Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 12:17 PM JST

PDB ID	:	8K4R
Title	:	Structure of VinM-VinL complex
Authors	:	Miyanaga, A.; Nagata, K.; Nakajima, J.; Chisuga, T.; Kudo, F.; Eguchi, T.
Deposited on	:	2023-07-20
Resolution	:	2.30 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:

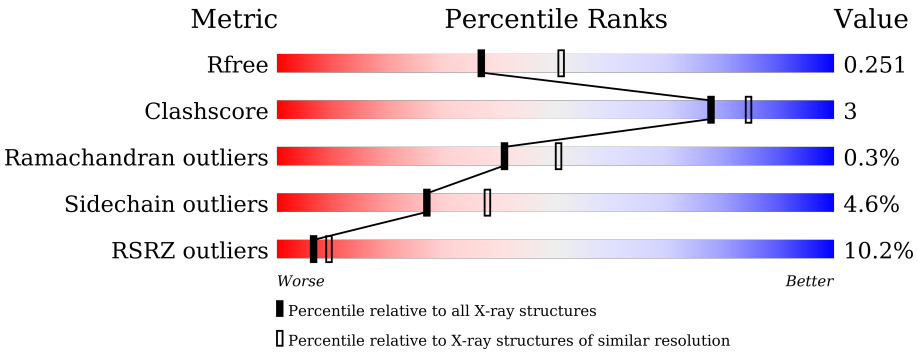
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	540	4% 83% 10% • 6%
1	C	540	11% 78% 7% • 14%
2	B	102	8% 66% 8% • 25%
2	D	102	21% 65% 11% • 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8725 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 Non-ribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3831	2427	695	698	11			
1	C	463	Total	C	N	O	S	0	0	0
			3520	2240	633	636	11			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q76KY3
A	-14	ASN	-	expression tag	UNP Q76KY3
A	-13	HIS	-	expression tag	UNP Q76KY3
A	-12	LYS	-	expression tag	UNP Q76KY3
A	-11	VAL	-	expression tag	UNP Q76KY3
A	-10	HIS	-	expression tag	UNP Q76KY3
A	-9	HIS	-	expression tag	UNP Q76KY3
A	-8	HIS	-	expression tag	UNP Q76KY3
A	-7	HIS	-	expression tag	UNP Q76KY3
A	-6	HIS	-	expression tag	UNP Q76KY3
A	-5	HIS	-	expression tag	UNP Q76KY3
A	-4	ILE	-	expression tag	UNP Q76KY3
A	-3	GLU	-	expression tag	UNP Q76KY3
A	-2	GLY	-	expression tag	UNP Q76KY3
A	-1	ARG	-	expression tag	UNP Q76KY3
A	0	HIS	-	expression tag	UNP Q76KY3
A	223	CYS	ASP	engineered mutation	UNP Q76KY3
C	-15	MET	-	initiating methionine	UNP Q76KY3
C	-14	ASN	-	expression tag	UNP Q76KY3
C	-13	HIS	-	expression tag	UNP Q76KY3
C	-12	LYS	-	expression tag	UNP Q76KY3
C	-11	VAL	-	expression tag	UNP Q76KY3
C	-10	HIS	-	expression tag	UNP Q76KY3
C	-9	HIS	-	expression tag	UNP Q76KY3
C	-8	HIS	-	expression tag	UNP Q76KY3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	HIS	-	expression tag	UNP Q76KY3
C	-6	HIS	-	expression tag	UNP Q76KY3
C	-5	HIS	-	expression tag	UNP Q76KY3
C	-4	ILE	-	expression tag	UNP Q76KY3
C	-3	GLU	-	expression tag	UNP Q76KY3
C	-2	GLY	-	expression tag	UNP Q76KY3
C	-1	ARG	-	expression tag	UNP Q76KY3
C	0	HIS	-	expression tag	UNP Q76KY3
C	223	CYS	ASP	engineered mutation	UNP Q76KY3

