expression tag	UNP Q2G1C0
C	255	HIS	-	expression tag	UNP Q2G1C0
C	256	HIS	-	expression tag	UNP Q2G1C0
C	257	HIS	-	expression tag	UNP Q2G1C0
C	258	HIS	-	expression tag	UNP Q2G1C0
C	259	HIS	-	expression tag	UNP Q2G1C0
C	260	HIS	-	expression tag	UNP Q2G1C0
C	261	HIS	-	expression tag	UNP Q2G1C0
D	239	GLY	-	expression tag	UNP Q2G1C0
D	240	GLY	-	expression tag	UNP Q2G1C0
D	241	SER	-	expression tag	UNP Q2G1C0
D	242	LEU	-	expression tag	UNP Q2G1C0
D	243	VAL	-	expression tag	UNP Q2G1C0
D	244	PRO	-	expression tag	UNP Q2G1C0
D	245	ARG	-	expression tag	UNP Q2G1C0
D	246	GLY	-	expression tag	UNP Q2G1C0
D	247	SER	-	expression tag	UNP Q2G1C0
D	248	ALA	-	expression tag	UNP Q2G1C0
D	249	ALA	-	expression tag	UNP Q2G1C0
D	250	ALA	-	expression tag	UNP Q2G1C0
D	251	ALA	-	expression tag	UNP Q2G1C0
D	252	LEU	-	expression tag	UNP Q2G1C0
D	253	GLU	-	expression tag	UNP Q2G1C0
D	254	HIS	-	expression tag	UNP Q2G1C0
D	255	HIS	-	expression tag	UNP Q2G1C0
D	256	HIS	-	expression tag	UNP Q2G1C0
D	257	HIS	-	expression tag	UNP Q2G1C0
D	258	HIS	-	expression tag	UNP Q2G1C0
D	259	HIS	-	expression tag	UNP Q2G1C0
D	260	HIS	-	expression tag	UNP Q2G1C0
D	261	HIS	-	expression tag	UNP Q2G1C0
E	239	GLY	-	expression tag	UNP Q2G1C0
E	240	GLY	-	expression tag	UNP Q2G1C0
E	241	SER	-	expression tag	UNP Q2G1C0
E	242	LEU	-	expression tag	UNP Q2G1C0
E	243	VAL	-	expression tag	UNP Q2G1C0
E	244	PRO	-	expression tag	UNP Q2G1C0
E	245	ARG	-	expression tag	UNP Q2G1C0
E	246	GLY	-	expression tag	UNP Q2G1C0
E	247	SER	-	expression tag	UNP Q2G1C0

Continued on next page...

Continued from previous page...

