



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:28 AM UTC

PDB ID : 2G9Z / pdb_00002g9z
Title : Thiamin pyrophosphokinase from *Candida albicans*
Authors : Abergel, C.; Santini, S.; Monchois, V.; Rousselle, T.; Claverie, J.M.; Bacterial targets at IGS-CNRS, France (BIGS)
Deposited on : 2006-03-07
Resolution : 1.96 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

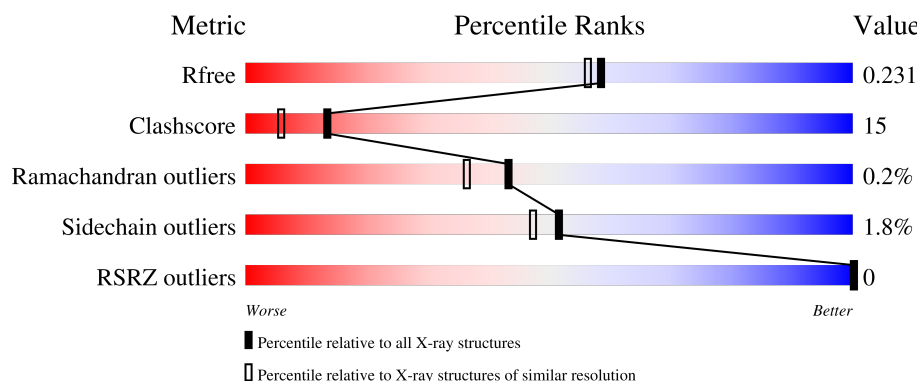
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	348	
1	B	348	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	707	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5365 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 thiamine pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2394	1536	384	464	10			
1	B	295	Total	C	N	O	S	0	0	0
			2381	1528	382	461	10			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q59N99
A	-11	ALA	-	expression tag	UNP Q59N99
A	-10	HIS	-	expression tag	UNP Q59N99
A	-9	HIS	-	expression tag	UNP Q59N99
A	-8	HIS	-	expression tag	UNP Q59N99
A	-7	HIS	-	expression tag	UNP Q59N99
A	-6	HIS	-	expression tag	UNP Q59N99
A	-5	HIS	-	expression tag	UNP Q59N99
A	-4	GLY	-	expression tag	UNP Q59N99
A	-3	HIS	-	expression tag	UNP Q59N99
A	-2	HIS	-	expression tag	UNP Q59N99
A	-1	HIS	-	expression tag	UNP Q59N99
A	0	GLN	-	expression tag	UNP Q59N99
A	1	LEU	-	expression tag	UNP Q59N99
A	327	GLN	-	expression tag	UNP Q59N99
A	328	LEU	-	expression tag	UNP Q59N99
A	329	ASP	-	expression tag	UNP Q59N99
A	330	GLY	-	expression tag	UNP Q59N99
A	331	ASP	-	expression tag	UNP Q59N99
A	332	LEU	-	expression tag	UNP Q59N99
A	333	GLU	-	expression tag	UNP Q59N99
A	334	ALA	-	expression tag	UNP Q59N99
A	335	ALA	-	expression tag	UNP Q59N99
B	-12	MET	-	expression tag	UNP Q59N99
B	-11	ALA	-	expression tag	UNP Q59N99

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q59N99
B	-9	HIS	-	expression tag	UNP Q59N99
B	-8	HIS	-	expression tag	UNP Q59N99
B	-7	HIS	-	expression tag	UNP Q59N99
B	-6	HIS	-	expression tag	UNP Q59N99
B	-5	HIS	-	expression tag	UNP Q59N99
B	-4	GLY	-	expression tag	UNP Q59N99
B	-3	HIS	-	expression tag	UNP Q59N99
B	-2	HIS	-	expression tag	UNP Q59N99
B	-1	HIS	-	expression tag	UNP Q59N99
B	0	GLN	-	expression tag	UNP Q59N99
B	1	LEU	-	expression tag	UNP Q59N99
B	327	GLN	-	expression tag	UNP Q59N99
B	328	LEU	-	expression tag	UNP Q59N99
B	329	ASP	-	expression tag	UNP Q59N99
B	330	GLY	-	expression tag	UNP Q59N99
B	331	ASP	-	expression tag	UNP Q59N99
B	332	LEU	-	expression tag	UNP Q59N99
B	333	GLU	-	expression tag	UNP Q59N99
B	334	ALA	-	expression tag	UNP Q59N99
B	335	ALA	-	expression tag	UNP Q59N99