- Molecule 2 is a protein called Acyl-carrier-protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	S	0	0	0
			633	404	100	127	2			
2	D	78	Total	C	N	O	S	0	0	0
			640	409	101	128	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q76KY4
B	-18	GLY	-	expression tag	UNP Q76KY4
B	-17	SER	-	expression tag	UNP Q76KY4
B	-16	SER	-	expression tag	UNP Q76KY4
B	-15	HIS	-	expression tag	UNP Q76KY4
B	-14	HIS	-	expression tag	UNP Q76KY4
B	-13	HIS	-	expression tag	UNP Q76KY4
B	-12	HIS	-	expression tag	UNP Q76KY4
B	-11	HIS	-	expression tag	UNP Q76KY4
B	-10	HIS	-	expression tag	UNP Q76KY4
B	-9	SER	-	expression tag	UNP Q76KY4
B	-8	SER	-	expression tag	UNP Q76KY4
B	-7	GLY	-	expression tag	UNP Q76KY4
B	-6	LEU	-	expression tag	UNP Q76KY4
B	-5	VAL	-	expression tag	UNP Q76KY4
B	-4	PRO	-	expression tag	UNP Q76KY4
B	-3	ARG	-	expression tag	UNP Q76KY4
B	-2	GLY	-	expression tag	UNP Q76KY4
B	-1	SER	-	expression tag	UNP Q76KY4
B	0	HIS	-	expression tag	UNP Q76KY4
D	-19	MET	-	initiating methionine	UNP Q76KY4

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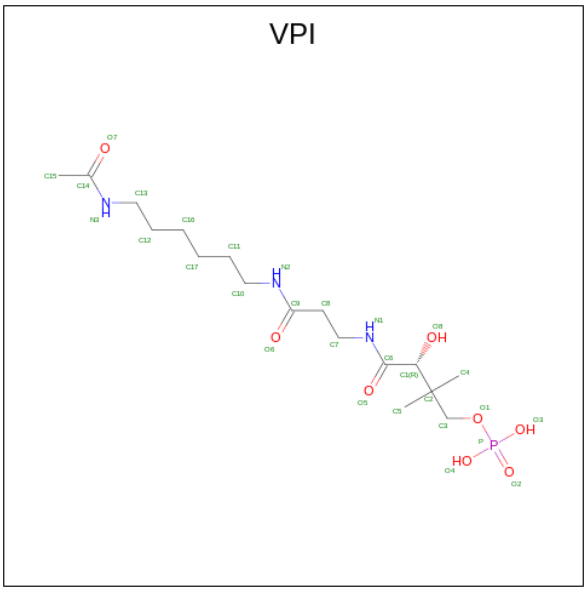
Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	GLY	-	expression tag	UNP Q76KY4
D	-17	SER	-	expression tag	UNP Q76KY4
D	-16	SER	-	expression tag	UNP Q76KY4
D	-15	HIS	-	expression tag	UNP Q76KY4
D	-14	HIS	-	expression tag	UNP Q76KY4
D	-13	HIS	-	expression tag	UNP Q76KY4
D	-12	HIS	-	expression tag	UNP Q76KY4
D	-11	HIS	-	expression tag	UNP Q76KY4
D	-10	HIS	-	expression tag	UNP Q76KY4
D	-9	SER	-	expression tag	UNP Q76KY4
D	-8	SER	-	expression tag	UNP Q76KY4
D	-7	GLY	-	expression tag	UNP Q76KY4
D	-6	LEU	-	expression tag	UNP Q76KY4
D	-5	VAL	-	expression tag	UNP Q76KY4
D	-4	PRO	-	expression tag	UNP Q76KY4
D	-3	ARG	-	expression tag	UNP Q76KY4
D	-2	GLY	-	expression tag	UNP Q76KY4
D	-1	SER	-	expression tag	UNP Q76KY4
D	0	HIS	-	expression tag	UNP Q76KY4

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is [(3 {R})-4-[[3-(6-acetamidohexylamino)-3-oxidanylidene-propyl]amino]-2,2-dimethyl-3-oxidanyl-4-oxidanylidene-butyl] dihydrogen phosphate (three-letter code: VPI) (formula: $C_{17}H_{34}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 28 17 3 7 1	0	0
4	D	1	Total C N O P 28 17 3 7 1	0	0

- Molecule 5 is water.