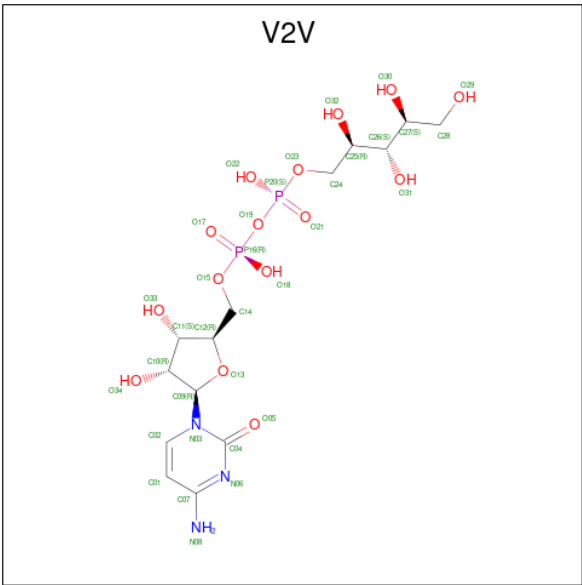
Chain	Residue	Modelled	Actual	Comment	Reference
E	248	ALA	-	expression tag	UNP Q2G1C0
E	249	ALA	-	expression tag	UNP Q2G1C0
E	250	ALA	-	expression tag	UNP Q2G1C0
E	251	ALA	-	expression tag	UNP Q2G1C0
E	252	LEU	-	expression tag	UNP Q2G1C0
E	253	GLU	-	expression tag	UNP Q2G1C0
E	254	HIS	-	expression tag	UNP Q2G1C0
E	255	HIS	-	expression tag	UNP Q2G1C0
E	256	HIS	-	expression tag	UNP Q2G1C0
E	257	HIS	-	expression tag	UNP Q2G1C0
E	258	HIS	-	expression tag	UNP Q2G1C0
E	259	HIS	-	expression tag	UNP Q2G1C0
E	260	HIS	-	expression tag	UNP Q2G1C0
E	261	HIS	-	expression tag	UNP Q2G1C0
F	239	GLY	-	expression tag	UNP Q2G1C0
F	240	GLY	-	expression tag	UNP Q2G1C0
F	241	SER	-	expression tag	UNP Q2G1C0
F	242	LEU	-	expression tag	UNP Q2G1C0
F	243	VAL	-	expression tag	UNP Q2G1C0
F	244	PRO	-	expression tag	UNP Q2G1C0
F	245	ARG	-	expression tag	UNP Q2G1C0
F	246	GLY	-	expression tag	UNP Q2G1C0
F	247	SER	-	expression tag	UNP Q2G1C0
F	248	ALA	-	expression tag	UNP Q2G1C0
F	249	ALA	-	expression tag	UNP Q2G1C0
F	250	ALA	-	expression tag	UNP Q2G1C0
F	251	ALA	-	expression tag	UNP Q2G1C0
F	252	LEU	-	expression tag	UNP Q2G1C0
F	253	GLU	-	expression tag	UNP Q2G1C0
F	254	HIS	-	expression tag	UNP Q2G1C0
F	255	HIS	-	expression tag	UNP Q2G1C0
F	256	HIS	-	expression tag	UNP Q2G1C0
F	257	HIS	-	expression tag	UNP Q2G1C0
F	258	HIS	-	expression tag	UNP Q2G1C0
F	259	HIS	-	expression tag	UNP Q2G1C0
F	260	HIS	-	expression tag	UNP Q2G1C0
F	261	HIS	-	expression tag	UNP Q2G1C0

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	C	1	Total	C	N	S	0	0
			3	1	1	1		
2	C	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		
2	E	1	Total	C	N	S	0	0
			3	1	1	1		
2	F	1	Total	C	N	S	0	0
			3	1	1	1		
2	F	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 3 is CDP-ribitol (three-letter code: V2V) (formula: $C_{14}H_{25}N_3O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			34	14	3	15	2		
3	E	1	Total	C	N	O	P	0	0
			34	14	3	15	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	281	Total	O	0	0
			281	281		
4	B	283	Total	O	0	0
			283	283		
4	C	212	Total	O	0	0
			212	212		
4	D	214	Total	O	0	0
			214	214		
4	E	213	Total	O	0	0
			213	213		
4	F	224	Total	O	0	0
			224	224		

- Molecule 1: Ribitol-5-phosphate cytidyltransferase 1



HIS
HIS
HIS
HIS
HIS
HIS
HIS

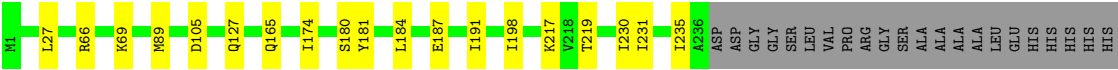
● Molecule 1: Ribitol-5-phosphate cytidyltransferase 1

Chain F:

83%

7%

10%



HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.73Å 138.60Å 109.53Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	50.65 – 1.80 50.65 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.65-1.80) 98.2 (50.65-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.170 , 0.217 0.169 , 0.216	Depositor DCC
R_{free} test set	6772 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	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	12400	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: V2V, SCN