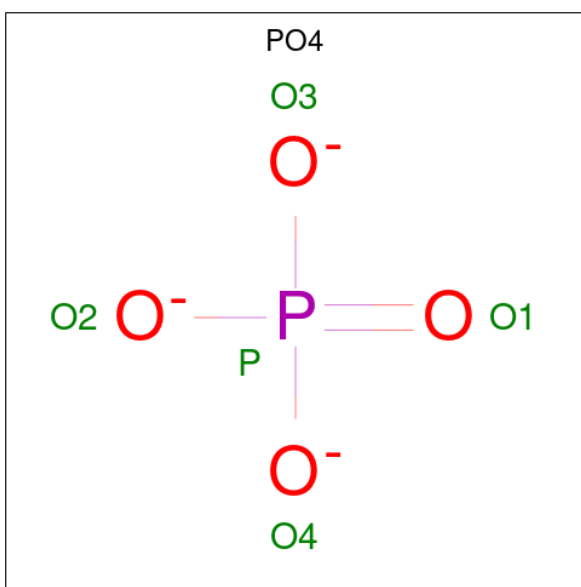
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

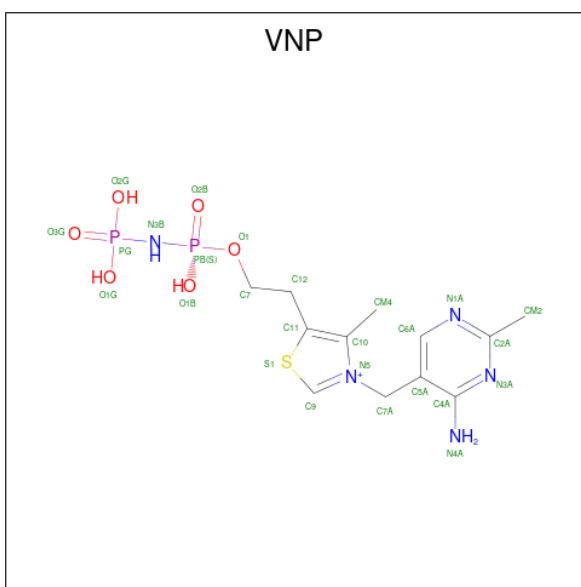
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-(2-{[HYDROXY (PHOSPHONOAMINO)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-UM (CCD ID: VNP) (formula: C₁₂H₂₀N₅O₆P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			26	12	5	6	2	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			26	12	5	6	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	265	Total	O	0	0
			265	265		
6	B	255	Total	O	0	0
			255	255		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.83Å 60.33Å 63.72Å 66.14° 89.94° 65.07°	Depositor
Resolution (Å)	29.44 – 1.96 29.44 – 1.96	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.44-1.96) 91.6 (29.44-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.187 , 0.236 0.185 , 0.231	Depositor DCC
R_{free} test set	4073 reflections (9.23%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.486 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5365	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% 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: VNP, MG, PO4, CL

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	0.35	0/2445	0.89	7/3319 (0.2%)
1	B	0.35	0/2432	0.90	8/3301 (0.2%)
All	All	0.35	0/4877	0.89	15/6620 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	GLU	N-CA-C	7.23	121.00	111.75
1	A	57	ASN	N-CA-C	7.04	121.19	108.17
1	B	302	ASN	N-CA-C	-7.01	101.48	110.53
1	B	57	ASN	N-CA-C	6.96	120.62	108.52
1	A	302	ASN	N-CA-C	-6.83	101.72	110.53
1	B	259	SER	N-CA-C	-6.54	105.03	114.12
1	A	233	ASP	N-CA-C	6.15	116.35	108.24
1	A	204	PHE	N-CA-C	6.01	117.83	111.28
1	B	233	ASP	N-CA-C	5.82	115.93	108.24
1	A	238	LEU	N-CA-C	-5.70	100.39	109.96
1	B	157	ASN	N-CA-C	5.55	117.00	111.07
1	A	37	PHE	N-CA-C	5.45	118.93	112.72
1	A	157	ASN	N-CA-C	5.25	117.41	111.11
1	B	204	PHE	N-CA-C	5.14	116.88	111.28
1	B	126	GLU	N-CA-C	-5.03	105.80	111.28

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	2394	0	2344	78	0
1	B	2381	0	2330	71	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	3	0
4	B	5	0	0	0	0
5	A	26	0	17	0	0
5	B	26	0	17	1	0
6	A	265	0	0	11	0
6	B	255	0	0	7	0
All	All	5365	0	4708	140	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 15.