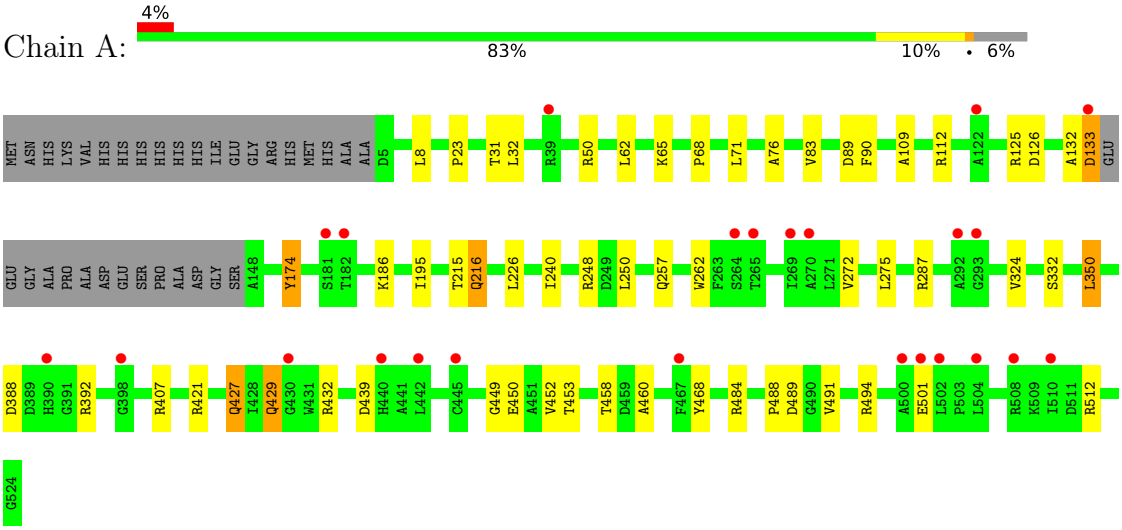
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	17	Total O 17 17	0	0
5	B	3	Total O 3 3	0	0
5	C	17	Total O 17 17	0	0
5	D	6	Total O 6 6	0	0

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.

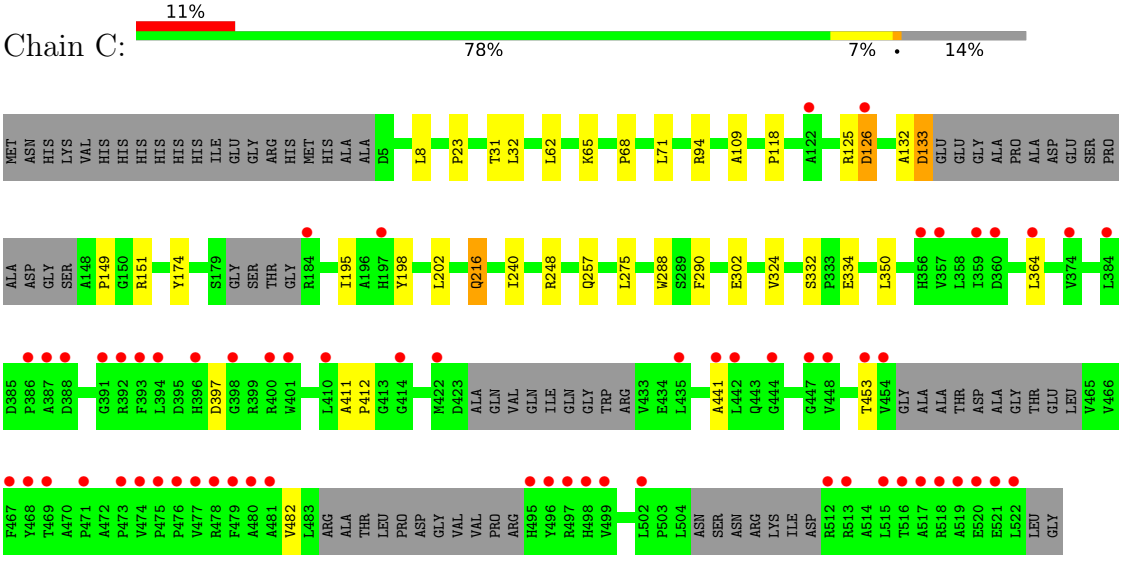
• Molecule 1: Non-ribosomal peptide synthetase