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	0.56	0/1839	0.64	0/2497
1	B	0.54	0/1838	0.66	0/2499
1	C	0.49	0/1849	0.62	0/2511
1	D	0.49	0/1835	0.61	0/2493
1	E	0.51	0/1802	0.62	0/2451
1	F	0.51	0/1870	0.62	0/2535
All	All	0.52	0/11033	0.63	0/14986

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	1812	0	1837	9	0
1	B	1811	0	1819	4	0
1	C	1822	0	1848	8	0
1	D	1808	0	1827	11	0
1	E	1776	0	1790	10	0
1	F	1843	0	1889	13	0
2	A	6	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
2	E	3	0	0	0	0
2	F	6	0	0	0	0
3	B	34	0	0	2	0
3	E	34	0	0	2	0
4	A	281	0	0	1	0
4	B	283	0	0	0	0
4	C	212	0	0	0	0
4	D	214	0	0	0	0
4	E	213	0	0	0	0
4	F	224	0	0	3	0
All	All	12400	0	11010	58	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 3.

All (58) 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)
3:B:301:V2V:C12	3:B:301:V2V:O13	1.65	1.25
3:E:301:V2V:C12	3:E:301:V2V:O13	1.66	1.23
1:E:176:LEU:HD11	1:E:204:LYS:HD3	1.56	0.86
3:B:301:V2V:O13	3:B:301:V2V:C14	2.47	0.61
1:F:127:GLN:NE2	4:F:403:HOH:O	2.33	0.60
1:D:142:ILE:HD11	1:D:213:LEU:HD22	1.84	0.58
1:F:184:LEU:HD21	1:F:198:ILE:HG23	1.86	0.57
1:E:132:TYR:CD2	1:E:207:ARG:HG3	2.40	0.56
3:E:301:V2V:O13	3:E:301:V2V:C14	2.50	0.55
1:E:132:TYR:CG	1:E:207:ARG:HG3	2.42	0.54
1:A:20:LEU:HD23	2:A:302:SCN:N	2.22	0.54
1:A:26:ASP:OD1	1:A:29:ASN:HA	2.08	0.53
1:B:142:ILE:O	1:B:160:ARG:NH1	2.42	0.53
1:A:67:LYS:HD3	1:A:68:PHE:CE2	2.43	0.53
1:D:230:ILE:HG23	1:D:235:ILE:HB	1.92	0.51
1:E:94:HIS:O	1:E:98:THR:HG23	2.11	0.51
1:D:230:ILE:HA	1:D:235:ILE:HD12	1.93	0.50
1:A:176:LEU:C	1:A:176:LEU:HD23	2.32	0.50
1:C:142:ILE:HG13	1:C:143:ASP:N	2.27	0.50
1:E:18:VAL:HG13	1:E:25:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:GLY:O	1:E:11:ILE:HG12	2.13	0.49
1:C:41:ILE:HD11	1:C:75:ILE:HD11	1.92	0.49
1:B:48:LYS:HE2	2:B:303:SCN:N	2.28	0.48
1:C:21:PRO:HB2	1:C:24:PHE:HD2	1.77	0.48
1:A:228:ASN:O	1:A:231:ILE:HG22	2.13	0.47
1:F:127:GLN:OE1	4:F:401:HOH:O	2.20	0.47
1:F:105:ASP:HB3	1:F:174:ILE:HD12	1.96	0.47
1:C:63:ASP:OD2	1:C:66:ARG:NH2	2.45	0.47
1:A:207:ARG:NH2	4:A:401:HOH:O	2.21	0.46