All (140) 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:138:GLN:HE22	4:A:707:PO4:P	1.93	0.90
1:B:58:GLN:HB2	1:B:198:ASN:HB3	1.53	0.87
1:A:248:LYS:HB3	1:A:252:MET:SD	2.15	0.85
1:A:58:GLN:HB2	1:A:198:ASN:HB3	1.57	0.85
1:A:122:LYS:O	1:A:126:GLU:HG3	1.77	0.84
1:B:122:LYS:O	1:B:126:GLU:HG3	1.80	0.82
1:A:252:MET:HE1	6:A:1019:HOH:O	1.85	0.76
1:A:294:MET:O	1:A:295:LEU:HB2	1.87	0.74
1:A:228:PHE:HB3	6:A:1014:HOH:O	1.88	0.72
1:A:138:GLN:NE2	4:A:707:PO4:O2	2.24	0.71
1:A:160:LYS:HE3	1:A:163:TRP:HA	1.75	0.69
1:B:258:GLY:HA3	6:B:975:HOH:O	1.93	0.69
1:A:277:ILE:CD1	1:A:291:LYS:HG2	2.22	0.69
1:B:56:LEU:HD12	1:B:199:ALA:HA	1.76	0.68
1:B:135:GLN:NE2	1:B:173:LEU:H	1.92	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLN:HE22	1:A:212:ASN:HD22	1.44	0.66
1:A:271:SER:HB2	1:B:295:LEU:HD13	1.79	0.65
1:B:218:ASN:OD1	1:B:239:LYS:HE2	1.97	0.64
1:B:155:GLN:HE22	1:B:187:VAL:CG2	2.10	0.64
1:B:277:ILE:CD1	1:B:291:LYS:HG2	2.27	0.64
1:A:135:GLN:NE2	1:A:173:LEU:H	1.96	0.63
1:B:101:GLN:HB2	1:B:104:ASP:OD2	1.99	0.62
1:B:171:ASP:OD1	1:B:175:LYS:HE3	1.99	0.62
1:B:58:GLN:HB2	1:B:198:ASN:CB	2.26	0.61
1:A:135:GLN:HE22	1:A:173:LEU:H	1.46	0.61
1:A:138:GLN:NE2	4:A:707:PO4:O4	2.34	0.60
1:B:249:ASN:O	1:B:252:MET:HG2	2.01	0.60
1:B:248:LYS:H	1:B:252:MET:HE3	1.67	0.58
1:B:135:GLN:HE22	1:B:173:LEU:H	1.52	0.58
1:B:187:VAL:HG23	1:B:187:VAL:O	2.03	0.58
1:A:58:GLN:HB2	1:A:198:ASN:CB	2.31	0.57
1:A:131:LYS:NZ	1:A:157:ASN:HD21	2.02	0.56
1:B:86:GLU:HG2	1:B:89:ASN:HD21	1.72	0.55
1:B:155:GLN:HE22	1:B:187:VAL:HG23	1.70	0.55
1:B:155:GLN:OE1	1:B:187:VAL:HG22	2.07	0.55
1:B:188:VAL:HG12	1:B:188:VAL:O	2.07	0.55
1:B:294:MET:O	1:B:295:LEU:HB2	2.06	0.55
1:A:245:ILE:N	1:A:245:ILE:HD12	2.22	0.55
1:A:277:ILE:HD13	1:A:291:LYS:HG2	1.90	0.54
1:B:156:LEU:O	1:B:159:THR:HG22	2.07	0.54
1:B:123:THR:HG21	6:B:1029:HOH:O	2.06	0.54
1:A:171:ASP:OD1	1:A:175:LYS:HE3	2.07	0.54
1:A:271:SER:HB2	1:B:295:LEU:CD1	2.38	0.54
1:B:245:ILE:HD12	1:B:245:ILE:N	2.23	0.54
1:A:209:GLN:NE2	1:A:213:GLN:HE21	2.06	0.53
1:B:277:ILE:HD13	1:B:291:LYS:HG2	1.90	0.53
1:B:65:ILE:HG22	1:B:69:LYS:HE3	1.90	0.53
1:A:89:ASN:HD22	1:A:102:ARG:HH22	1.56	0.53
1:A:270:LEU:O	1:B:294:MET:HG3	2.09	0.53
1:B:135:GLN:HB2	1:B:145:LYS:HD3	1.91	0.53
1:A:326:VAL:O	1:A:326:VAL:HG22	2.08	0.52
1:B:131:LYS:NZ	1:B:157:ASN:HD21	2.06	0.52
1:A:209:GLN:HE21	1:A:213:GLN:HE21	1.55	0.52
1:B:252:MET:HB3	6:B:1008:HOH:O	2.09	0.52
1:A:62:ILE:HD13	1:A:197:LEU:HD21	1.91	0.52
1:A:101:GLN:HB2	1:A:104:ASP:OD2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:HB3	6:A:1029:HOH:O	2.08	0.51
1:A:89:ASN:ND2	1:A:102:ARG:NH2	2.58	0.51
1:B:248:LYS:N	1:B:252:MET:HE3	2.24	0.51
1:A:203:ARG:CZ	1:B:264:THR:HG21	2.41	0.51
1:A:230:THR:HG22	6:A:1014:HOH:O	2.10	0.51
1:A:209:GLN:NE2	1:A:212:ASN:HD22	2.07	0.50
1:A:294:MET:HG3	1:B:270:LEU:O	2.11	0.50
1:B:233:ASP:HB3	1:B:323:GLU:HA	1.92	0.50
1:B:56:LEU:HD12	1:B:199:ALA:CA	2.41	0.50
1:A:264:THR:HG21	1:B:203:ARG:CZ	2.42	0.50
1:A:223:LYS:HE3	6:A:996:HOH:O	2.12	0.49
1:B:65:ILE:HD12	1:B:105:TYR:CZ	2.48	0.49
1:A:213:GLN:O	1:A:217:MET:HG3	2.13	0.49
1:B:267:LEU:HD12	1:B:267:LEU:N	2.28	0.49
1:A:111:VAL:HG23	1:A:112:GLY:N	2.28	0.48
1:B:114:PHE:CE2	1:B:134:ARG:HB2	2.48	0.48
1:A:249:ASN:HA	1:A:307:GLU:O	2.14	0.48
1:B:209:GLN:HE22	1:B:212:ASN:HD22	1.60	0.48
1:A:223:LYS:HB2	6:A:863:HOH:O	2.13	0.48
1:B:209:GLN:HG3	6:B:1001:HOH:O	2.13	0.48
1:A:255:LYS:O	1:A:256:ASP:C	2.57	0.48
1:A:267:LEU:HD12	1:A:267:LEU:N	2.28	0.48
1:A:114:PHE:HD2	1:A:134:ARG:HD2	1.78	0.48
1:A:135:GLN:HB2	1:A:145:LYS:HD3	1.95	0.48
1:B:65:ILE:CG2	1:B:69:LYS:HE3	2.43	0.48
1:B:255:LYS:O	1:B:256:ASP:C	2.57	0.48
1:A:252:MET:HE2	6:A:929:HOH:O	2.15	0.47
1:B:155:GLN:HE22	1:B:187:VAL:HG22	1.79	0.47
1:B:248:LYS:H	1:B:252:MET:CE	2.27	0.47
1:A:89:ASN:ND2	1:A:102:ARG:HH22	2.14	0.46
1:A:301:SER:O	5:B:601:VNP:H7A2	2.15	0.46
1:B:140:TYR:O	1:B:145:LYS:HE3	2.14	0.46
1:B:255:LYS:HE3	6:B:1005:HOH:O	2.15	0.46
1:A:266:GLY:C	1:A:267:LEU:HD12	2.40	0.46
1:A:89:ASN:HD22	1:A:102:ARG:NH2	2.14	0.46
1:A:279:ASN:OD1	1:A:288:ARG:HA	2.15	0.46
1:B:266:GLY:C	1:B:267:LEU:HD12	2.41	0.46
1:A:208:VAL:HG21	1:B:268:LEU:HD13	1.97	0.45
1:A:228:PHE:HB2	1:A:235:ILE:HB	1.97	0.45
1:A:295:LEU:CD2	1:B:271:SER:HB2	2.47	0.45
1:A:284:LYS:HB2	1:A:303:ARG:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:HE22	1:B:172:GLY:N	2.14	0.45
1:B:267:LEU:HD22	1:B:278:LEU:HD13	1.98	0.45
1:A:274:THR:HG21	6:A:832:HOH:O	2.17	0.45
1:B:162:ASN:HB2	1:B:165:GLU:HG3	1.98	0.45
1:B:209:GLN:NE2	1:B:213:GLN:HE21	2.16	0.44
1:A:164:PHE:O	1:A:167:ILE:HG23	2.17	0.44
1:B:111:VAL:HG23	1:B:112:GLY:N	2.33	0.44
1:A:239:LYS:O	1:A:240:LYS:C	2.61	0.44
1:A:215:TYR:CE1	1:A:271:SER:HB3	2.53	0.44
1:A:119:PRO:HA	1:A:122:LYS:HE2	1.99	0.44
1:B:155:GLN:NE2	1:B:187:VAL:HG22	2.33	0.43
1:A:252:MET:CE	6:A:929:HOH:O	2.66	0.43
1:B:213:GLN:O	1:B:217:MET:HG3	2.19	0.43
1:B:297:GLN:HG2	6:B:857:HOH:O	2.18	0.43
1:A:218:ASN:OD1	1:A:239:LYS:HE2	2.18	0.43
1:B:74:ILE:HD12	1:B:74:ILE:N	2.34	0.43
1:B:169:GLU:HG3	6:B:999:HOH:O	2.17	0.43
1:B:249:ASN:HA	1:B:307:GLU:O	2.19	0.43
1:A:23:PRO:HG3	1:A:311:ILE:HD13	2.01	0.43
1:B:50:HIS:HB2	1:B:191:ASP:O	2.18	0.43
1:B:64:LEU:HD21	1:B:84:LEU:CD1	2.49	0.43
1:A:206:GLN:HG3	6:A:846:HOH:O	2.18	0.42
1:A:118:SER:OG	1:A:121:VAL:HG23	2.19	0.42
1:A:65:ILE:HD12	1:A:65:ILE:N	2.35	0.42
1:A:131:LYS:NZ	1:A:157:ASN:ND2	2.66	0.42
1:A:254:HIS:O	1:A:255:LYS:C	2.62	0.42
1:A:267:LEU:HD22	1:A:278:LEU:HD13	2.00	0.42
1:B:239:LYS:O	1:B:240:LYS:C	2.63	0.42
1:B:262:THR:HA	1:B:263:PRO:HD3	1.89	0.42
1:A:171:ASP:OD1	1:A:171:ASP:N	2.51	0.42
1:A:188:VAL:O	1:A:188:VAL:HG22	2.18	0.42
1:B:209:GLN:HE21	1:B:213:GLN:HE21	1.68	0.41
1:B:35:GLN:HB3	1:B:38:VAL:HG23	2.02	0.41
1:B:252:MET:HG3	1:B:253:PHE:HD1	1.86	0.41
1:A:144:THR:HG23	6:A:1054:HOH:O	2.19	0.41
1:A:18:LEU:C	1:A:19:ILE:HD12	2.46	0.41
1:A:262:THR:HA	1:A:263:PRO:HD3	1.90	0.41
1:A:295:LEU:HD21	1:B:271:SER:HB2	2.03	0.41
1:B:223:LYS:HA	1:B:223:LYS:HD3	1.91	0.41
1:A:233:ASP:HB3	1:A:323:GLU:HA	2.02	0.40
1:A:248:LYS:N	1:A:252:MET:SD	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:O	1:A:86:GLU:HG3	2.21	0.40
1:A:165:GLU:O	1:A:166:SER:HB2	2.20	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	289/348 (83%)	274 (95%)	14 (5%)	1 (0%)	36	28
1	B	287/348 (82%)	274 (96%)	13 (4%)	0	100	100
All	All	576/696 (83%)	548 (95%)	27 (5%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASN

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	277/323 (86%)	272 (98%)	5 (2%)	51	47
1	B	275/323 (85%)	270 (98%)	5 (2%)	51	47
All	All	552/646 (85%)	542 (98%)	10 (2%)	51	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	111	VAL
1	A	156	LEU
1	A	176	LEU
1	A	316	ASP
1	B	67	LEU
1	B	111	VAL
1	B	156	LEU
1	B	189	ASP
1	B	316	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	35	GLN
1	A	51	ASN
1	A	58	GLN
1	A	89	ASN
1	A	135	GLN
1	A	138	GLN
1	A	157	ASN
1	A	158	HIS
1	A	206	GLN
1	A	209	GLN
1	A	213	GLN
1	B	10	GLN
1	B	51	ASN
1	B	89	ASN
1	B	135	GLN
1	B	157	ASN
1	B	158	HIS
1	B	206	GLN
1	B	209	GLN
1	B	249	ASN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
5	VNP	B	601	2	27,27,27	2.28	5 (18%)	35,40,40	2.19	13 (37%)
4	PO4	B	708	2	4,4,4	1.76	2 (50%)	6,6,6	0.45	0
4	PO4	A	707	2	4,4,4	1.77	1 (25%)	6,6,6	0.48	0
5	VNP	A	602	2	27,27,27	2.27	5 (18%)	35,40,40	2.17	12 (34%)