Chain A:



• Molecule 1: Non-ribosomal peptide synthetase

Chain C:

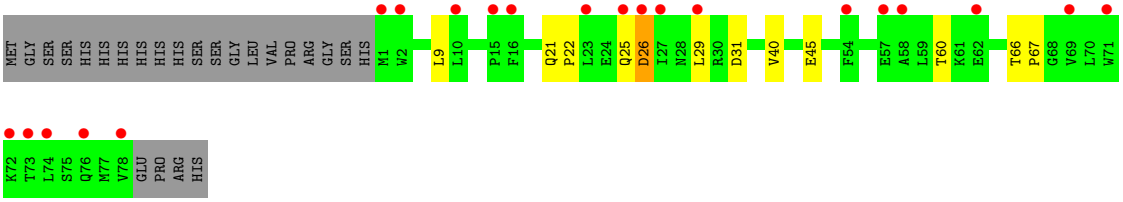


• Molecule 2: Acyl-carrier-protein

Chain B:

• Molecule 2: Acyl-carrier-protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.50Å 72.99Å 80.21Å 94.18° 90.87° 103.34°	Depositor
Resolution (Å)	46.04 – 2.30 46.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.04-2.30) 97.9 (46.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.207 , 0.251 0.211 , 0.251	Depositor DCC
R_{free} test set	2703 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8725	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: VPI, NA

