



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:57 PM BST

PDB ID : 4KQR
Title : CRYSTAL STRUCTURE OF PENICILLIN-BINDING PROTEIN 3 FROM PSEUDOMONAS AERUGINOSA IN COMPLEX WITH (5S)-Penicilloic Acid
Authors : Nettleship, J.E.; Stuart, D.I.; Owens, R.J.; Ren, J.
Deposited on : 2013-05-15
Resolution : 2.01 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 : 2.13.1
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) : 2.13.1

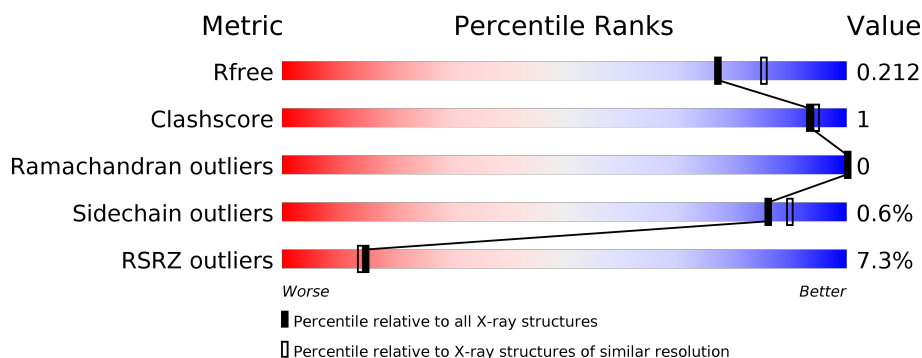
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	564	<div> <div>3%</div> <div>89%</div> <div>8%</div> </div>
1	B	564	<div> <div>11%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8647 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 Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			3973	2503	722	736	12			
1	B	518	Total	C	N	O	S	0	0	0
			3956	2494	717	733	12			

There are 38 discrepancies between the modelled and reference sequences:

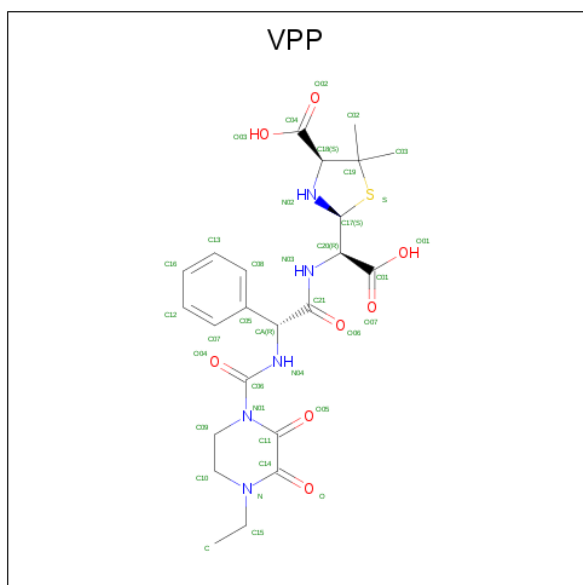
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	EXPRESSION TAG	UNP G3XD46
A	17	ALA	-	EXPRESSION TAG	UNP G3XD46
A	18	HIS	-	EXPRESSION TAG	UNP G3XD46
A	19	HIS	-	EXPRESSION TAG	UNP G3XD46
A	20	HIS	-	EXPRESSION TAG	UNP G3XD46
A	21	HIS	-	EXPRESSION TAG	UNP G3XD46
A	22	HIS	-	EXPRESSION TAG	UNP G3XD46
A	23	HIS	-	EXPRESSION TAG	UNP G3XD46
A	24	SER	-	EXPRESSION TAG	UNP G3XD46
A	25	SER	-	EXPRESSION TAG	UNP G3XD46
A	26	GLY	-	EXPRESSION TAG	UNP G3XD46
A	27	LEU	-	EXPRESSION TAG	UNP G3XD46
A	28	GLU	-	EXPRESSION TAG	UNP G3XD46
A	29	VAL	-	EXPRESSION TAG	UNP G3XD46
A	30	LEU	-	EXPRESSION TAG	UNP G3XD46
A	31	PHE	-	EXPRESSION TAG	UNP G3XD46
A	32	GLN	-	EXPRESSION TAG	UNP G3XD46
A	33	GLY	-	EXPRESSION TAG	UNP G3XD46
A	34	PRO	-	EXPRESSION TAG	UNP G3XD46
B	16	MET	-	EXPRESSION TAG	UNP G3XD46
B	17	ALA	-	EXPRESSION TAG	UNP G3XD46
B	18	HIS	-	EXPRESSION TAG	UNP G3XD46
B	19	HIS	-	EXPRESSION TAG	UNP G3XD46
B	20	HIS	-	EXPRESSION TAG	UNP G3XD46
B	21	HIS	-	EXPRESSION TAG	UNP G3XD46