1:B:56:GLN:HG2	1:B:57:TRP:CD1	2.50	0.46
1:D:128:ALA:HB3	1:D:135:VAL:HG21	1.98	0.46
1:F:230:ILE:HA	1:F:235:ILE:HD12	1.98	0.45
1:E:43:ILE:HG13	1:E:122:ILE:HG21	1.99	0.45
1:D:43:ILE:HG13	1:D:122:ILE:HG21	2.00	0.44
1:D:22:LYS:HD3	2:D:302:SCN:C	2.47	0.44
1:B:113:VAL:HG23	1:B:217:LYS:HG3	1.99	0.44
1:E:178:LYS:HB3	1:E:178:LYS:HE2	1.73	0.43
1:F:69:LYS:HA	1:F:69:LYS:HD2	1.83	0.43
1:A:105:ASP:HB3	1:A:174:ILE:HD12	2.00	0.43
1:D:21:PRO:HB2	1:D:24:PHE:HD2	1.84	0.43
1:F:217:LYS:HG2	1:F:219:THR:HG23	2.01	0.42
1:C:168:THR:HB	1:C:169:PRO:HA	2.01	0.42
1:F:181:TYR:HA	1:F:184:LEU:HD23	2.02	0.42
1:D:37:LEU:HD11	1:D:51:ILE:HD11	2.02	0.41
1:D:168:THR:HB	1:D:169:PRO:HA	2.01	0.41
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.88	0.41
1:A:165:GLN:HE21	1:A:165:GLN:HB3	1.77	0.41
1:F:187:GLU:O	1:F:191:ILE:HG12	2.21	0.41
1:E:113:VAL:HG23	1:E:217:LYS:HG3	2.02	0.41
1:C:164:TYR:CE2	1:D:148:SER:HB3	2.56	0.41
1:F:66:ARG:HD2	4:F:404:HOH:O	2.21	0.41
1:C:54:PRO:HD2	1:C:57:TRP:CE3	2.56	0.41
1:F:89:MET:HG3	1:F:181:TYR:CD1	2.56	0.41
1:D:141:ALA:HA	1:D:165:GLN:HG3	2.02	0.40
1:F:27:LEU:HD11	1:F:231:ILE:HG13	2.04	0.40
1:A:21:PRO:HB2	1:A:24:PHE:HD2	1.87	0.40
1:F:180:SER:O	1:F:184:LEU:HD22	2.21	0.40
1:E:110:HIS:CE1	1:E:117:LEU:HD13	2.55	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	231/261 (88%)	224 (97%)	7 (3%)	0	100	100
1	B	234/261 (90%)	229 (98%)	5 (2%)	0	100	100
1	C	234/261 (90%)	228 (97%)	6 (3%)	0	100	100
1	D	234/261 (90%)	230 (98%)	4 (2%)	0	100	100
1	E	226/261 (87%)	222 (98%)	4 (2%)	0	100	100
1	F	234/261 (90%)	228 (97%)	6 (3%)	0	100	100
All	All	1393/1566 (89%)	1361 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/227 (89%)	202 (100%)	0	100	100
1	B	198/227 (87%)	198 (100%)	0	100	100
1	C	201/227 (88%)	201 (100%)	0	100	100
1	D	197/227 (87%)	196 (100%)	1 (0%)	88	87
1	E	196/227 (86%)	195 (100%)	1 (0%)	88	87
1	F	205/227 (90%)	204 (100%)	1 (0%)	88	87
All	All	1199/1362 (88%)	1196 (100%)	3 (0%)	92	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	190	SER
1	E	165	GLN
1	F	165	GLN