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	0.66	0/3931	0.84	1/5377 (0.0%)
1	C	0.64	0/3611	0.80	0/4934
2	B	0.68	0/646	0.76	0/878
2	D	0.66	0/653	0.75	0/888
All	All	0.66	0/8841	0.81	1/12077 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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	3831	0	3774	27	0
1	C	3520	0	3460	16	0
2	B	633	0	609	7	0
2	D	640	0	618	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	0	0	0
4	D	28	0	0	0	0
5	A	17	0	0	0	0
5	B	3	0	0	0	0
5	C	17	0	0	0	0
5	D	6	0	0	0	0
All	All	8725	0	8461	50	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 (50) 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:65:LYS:HD3	1:A:216:GLN:OE1	1.89	0.72
1:C:65:LYS:HD3	1:C:216:GLN:OE1	1.92	0.68
1:A:489:ASP:OD2	2:B:30:ARG:NH1	2.27	0.67
1:C:133:ASP:N	1:C:133:ASP:OD1	2.34	0.61
1:A:133:ASP:N	1:A:133:ASP:OD1	2.33	0.60
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.88	0.56
2:D:26:ASP:HA	2:D:66:THR:HB	1.89	0.55
1:C:68:PRO:HB3	1:C:132:ALA:HB1	1.89	0.54
1:A:427:GLN:NE2	1:A:429:GLN:O	2.41	0.54
1:A:240:ILE:CD1	1:A:257:GLN:HB3	2.38	0.54
1:A:8:LEU:HD13	1:A:195:ILE:HG21	1.90	0.53
1:C:240:ILE:CD1	1:C:257:GLN:HB3	2.41	0.51
1:A:32:LEU:HD21	1:A:71:LEU:HD21	1.92	0.50
1:A:68:PRO:HB3	1:A:132:ALA:HB1	1.94	0.50
1:A:427:GLN:NE2	1:A:427:GLN:O	2.45	0.50
2:D:29:LEU:HD21	2:D:67:PRO:HG3	1.94	0.49
2:B:29:LEU:HD21	2:B:67:PRO:HG3	1.94	0.49
2:B:26:ASP:HA	2:B:66:THR:HB	1.95	0.49
1:C:8:LEU:HD13	1:C:195:ILE:HG21	1.94	0.48
2:D:9:LEU:HD11	2:D:45:GLU:HG2	1.97	0.46
1:A:458:THR:HG22	1:A:460:ALA:H	1.79	0.46
1:A:439:ASP:OD2	1:A:512:ARG:NH2	2.48	0.46
1:A:489:ASP:OD2	2:B:30:ARG:CZ	2.64	0.45
1:A:275:LEU:CD1	2:B:40:VAL:HG12	2.48	0.44
1:A:484:ARG:NH2	2:B:30:ARG:O	2.51	0.44
1:A:250:LEU:HD22	1:A:272:VAL:HG21	1.99	0.43
2:B:43:LEU:CD1	2:B:54:PHE:CD2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:CE1	1:A:488:PRO:HB3	2.53	0.43
1:C:118:PRO:HA	1:C:149:PRO:HG2	1.99	0.43
1:A:174:TYR:CE2	1:A:226:LEU:HD21	2.54	0.43
1:C:32:LEU:HD21	1:C:71:LEU:HD21	1.99	0.43
1:C:126:ASP:O	1:C:151:ARG:HD2	2.19	0.42
1:C:441:ALA:O	1:C:482:VAL:HG11	2.20	0.42
1:A:62:LEU:O	1:A:109:ALA:HA	2.20	0.42
1:C:62:LEU:O	1:C:109:ALA:HA	2.19	0.42
1:A:76:ALA:HB3	1:A:83:VAL:HG22	2.02	0.41
1:A:89:ASP:HB3	1:A:112:ARG:NH2	2.35	0.41
1:C:275:LEU:CD1	2:D:40:VAL:HG12	2.50	0.41
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.90	0.41
1:A:429:GLN:HE21	1:A:429:GLN:HB3	1.67	0.41
1:C:288:TRP:HB3	1:C:290:PHE:CE2	2.56	0.41
1:A:215:THR:HG21	1:A:262:TRP:CE3	2.55	0.41
1:C:198:TYR:CZ	1:C:202:LEU:HD11	2.56	0.41
1:C:23:PRO:HB3	1:C:31:THR:HG23	2.02	0.40
1:C:397:ASP:OD1	1:C:397:ASP:O	2.39	0.40
1:A:23:PRO:HB3	1:A:31:THR:HG23	2.03	0.40
1:A:186:LYS:HG2	1:A:388:ASP:CG	2.41	0.40
1:A:450:GLU:O	1:A:468:TYR:HA	2.21	0.40
1:A:174:TYR:CZ	1:A:226:LEU:HD21	2.56	0.40
2:D:21:GLN:HA	2:D:22:PRO:HD3	1.94	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	502/540 (93%)	486 (97%)	14 (3%)	2 (0%)	34 42
1	C	449/540 (83%)	437 (97%)	11 (2%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	75/102 (74%)	72 (96%)	3 (4%)	0	100 100
2	D	76/102 (74%)	71 (93%)	5 (7%)	0	100 100
All	All	1102/1284 (86%)	1066 (97%)	33 (3%)	3 (0%)	41 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	324	VAL
1	A	324	VAL
1	A	449	GLY

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	386/412 (94%)	366 (95%)	20 (5%)	23 32
1	C	355/412 (86%)	342 (96%)	13 (4%)	34 48
2	B	71/93 (76%)	67 (94%)	4 (6%)	21 29
2	D	72/93 (77%)	68 (94%)	4 (6%)	21 29
All	All	884/1010 (88%)	843 (95%)	41 (5%)	27 38

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	125	ARG
1	A	126	ASP
1	A	133	ASP
1	A	174	TYR
1	A	216	GLN
1	A	248	ARG
1	A	332	SER
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	392	ARG
1	A	407	ARG
1	A	421	ARG
1	A	427	GLN
1	A	429	GLN
1	A	432	ARG
1	A	452	VAL
1	A	453	THR
1	A	491	VAL
1	A	494	ARG
1	A	501	GLU
2	B	26	ASP
2	B	30	ARG
2	B	37	LEU
2	B	61	LYS
1	C	94	ARG
1	C	125	ARG
1	C	126	ASP
1	C	133	ASP
1	C	174	TYR
1	C	216	GLN
1	C	248	ARG
1	C	302	GLU
1	C	332	SER
1	C	334	GLU
1	C	350	LEU
1	C	364	LEU
1	C	453	THR
2	D	25	GLN
2	D	26	ASP
2	D	31	ASP
2	D	60	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	GLN
1	A	429	GLN
1	C	396	HIS