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Chain	Residue	Modelled	Actual	Comment	Reference
B	22	HIS	-	EXPRESSION TAG	UNP G3XD46
B	23	HIS	-	EXPRESSION TAG	UNP G3XD46
B	24	SER	-	EXPRESSION TAG	UNP G3XD46
B	25	SER	-	EXPRESSION TAG	UNP G3XD46
B	26	GLY	-	EXPRESSION TAG	UNP G3XD46
B	27	LEU	-	EXPRESSION TAG	UNP G3XD46
B	28	GLU	-	EXPRESSION TAG	UNP G3XD46
B	29	VAL	-	EXPRESSION TAG	UNP G3XD46
B	30	LEU	-	EXPRESSION TAG	UNP G3XD46
B	31	PHE	-	EXPRESSION TAG	UNP G3XD46
B	32	GLN	-	EXPRESSION TAG	UNP G3XD46
B	33	GLY	-	EXPRESSION TAG	UNP G3XD46
B	34	PRO	-	EXPRESSION TAG	UNP G3XD46

- Molecule 2 is (2S,4S)-2-[(R)-carboxy{[(2R)-2-{[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino}-2-phenylacetyl]amino}methyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: VPP) (formula: C₂₃H₂₉N₅O₈S).

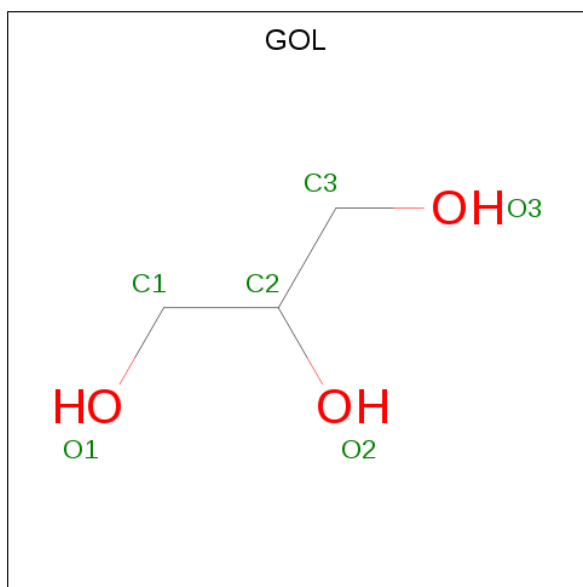


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	23	5	8	1		
2	B	1	Total	C	N	O	S	0	0
			37	23	5	8	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

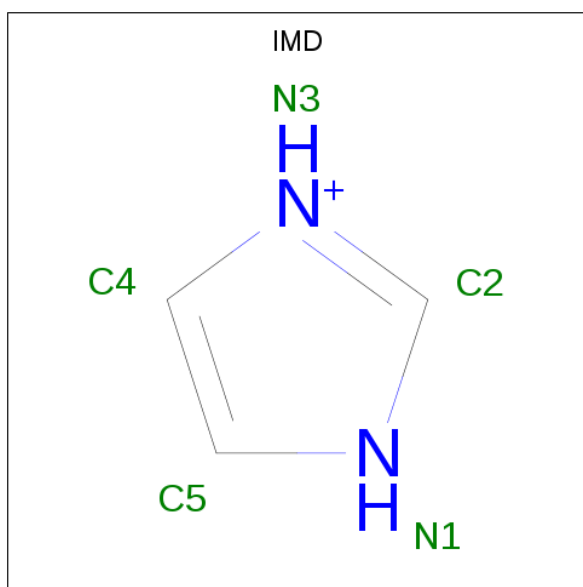
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Cl	0	0
			3	3		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

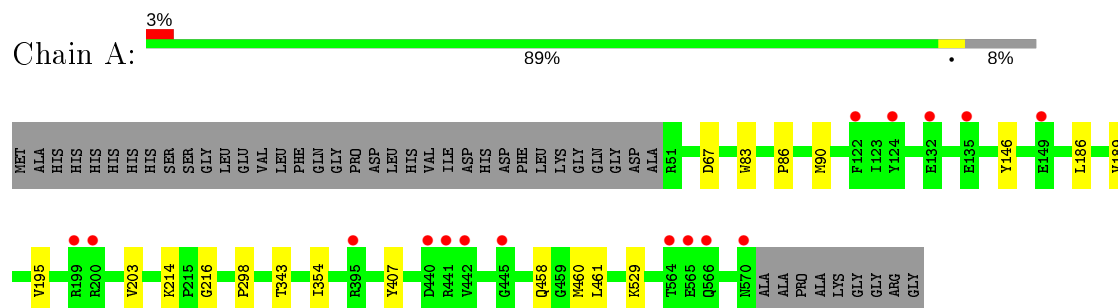
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	307	Total	O	0	0
			307	307		
6	B	263	Total	O	0	0
			263	263		