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
5	VNP	B	601	2	-	2/14/17/17	0/2/2/2
5	VNP	A	602	2	-	3/14/17/17	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	VNP	C11-C10	8.69	1.53	1.35
5	A	602	VNP	C11-C10	8.66	1.53	1.35
5	A	602	VNP	C11-S1	3.83	1.82	1.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	VNP	C11-S1	3.79	1.82	1.72
5	B	601	VNP	PB-O1B	-3.19	1.48	1.56
5	A	602	VNP	PB-O1B	-3.15	1.48	1.56
5	A	602	VNP	C10-N5	-2.80	1.34	1.39
5	B	601	VNP	C10-N5	-2.79	1.34	1.39
4	B	708	PO4	P-O3	-2.12	1.48	1.54
4	A	707	PO4	P-O2	-2.07	1.48	1.54
5	B	601	VNP	C9-S1	2.05	1.75	1.69
5	A	602	VNP	C9-S1	2.04	1.75	1.69
4	B	708	PO4	P-O4	-2.01	1.48	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	VNP	C10-C11-S1	-6.62	100.25	110.56
5	A	602	VNP	C10-C11-S1	-6.58	100.31	110.56
5	B	601	VNP	C12-C11-C10	-4.68	116.42	128.17
5	A	602	VNP	C12-C11-C10	-4.63	116.55	128.17
5	B	601	VNP	O1B-PB-O2B	3.63	117.66	109.87
5	A	602	VNP	O1B-PB-O2B	3.53	117.44	109.87
5	B	601	VNP	N1A-C2A-N3A	-3.19	120.22	125.53
5	A	602	VNP	N1A-C2A-N3A	-3.16	120.27	125.53
5	A	602	VNP	C6A-N1A-C2A	2.97	120.96	116.07
5	B	601	VNP	C6A-N1A-C2A	2.95	120.92	116.07
5	A	602	VNP	C9-S1-C11	2.40	92.80	91.22
5	B	601	VNP	C7A-C5A-C4A	2.37	126.67	122.36
5	B	601	VNP	C7A-C5A-C6A	-2.34	116.29	120.69
5	A	602	VNP	C7A-C5A-C6A	-2.34	116.30	120.69
5	A	602	VNP	CM2-C2A-N1A	2.33	119.68	117.20
5	B	601	VNP	S1-C9-N5	-2.30	109.39	112.30
5	B	601	VNP	CM2-C2A-N1A	2.25	119.60	117.20
5	B	601	VNP	O2B-PB-N3B	-2.24	108.47	111.77
5	B	601	VNP	C9-S1-C11	2.23	92.69	91.22
5	A	602	VNP	C9-N5-C10	2.22	117.06	114.06
5	A	602	VNP	C7A-C5A-C4A	2.22	126.41	122.36
5	A	602	VNP	S1-C9-N5	-2.22	109.49	112.30
5	B	601	VNP	C9-N5-C10	2.15	116.96	114.06
5	A	602	VNP	O2B-PB-N3B	-2.04	108.77	111.77
5	B	601	VNP	CM2-C2A-N3A	2.04	120.17	117.13