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	VPI	B	101	2,1	22,27,28	0.92	1 (4%)	27,34,37	1.39	3 (11%)
4	VPI	D	101	2,1	22,27,28	0.59	0	27,34,37	1.39	3 (11%)

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	VPI	B	101	2,1	-	12/31/33/34	-
4	VPI	D	101	2,1	-	11/31/33/34	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	101	VPI	P-O1	-2.08	1.56	1.62

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	101	VPI	C4-C2-C1	4.82	117.18	108.82
4	B	101	VPI	C4-C2-C1	3.34	114.61	108.82
4	D	101	VPI	C4-C2-C3	-3.31	102.83	108.23
4	B	101	VPI	C4-C2-C3	-2.67	103.88	108.23
4	D	101	VPI	O6-C9-C8	-2.33	117.76	122.02
4	B	101	VPI	C5-C2-C4	2.22	113.69	109.17

There are no chirality outliers.

All (23) torsion outliers are listed below:

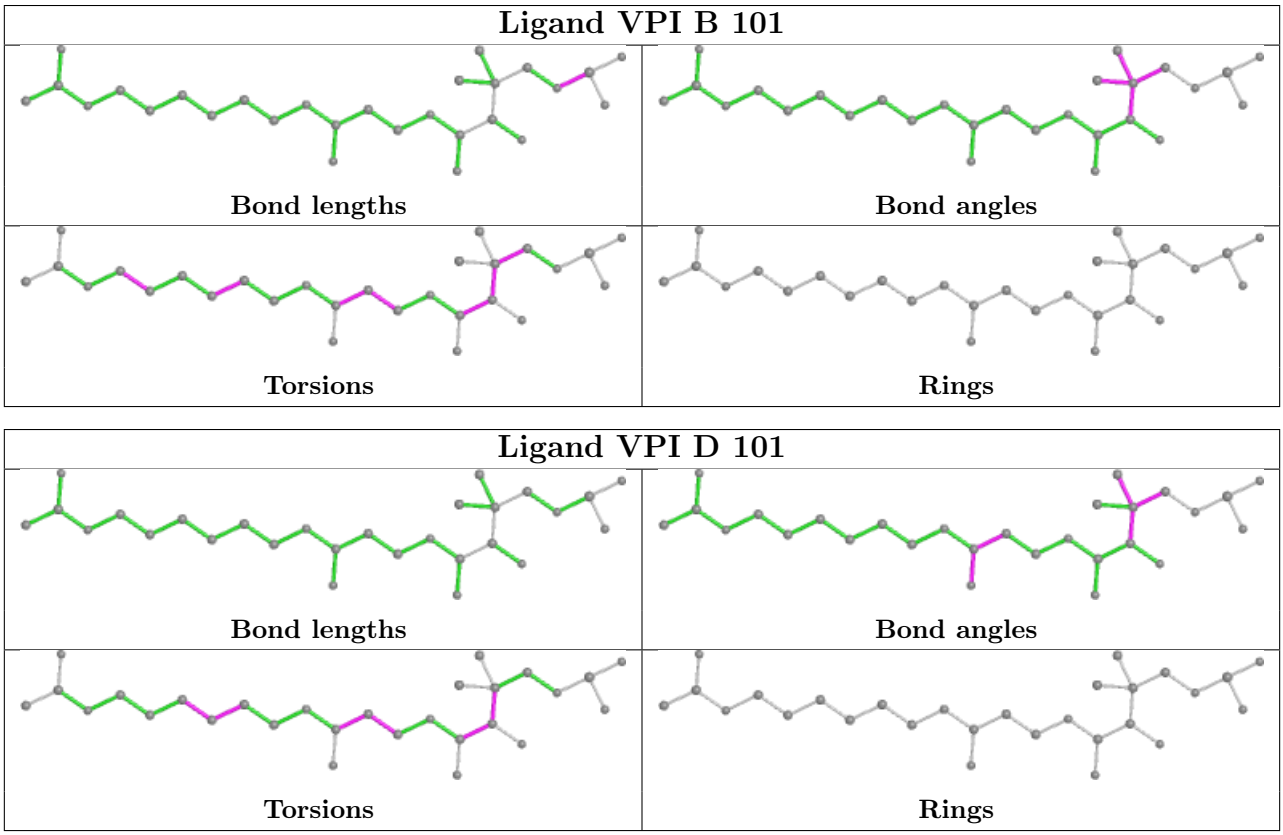
Mol	Chain	Res	Type	Atoms
4	B	101	VPI	C6-C1-C2-C4
4	B	101	VPI	C6-C1-C2-C3
4	B	101	VPI	O8-C1-C2-C4
4	B	101	VPI	O8-C1-C2-C3
4	D	101	VPI	N1-C7-C8-C9
4	D	101	VPI	C6-C1-C2-C4
4	D	101	VPI	C6-C1-C2-C3
4	D	101	VPI	O8-C1-C2-C4
4	D	101	VPI	O8-C1-C2-C5
4	D	101	VPI	O8-C1-C2-C3
4	B	101	VPI	C10-C11-C17-C16
4	B	101	VPI	C7-C8-C9-O6
4	B	101	VPI	O8-C1-C2-C5
4	D	101	VPI	C12-C16-C17-C11
4	D	101	VPI	C7-C8-C9-O6
4	B	101	VPI	N1-C7-C8-C9
4	D	101	VPI	C7-C8-C9-N2
4	B	101	VPI	C1-C2-C3-O1
4	D	101	VPI	C10-C11-C17-C16
4	B	101	VPI	C7-C8-C9-N2
4	D	101	VPI	O8-C1-C6-O5
4	B	101	VPI	O8-C1-C6-N1
4	B	101	VPI	C16-C12-C13-N3