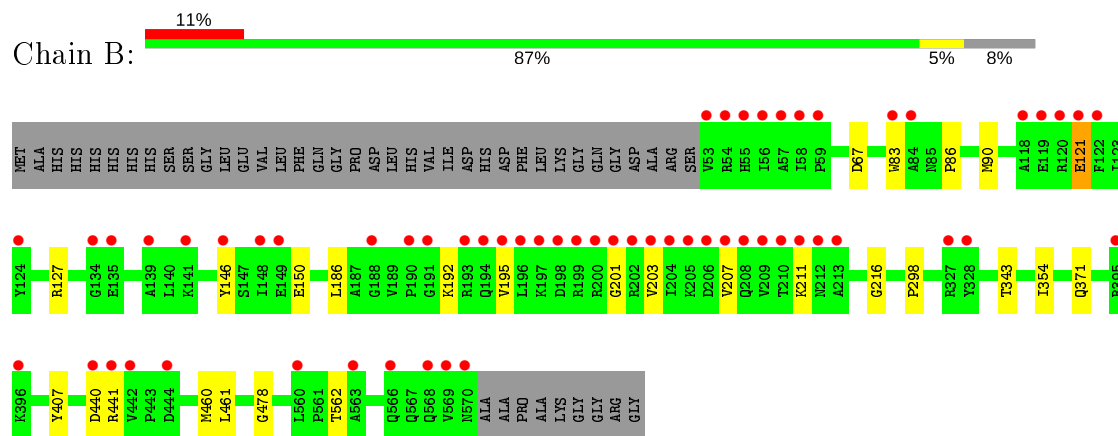
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Penicillin-binding protein 3



- Molecule 1: Penicillin-binding protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.20Å 75.45Å 83.22Å 70.77° 85.40° 85.06°	Depositor
Resolution (Å)	47.36 – 2.01 47.32 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.36-2.01) 95.5 (47.32-2.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.185 , 0.207 0.190 , 0.212	Depositor DCC
R_{free} test set	4164 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.1	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	0.95	EDS
Total number of atoms	8647	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: GOL, CL, VPP, IMD

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	0.38	0/4050	0.58	0/5495
1	B	0.37	0/4033	0.57	0/5473
All	All	0.38	0/8083	0.58	0/10968

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	3973	0	4029	10	0
1	B	3956	0	4011	13	0
2	A	37	0	27	0	0
2	B	37	0	27	0	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
4	A	30	0	40	1	0
4	B	24	0	32	0	0
5	A	10	0	10	0	0
5	B	5	0	5	0	0
6	A	307	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	263	0	0	1	0
All	All	8647	0	8181	23	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 1.