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SCN	E	302	-	1,2,2	0.41	0	0,1,1	0.00	-
2	SCN	B	302	-	1,2,2	0.46	0	0,1,1	0.00	-
2	SCN	C	302	-	1,2,2	0.61	0	0,1,1	0.00	-
2	SCN	B	303	-	1,2,2	0.43	0	0,1,1	0.00	-
3	V2V	B	301	-	30,35,35	3.71	14 (46%)	37,52,52	1.54	4 (10%)
3	V2V	E	301	-	30,35,35	3.89	15 (50%)	37,52,52	1.20	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCN	C	301	-	1,2,2	0.43	0	0,1,1	0.00	-
2	SCN	D	301	-	1,2,2	0.75	0	0,1,1	0.00	-
2	SCN	D	302	-	1,2,2	0.61	0	0,1,1	0.00	-
2	SCN	F	302	-	1,2,2	0.47	0	0,1,1	0.00	-
2	SCN	F	301	-	1,2,2	0.42	0	0,1,1	0.00	-
2	SCN	A	301	-	1,2,2	0.48	0	0,1,1	0.00	-
2	SCN	A	302	-	1,2,2	1.16	0	0,1,1	0.00	-

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	V2V	B	301	-	-	6/30/48/48	0/2/2/2
3	V2V	E	301	-	-	5/30/48/48	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	V2V	O13-C12	9.47	1.66	1.45
3	B	301	V2V	O13-C12	9.17	1.65	1.45
3	B	301	V2V	O13-C09	-8.72	1.28	1.41
3	E	301	V2V	C11-C12	-8.27	1.31	1.53
3	E	301	V2V	O13-C09	-8.17	1.29	1.41
3	B	301	V2V	C11-C12	-7.71	1.33	1.53
3	B	301	V2V	C02-N03	7.58	1.45	1.35
3	E	301	V2V	C02-N03	7.40	1.45	1.35
3	E	301	V2V	C07-N06	6.10	1.45	1.35
3	B	301	V2V	C07-N06	5.06	1.43	1.35
3	E	301	V2V	C04-N06	5.00	1.48	1.38
3	E	301	V2V	C24-C25	4.78	1.58	1.51
3	E	301	V2V	C02-C01	4.71	1.48	1.38
3	B	301	V2V	C10-C09	4.55	1.60	1.53
3	B	301	V2V	C04-N06	4.20	1.46	1.38
3	B	301	V2V	C24-C25	4.10	1.57	1.51
3	E	301	V2V	O34-C10	-3.55	1.34	1.43
3	E	301	V2V	C07-N08	3.52	1.45	1.35
3	B	301	V2V	C02-C01	3.49	1.45	1.38
3	E	301	V2V	C01-C07	3.11	1.48	1.41
3	B	301	V2V	C07-N08	3.04	1.44	1.35
3	E	301	V2V	C10-C09	2.82	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	V2V	O33-C11	2.72	1.49	1.43
3	B	301	V2V	P16-O15	2.60	1.69	1.59
3	B	301	V2V	O33-C11	2.38	1.48	1.43
3	B	301	V2V	C01-C07	2.33	1.46	1.41
3	E	301	V2V	P16-O15	2.28	1.68	1.59
3	E	301	V2V	C11-C10	2.13	1.59	1.53
3	B	301	V2V	C11-C10	2.02	1.58	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	V2V	C04-N06-C07	5.65	122.07	116.34
3	E	301	V2V	C04-N06-C07	3.49	119.88	116.34
3	B	301	V2V	N08-C07-N06	2.66	120.70	116.49
3	E	301	V2V	O13-C09-C10	-2.29	103.58	106.93
3	B	301	V2V	O13-C12-C14	-2.20	102.15	109.37
3	B	301	V2V	O13-C09-C10	-2.05	103.92	106.93

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	V2V	C10-C09-N03-C02
3	E	301	V2V	C10-C09-N03-C02
3	B	301	V2V	O31-C26-C27-C28
3	B	301	V2V	C25-C26-C27-C28
3	B	301	V2V	O31-C26-C27-O30
3	E	301	V2V	O31-C26-C27-O30
3	E	301	V2V	O31-C26-C27-C28
3	B	301	V2V	C25-C26-C27-O30
3	E	301	V2V	C25-C26-C27-C28
3	E	301	V2V	C25-C26-C27-O30
3	B	301	V2V	C24-O23-P20-O21

There are no ring outliers.