There are no chirality outliers.

All (5) torsion outliers are listed below:

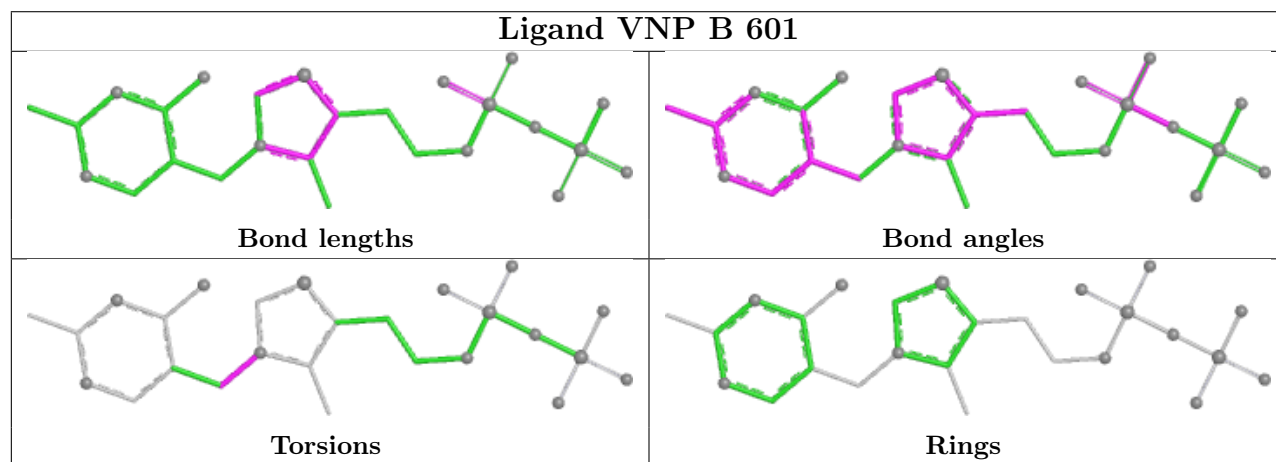
Mol	Chain	Res	Type	Atoms
5	A	602	VNP	C5A-C7A-N5-C9
5	B	601	VNP	C5A-C7A-N5-C9
5	A	602	VNP	C5A-C7A-N5-C10
5	B	601	VNP	C5A-C7A-N5-C10
5	A	602	VNP	PB-N3B-PG-O3G