All (23) 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:478:GLY:H	1:B:562:THR:HG23	1.55	0.72
1:A:343:THR:HA	1:A:460:MET:HE2	1.85	0.58
1:B:343:THR:HA	1:B:460:MET:HE2	1.85	0.57
1:A:458:GLN:OE1	4:A:606:GOL:H11	2.04	0.57
1:B:562:THR:HG21	6:B:772:HOH:O	2.13	0.48
1:A:189:VAL:CG1	1:A:214:LYS:HB3	2.44	0.47
1:A:186:LEU:O	1:A:216:GLY:HA3	2.17	0.44
1:B:354:ILE:HG21	1:B:407:TYR:HB3	1.99	0.44
1:A:298:PRO:HG3	1:A:461:LEU:HD21	2.00	0.44
1:B:121:GLU:HG3	1:B:201:GLY:HA3	2.00	0.43
1:B:186:LEU:O	1:B:216:GLY:HA3	2.18	0.43
1:A:354:ILE:HG21	1:A:407:TYR:HB3	2.00	0.43
1:B:298:PRO:HG3	1:B:461:LEU:HD21	2.01	0.43
1:B:86:PRO:O	1:B:90:MET:HG2	2.20	0.42
1:A:195:VAL:HG13	1:A:203:VAL:HG13	2.02	0.42
1:B:440:ASP:OD1	1:B:441:ARG:N	2.53	0.41
1:B:127:ARG:NH2	1:B:150:GLU:OE1	2.54	0.41
1:B:83:TRP:CE2	1:B:146:TYR:HB2	2.55	0.41
1:A:86:PRO:O	1:A:90:MET:HG2	2.20	0.41
1:A:529:LYS:HD3	6:A:960:HOH:O	2.21	0.41
1:A:83:TRP:CE2	1:A:146:TYR:HB2	2.55	0.41
1:B:195:VAL:HG13	1:B:203:VAL:HG13	2.03	0.40
1:B:192:LYS:HB3	1:B:211:LYS:HG2	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	518/564 (92%)	508 (98%)	10 (2%)	0	100	100
1	B	516/564 (92%)	506 (98%)	10 (2%)	0	100	100
All	All	1034/1128 (92%)	1014 (98%)	20 (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	416/448 (93%)	415 (100%)	1 (0%)	93	95
1	B	414/448 (92%)	410 (99%)	4 (1%)	76	81
All	All	830/896 (93%)	825 (99%)	5 (1%)	86	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	B	67	ASP
1	B	121	GLU
1	B	207	VAL
1	B	371	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	B	336	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	605	-	5,5,5	0.35	0	5,5,5	0.22	0
5	IMD	B	609	-	3,5,5	0.32	0	4,5,5	0.62	0
4	GOL	A	606	-	5,5,5	0.36	0	5,5,5	0.32	0
2	VPP	A	601	-	30,39,39	2.37	8 (26%)	37,57,57	1.06	2 (5%)
5	IMD	A	610	-	3,5,5	0.33	0	4,5,5	0.61	0
4	GOL	B	607	-	5,5,5	0.48	0	5,5,5	0.71	0
4	GOL	A	607	-	5,5,5	0.53	0	5,5,5	0.31	0
5	IMD	A	609	-	3,5,5	0.34	0	4,5,5	0.57	0
4	GOL	A	608	-	5,5,5	0.39	0	5,5,5	0.30	0
4	GOL	B	605	-	5,5,5	0.24	0	5,5,5	0.15	0
4	GOL	A	604	-	5,5,5	0.29	0	5,5,5	0.65	0
4	GOL	B	606	-	5,5,5	0.29	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VPP	B	601	-	30,39,39	2.27	8 (26%)	37,57,57	1.12	2 (5%)
4	GOL	B	608	-	5,5,5	0.35	0	5,5,5	0.34	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	605	-	-	4/4/4/4	-
5	IMD	B	609	-	-	-	0/1/1/1
4	GOL	A	606	-	-	0/4/4/4	-
2	VPP	A	601	-	-	0/22/66/66	0/3/3/3
5	IMD	A	610	-	-	-	0/1/1/1
4	GOL	B	607	-	-	2/4/4/4	-
4	GOL	A	607	-	-	3/4/4/4	-
5	IMD	A	609	-	-	-	0/1/1/1
4	GOL	A	608	-	-	4/4/4/4	-
4	GOL	B	605	-	-	2/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	B	606	-	-	0/4/4/4	-
2	VPP	B	601	-	-	1/22/66/66	0/3/3/3
4	GOL	B	608	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	VPP	C14-N	6.36	1.42	1.35
2	A	601	VPP	C14-C11	-6.02	1.43	1.53
2	B	601	VPP	C14-N	5.79	1.42	1.35
2	B	601	VPP	C14-C11	-5.44	1.44	1.53
2	B	601	VPP	C21-N03	4.90	1.44	1.34
2	A	601	VPP	C21-N03	4.86	1.44	1.34
2	B	601	VPP	C06-N04	4.12	1.44	1.35
2	A	601	VPP	C06-N04	4.04	1.44	1.35
2	B	601	VPP	C19-S	-3.49	1.78	1.85
2	A	601	VPP	C19-S	-3.17	1.78	1.85
2	A	601	VPP	C20-N03	-2.47	1.41	1.46
2	A	601	VPP	C17-S	-2.47	1.78	1.84
2	B	601	VPP	C17-S	-2.41	1.78	1.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	VPP	C20-N03	-2.24	1.42	1.46
2	A	601	VPP	C18-N02	2.11	1.49	1.46
2	B	601	VPP	C11-N01	2.04	1.43	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	VPP	N04-C06-N01	4.14	120.06	114.04
2	B	601	VPP	N04-C06-N01	4.06	119.94	114.04
2	B	601	VPP	O-C14-N	-2.86	120.68	123.66
2	A	601	VPP	C10-C09-N01	2.17	112.88	108.78

There are no chirality outliers.

All (20) torsion outliers are listed below:

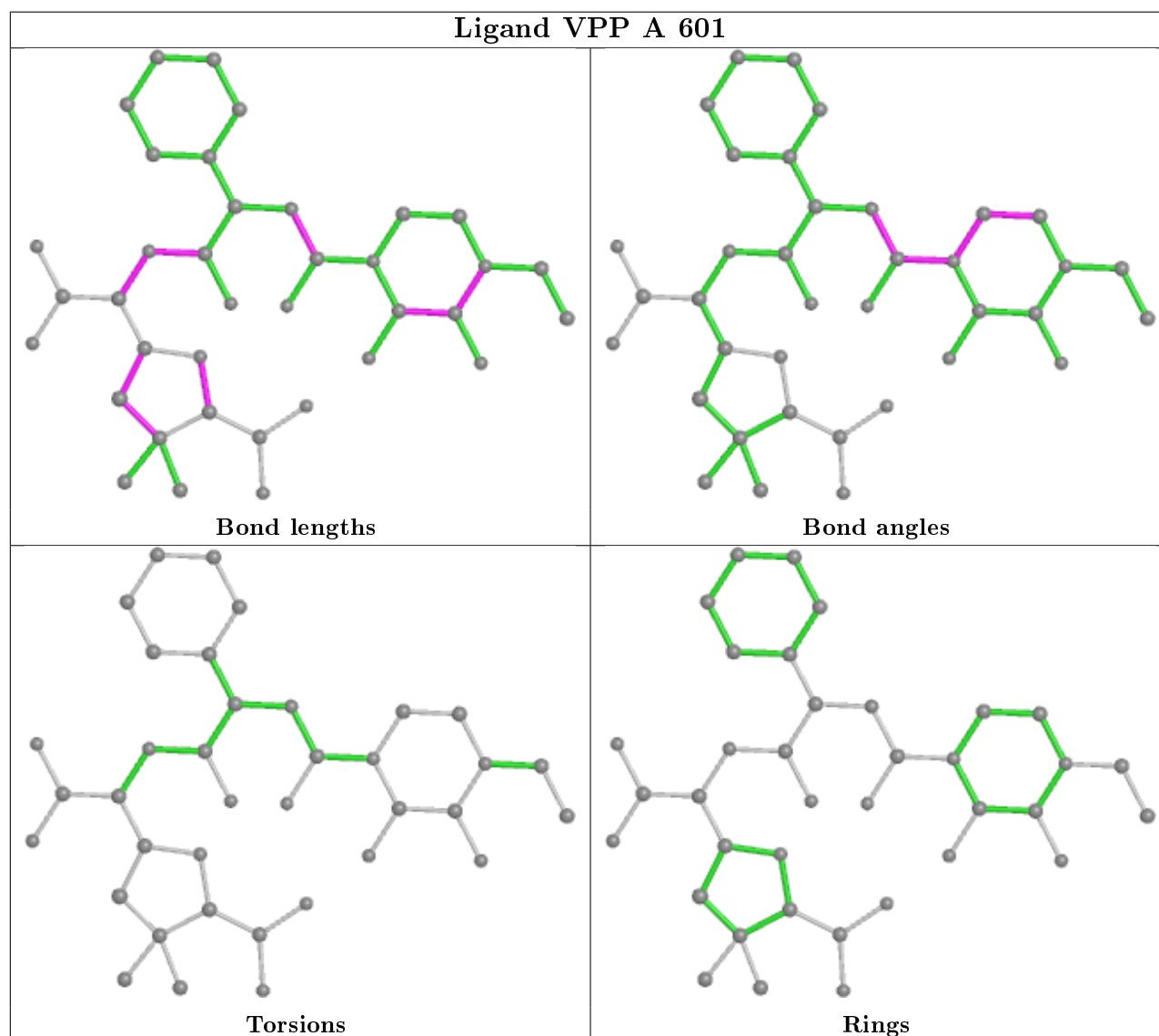
Mol	Chain	Res	Type	Atoms
4	A	605	GOL	O1-C1-C2-O2
4	A	605	GOL	O1-C1-C2-C3
4	A	605	GOL	C1-C2-C3-O3
4	A	607	GOL	O1-C1-C2-C3
4	B	607	GOL	O1-C1-C2-C3
4	A	604	GOL	O1-C1-C2-O2
4	A	604	GOL	O1-C1-C2-C3
4	B	608	GOL	O1-C1-C2-C3
4	A	607	GOL	O1-C1-C2-O2
4	A	608	GOL	O2-C2-C3-O3
4	B	605	GOL	O1-C1-C2-C3
4	A	608	GOL	O1-C1-C2-C3
4	A	608	GOL	C1-C2-C3-O3
4	B	608	GOL	O1-C1-C2-O2
4	A	605	GOL	O2-C2-C3-O3
4	B	607	GOL	O1-C1-C2-O2
4	A	607	GOL	O2-C2-C3-O3
4	B	605	GOL	O1-C1-C2-O2
2	B	601	VPP	C21-CA-N04-C06
4	A	608	GOL	O1-C1-C2-O2