5 monomers are involved in 7 short contacts:

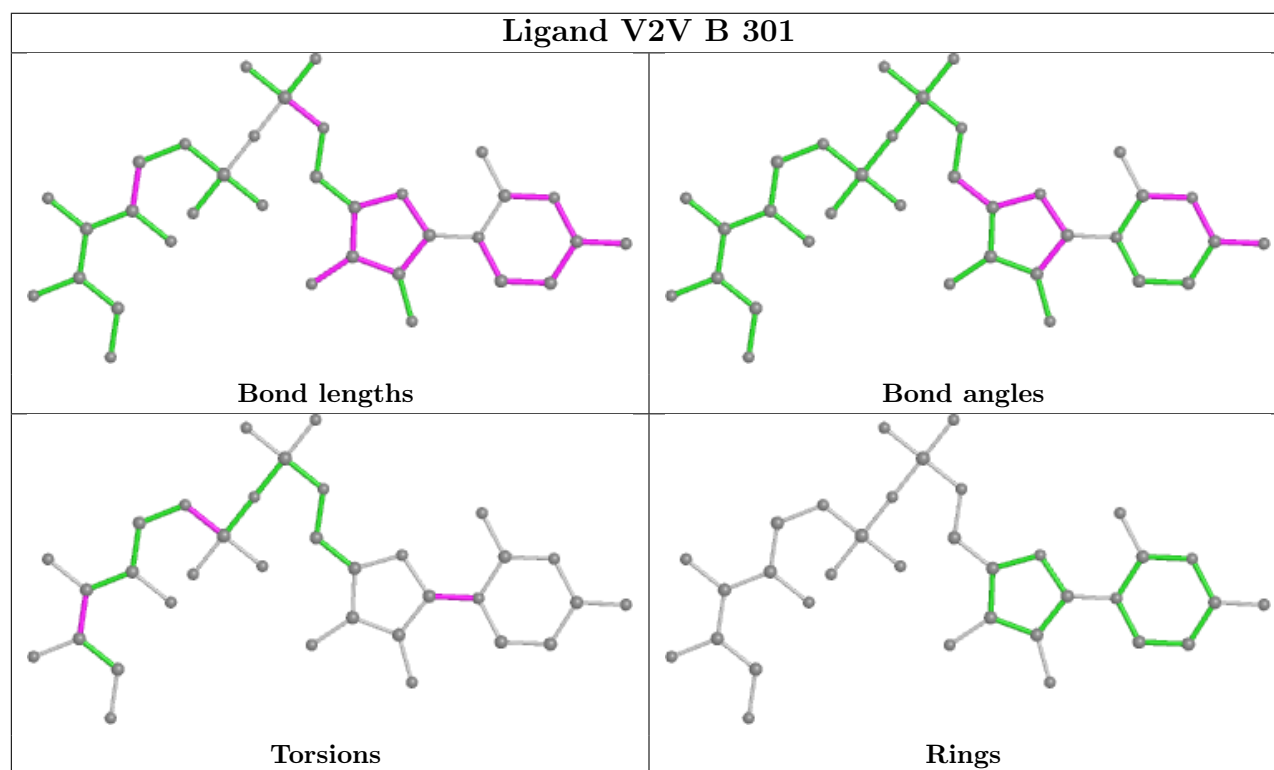
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	SCN	1	0
3	B	301	V2V	2	0
3	E	301	V2V	2	0