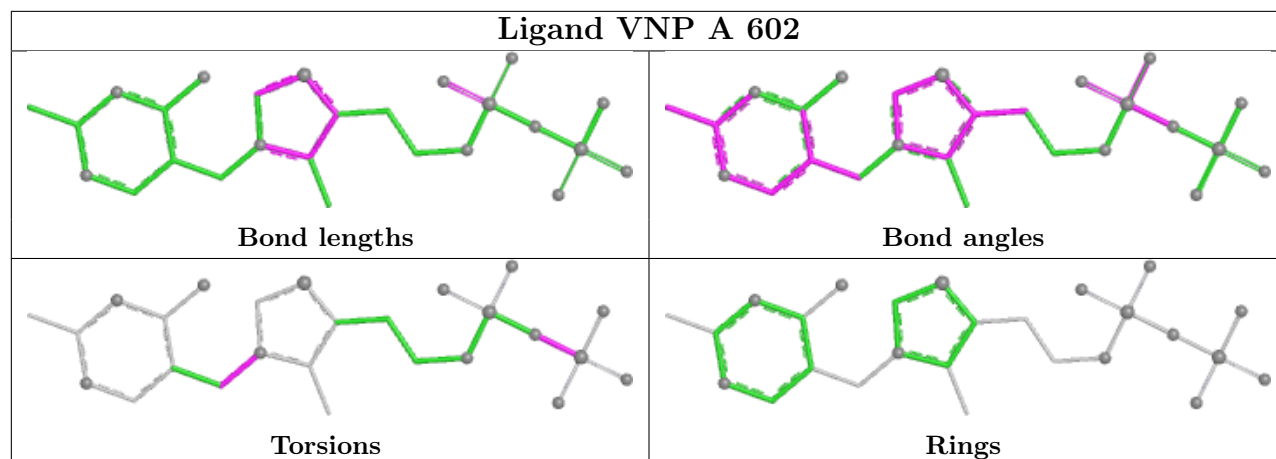
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	VNP	1	0
4	A	707	PO4	3	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	297/348 (85%)	-1.20	0 100 100	11, 24, 46, 56	11 (3%)
1	B	295/348 (84%)	-1.21	0 100 100	11, 24, 46, 57	10 (3%)
All	All	592/696 (85%)	-1.21	0 100 100	11, 24, 46, 57	21 (3%)

There are no RSRZ outliers to report.

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.