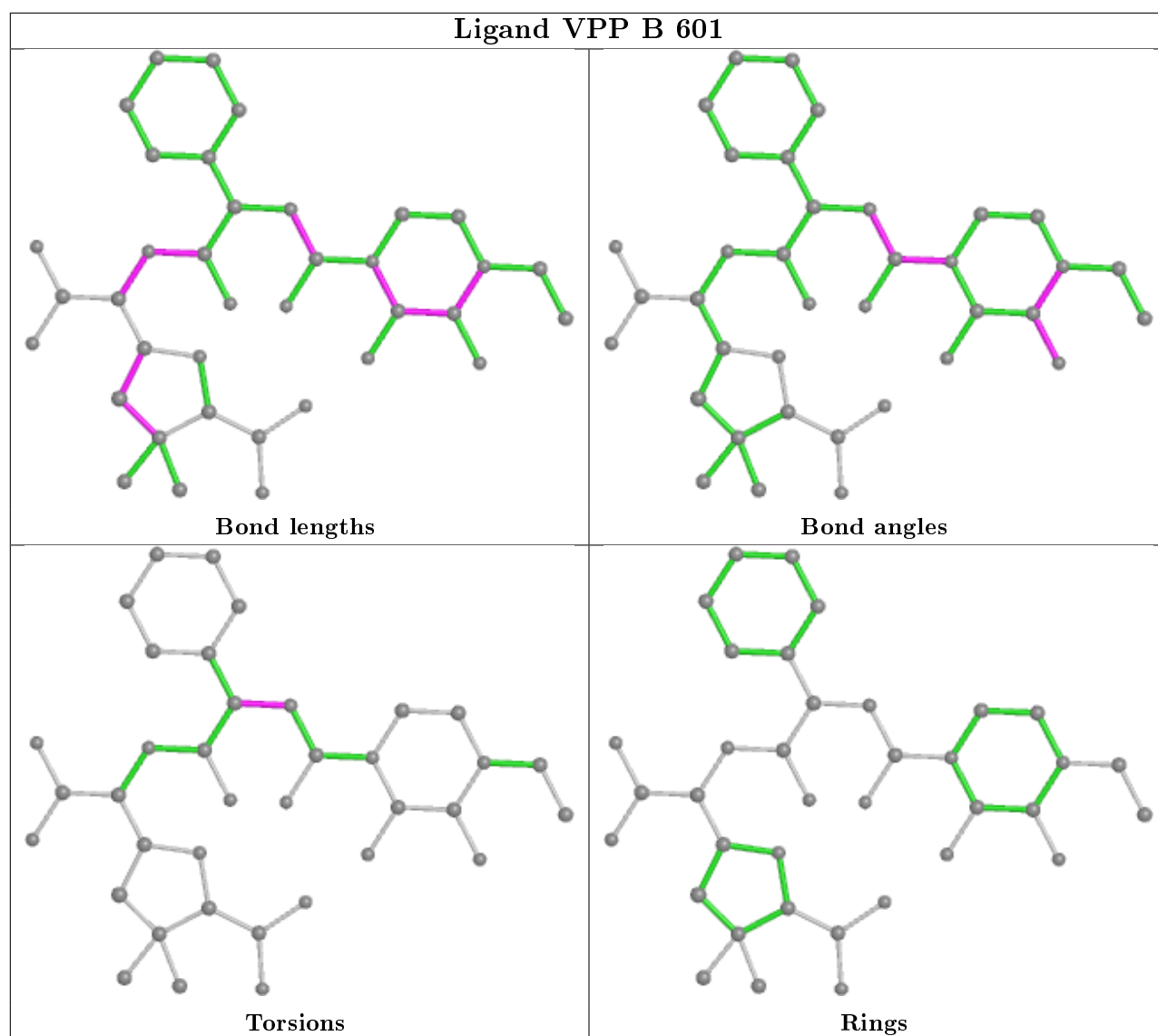
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	GOL	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	520/564 (92%)	-0.00	16 (3%) 49 48	12, 26, 59, 98	0
1	B	518/564 (91%)	0.47	60 (11%) 4 4	13, 30, 89, 129	0
All	All	1038/1128 (92%)	0.23	76 (7%) 15 14	12, 28, 73, 129	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	VAL	7.5
1	B	195	VAL	6.9
1	B	55	HIS	6.8
1	B	56	ILE	6.7
1	B	200	ARG	6.4
1	B	196	LEU	6.3
1	B	395	ARG	5.9
1	B	199	ARG	5.8
1	B	204	ILE	5.3
1	B	207	VAL	5.2
1	B	53	VAL	4.8
1	B	206	ASP	4.7
1	B	120	ARG	4.7
1	B	122	PHE	4.4
1	B	205	LYS	4.3
1	B	58	ILE	4.3
1	B	202	ARG	4.3
1	B	569	VAL	4.3
1	B	146	TYR	4.2
1	B	124	TYR	4.2
1	B	328	TYR	4.2
1	B	201	GLY	4.0
1	B	208	GLN	3.8
1	A	199	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	441	ARG	3.7
1	B	119	GLU	3.6
1	B	139	ALA	3.6
1	A	200	ARG	3.6
1	B	213	ALA	3.5
1	B	135	GLU	3.5
1	B	197	LYS	3.3
1	B	441	ARG	3.2
1	B	440	ASP	3.2
1	B	211	LYS	3.2
1	B	194	GLN	3.2
1	A	132	GLU	3.2
1	B	210	THR	3.2
1	A	570	ASN	3.1
1	A	440	ASP	3.1
1	B	57	ALA	3.0
1	B	212	ASN	3.0
1	A	122	PHE	2.9
1	B	149	GLU	2.9
1	B	209	VAL	2.9
1	B	193	ARG	2.8
1	B	118	ALA	2.8
1	A	135	GLU	2.8
1	B	190	PRO	2.7
1	B	141	LYS	2.7
1	B	54	ARG	2.7
1	B	327	ARG	2.7
1	B	560	LEU	2.7
1	B	59	PRO	2.6
1	B	570	ASN	2.6
1	B	83	TRP	2.6
1	B	568	GLN	2.6
1	B	191	GLY	2.5
1	B	442	VAL	2.5
1	B	198	ASP	2.5
1	B	444	ASP	2.4
1	A	565	GLU	2.4
1	A	124	TYR	2.3
1	B	188	GLY	2.3
1	A	566	GLN	2.3
1	A	442	VAL	2.3
1	B	396	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	148	ILE	2.2
1	B	563	ALA	2.2
1	A	564	THR	2.2
1	A	395	ARG	2.2
1	B	566	GLN	2.1
1	A	445	GLY	2.1
1	B	84	ALA	2.1
1	A	149	GLU	2.1
1	B	121	GLU	2.0
1	B	134	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