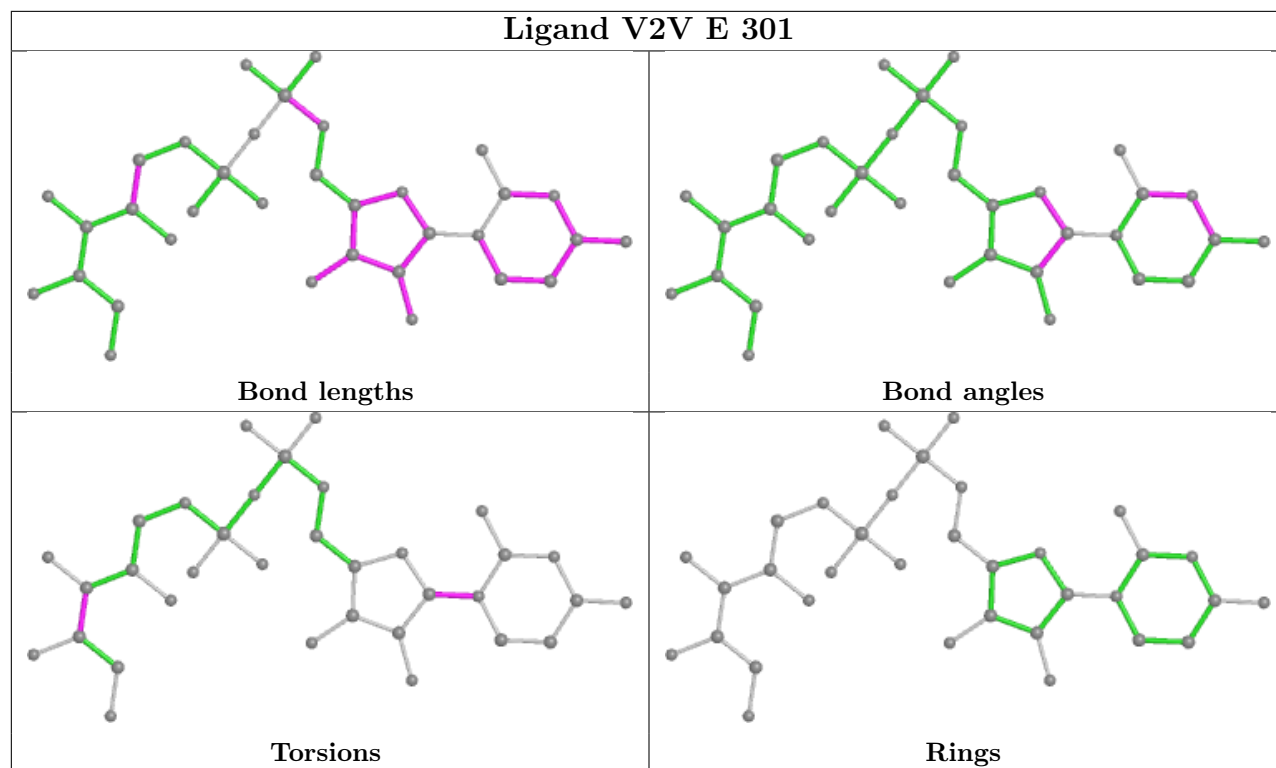
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	SCN	1	0
2	A	302	SCN	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 [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	233/261 (89%)	-0.58	0	100	100	16, 23, 42, 57	0
1	B	236/261 (90%)	-0.55	2 (0%)	86	84	15, 24, 49, 85	0
1	C	236/261 (90%)	-0.47	3 (1%)	77	74	18, 32, 63, 76	0
1	D	236/261 (90%)	-0.51	2 (0%)	86	84	20, 31, 61, 77	0
1	E	230/261 (88%)	-0.45	2 (0%)	84	82	18, 31, 57, 86	0
1	F	236/261 (90%)	-0.54	0	100	100	18, 28, 55, 84	0
All	All	1407/1566 (89%)	-0.52	9 (0%)	89	87	15, 28, 55, 86	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	PRO	4.9
1	D	185	SER	2.8
1	E	11	ILE	2.8
1	D	191	ILE	2.7
1	E	18	VAL	2.7
1	C	161	ASN	2.4
1	B	13	SER	2.4
1	C	193	SER	2.2
1	C	235	ILE	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 monosaccharides in this entry.