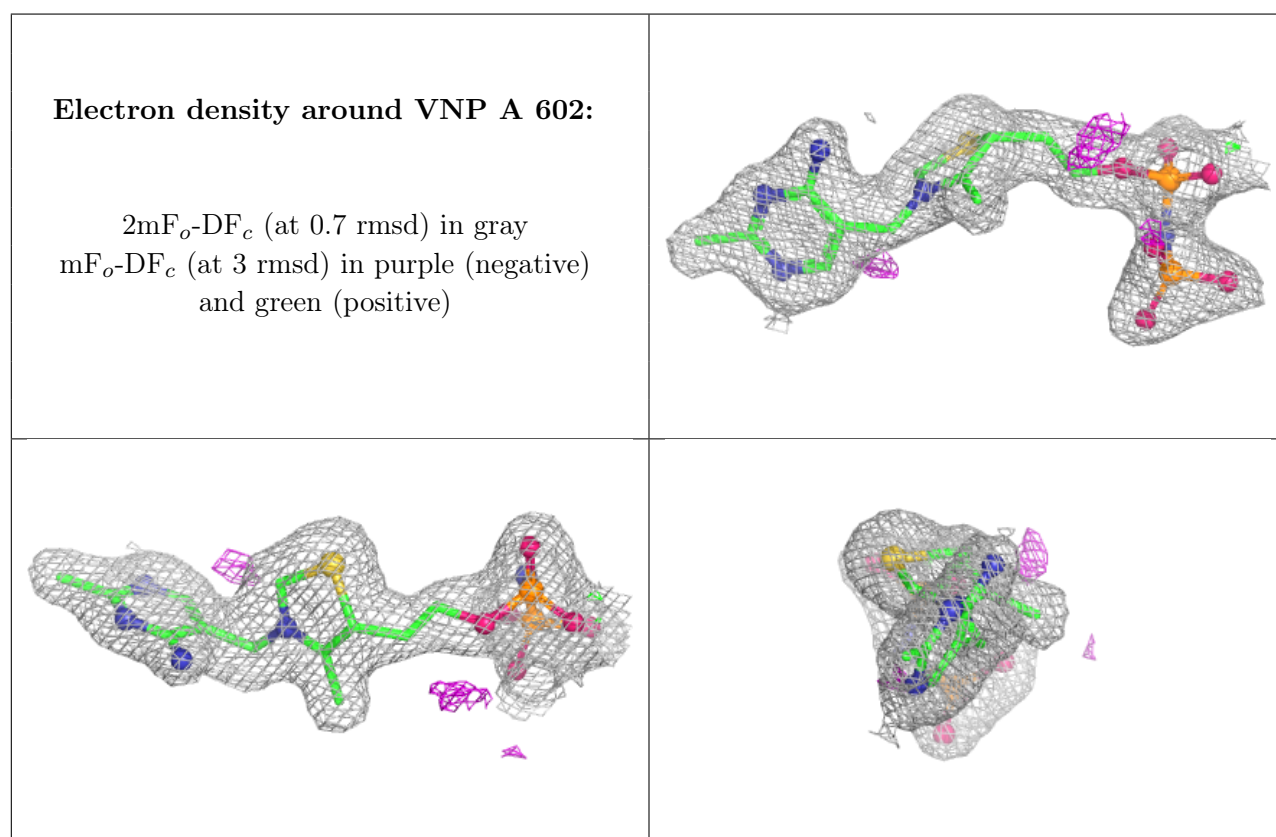
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	702	1/1	0.98	0.03	24,24,24,24	0
2	MG	A	801	1/1	0.99	0.08	14,14,14,14	0
2	MG	B	802	1/1	0.99	0.06	17,17,17,17	0
3	CL	A	705	1/1	0.99	0.02	31,31,31,31	0
3	CL	B	706	1/1	0.99	0.05	28,28,28,28	0
4	PO4	B	708	5/5	0.99	0.05	27,30,31,33	0
2	MG	B	701	1/1	1.00	0.01	20,20,20,20	0

Continued on next page...

Continued from previous page...

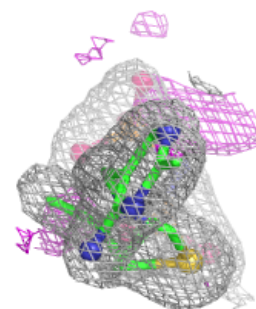
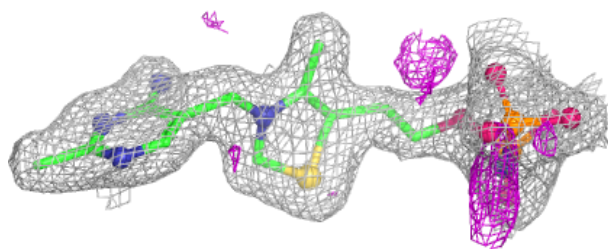
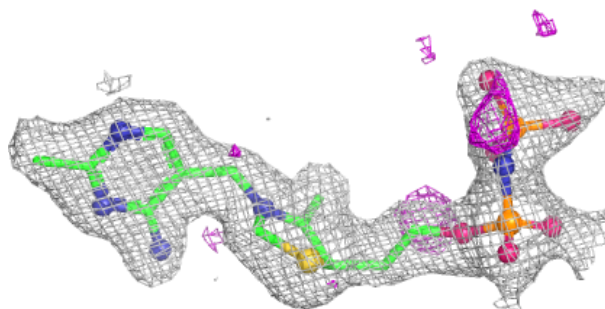
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	703	1/1	1.00	0.02	23,23,23,23	0
4	PO4	A	707	5/5	1.00	0.05	28,32,34,34	1
2	MG	A	704	1/1	1.00	0.02	25,25,25,25	0
5	VNP	A	602	26/26	1.00	0.03	12,17,25,27	0
5	VNP	B	601	26/26	1.00	0.02	12,17,23,26	0

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 VNP B 601:

$2mF_o-DF_c$ (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.