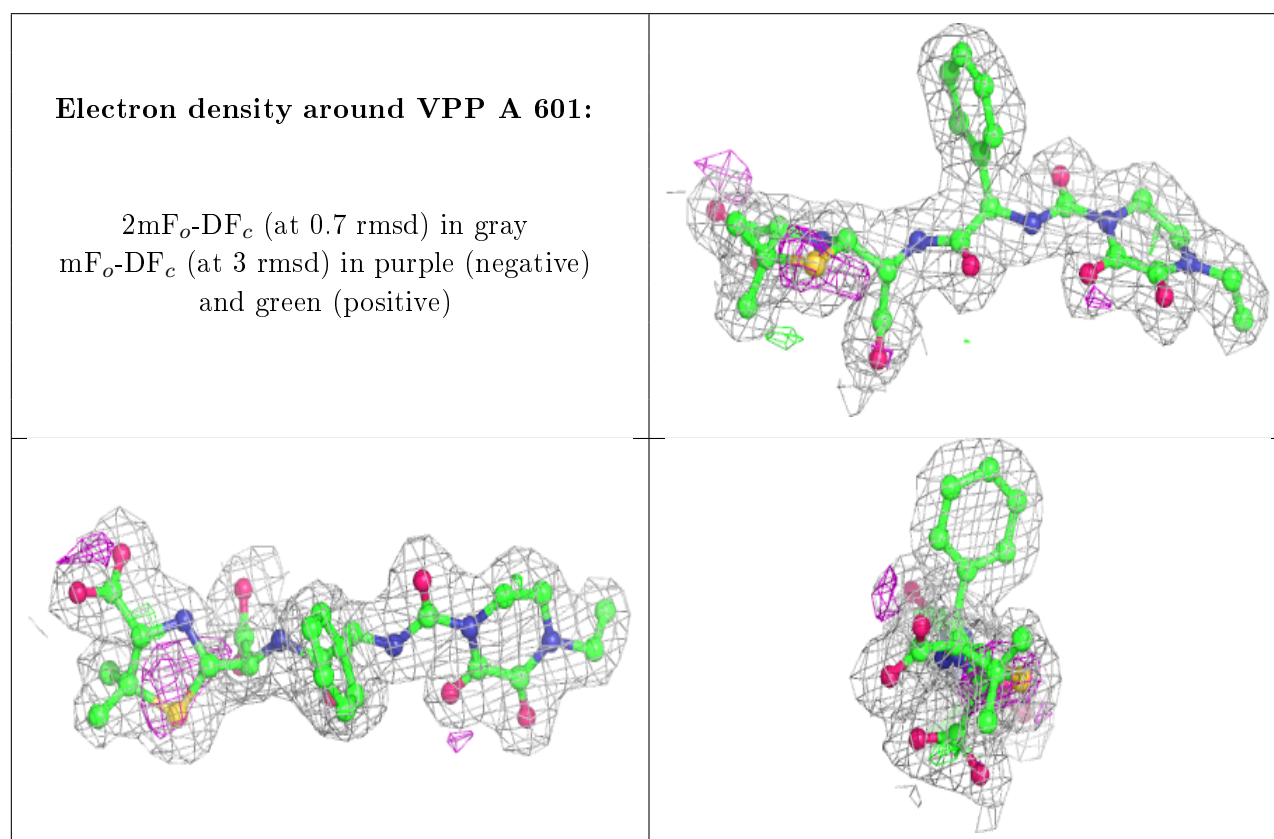
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	606	6/6	0.56	0.34	68,70,71,73	0
4	GOL	B	607	6/6	0.71	0.19	41,42,44,46	0
4	GOL	A	608	6/6	0.72	0.26	43,47,49,54	0
4	GOL	B	608	6/6	0.81	0.24	49,50,51,52	0
5	IMD	B	609	5/5	0.84	0.15	58,59,59,60	0
5	IMD	A	609	5/5	0.84	0.16	47,47,48,49	0
5	IMD	A	610	5/5	0.85	0.18	63,64,64,64	0
4	GOL	B	606	6/6	0.86	0.14	65,66,68,69	0
4	GOL	A	605	6/6	0.87	0.19	44,48,51,54	0
4	GOL	A	607	6/6	0.88	0.13	37,40,44,48	0
4	GOL	A	604	6/6	0.91	0.16	29,31,32,33	0
2	VPP	A	601	37/37	0.95	0.10	18,20,25,27	0
3	CL	A	602	1/1	0.95	0.08	38,38,38,38	0