6.4 Ligands

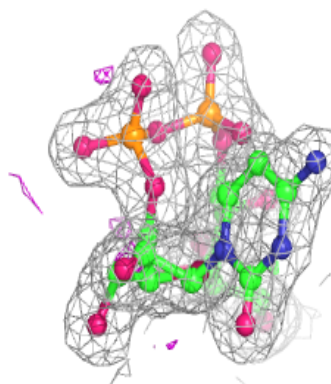
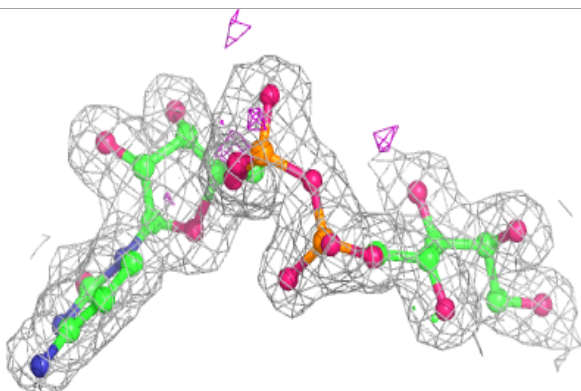
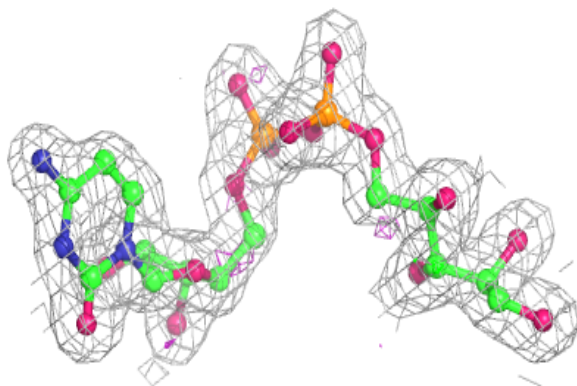
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SCN	B	303	3/3	0.95	0.11	46,46,50,55	0
2	SCN	F	302	3/3	0.95	0.10	45,45,52,60	0
3	V2V	E	301	34/34	0.96	0.08	20,25,29,30	0
2	SCN	D	302	3/3	0.97	0.09	53,53,61,67	0
2	SCN	E	302	3/3	0.98	0.17	42,42,48,55	0
2	SCN	D	301	3/3	0.98	0.10	23,23,24,25	0
3	V2V	B	301	34/34	0.98	0.08	15,20,23,24	0
2	SCN	B	302	3/3	0.98	0.10	37,37,42,45	0
2	SCN	C	301	3/3	0.99	0.07	21,21,23,24	0
2	SCN	F	301	3/3	0.99	0.07	21,21,23,24	0
2	SCN	C	302	3/3	0.99	0.25	40,40,50,59	0
2	SCN	A	301	3/3	0.99	0.08	22,22,24,26	0
2	SCN	A	302	3/3	0.99	0.07	27,27,29,32	0

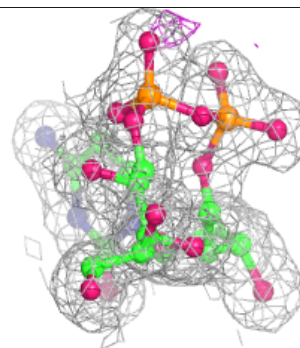
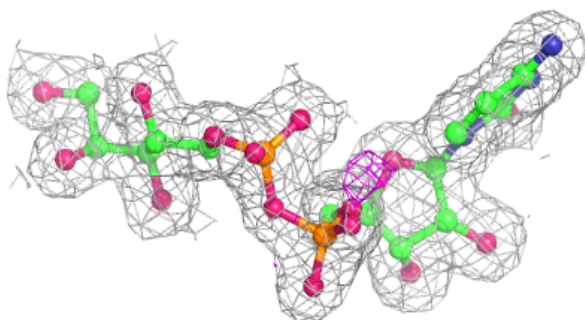
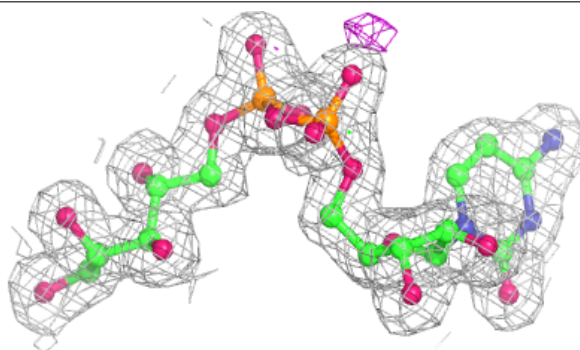
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V2V E 301:

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

**Electron density around V2V B 301:**

$2mF_o-DF_c$ (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.