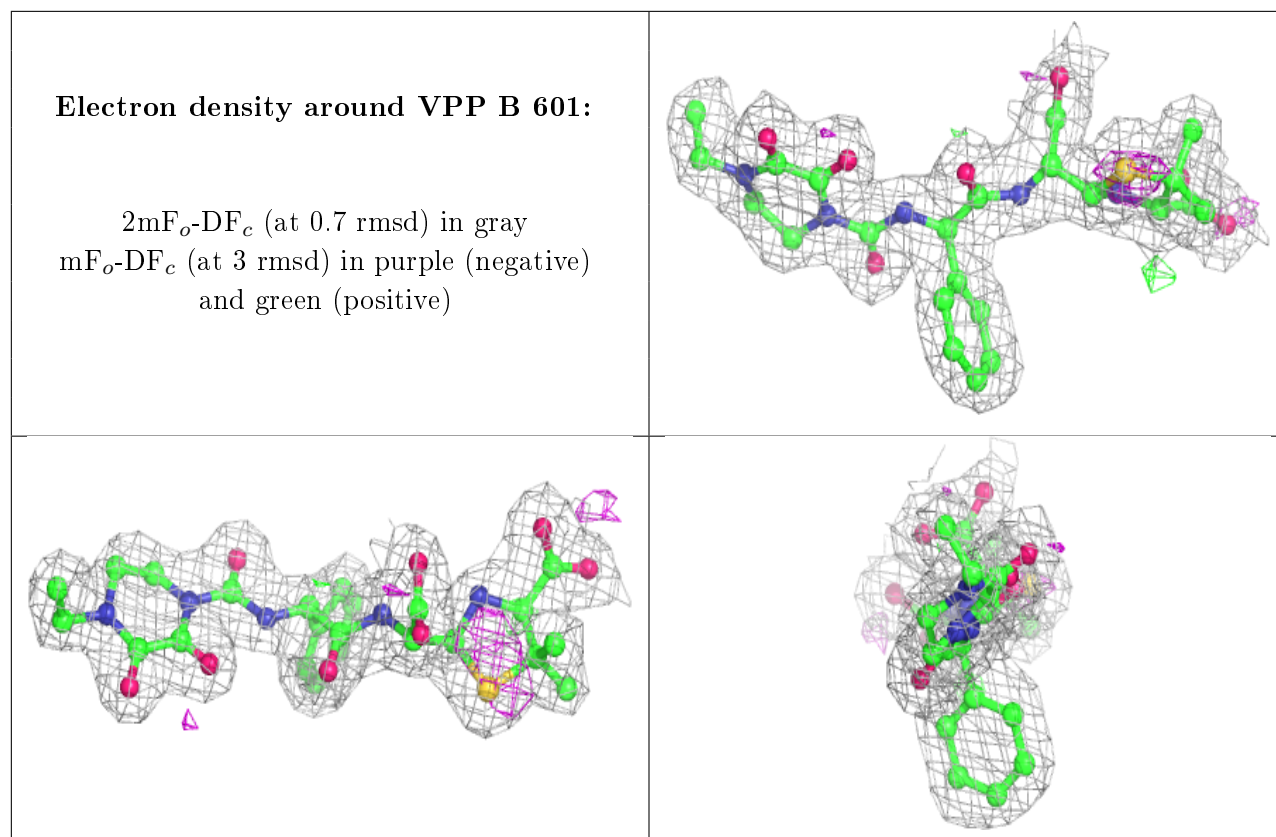
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	B	604	1/1	0.95	0.10	45,45,45,45	0
2	VPP	B	601	37/37	0.96	0.10	22,25,27,30	0
4	GOL	B	605	6/6	0.96	0.10	26,28,29,32	0
3	CL	B	602	1/1	0.98	0.09	32,32,32,32	0
3	CL	B	603	1/1	0.98	0.05	40,40,40,40	0
3	CL	A	603	1/1	0.98	0.10	38,38,38,38	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.