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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, 95^{th} 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	506/540 (93%)	0.51	24 (4%) 31 38	38, 55, 77, 96	0
1	C	463/540 (85%)	0.80	62 (13%) 3 4	38, 59, 95, 114	0
2	B	77/102 (75%)	0.73	8 (10%) 6 9	48, 68, 89, 101	0
2	D	78/102 (76%)	1.22	21 (26%) 0 0	45, 76, 96, 100	0
All	All	1124/1284 (87%)	0.69	115 (10%) 6 9	38, 58, 91, 114	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	496	TYR	6.6
2	D	76	GLN	5.9
1	C	522	LEU	4.9
1	C	517	ALA	4.8
1	C	444	GLY	4.6
1	C	477	VAL	4.5
1	C	393	PHE	4.5
2	D	72	LYS	4.4
1	C	386	PRO	4.3
1	C	498	HIS	4.2
1	C	391	GLY	4.2
1	C	497	ARG	4.1
1	C	469	THR	4.0
1	C	513	ARG	3.9
1	C	499	VAL	3.9
1	A	500	ALA	3.9
1	C	479	PHE	3.9
2	B	57	GLU	3.9
1	C	495	HIS	3.8
1	C	468	TYR	3.8
1	C	518	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	512	ARG	3.6
1	C	396	HIS	3.6
1	C	475	PRO	3.6
1	A	501	GLU	3.5
1	A	445	CYS	3.5
1	A	182	THR	3.5
1	C	519	ALA	3.5
1	C	521	GLU	3.5
1	C	481	ALA	3.5
1	C	516	THR	3.4
2	D	62	GLU	3.4
1	C	435	LEU	3.4
1	C	442	LEU	3.4
2	B	76	GLN	3.3
2	B	72	LYS	3.3
1	C	359	ILE	3.3
2	B	1	MET	3.3
1	C	410	LEU	3.3
1	C	454	VAL	3.1
1	C	360	ASP	3.1
1	C	480	ALA	3.1
1	C	394	LEU	3.1
1	C	478	ARG	3.1
1	C	392	ARG	3.1
1	C	515	LEU	3.1
1	C	471	PRO	3.1
1	C	476	PRO	3.1
1	A	510	ILE	3.1
2	D	54	PHE	3.1
1	C	184	ARG	3.0
2	D	10	LEU	2.9
1	C	453	THR	2.9
1	A	292	ALA	2.9
2	B	77	MET	2.9
2	D	78	VAL	2.9
2	D	58	ALA	2.8
1	C	387	ALA	2.8
1	C	384	LEU	2.8
2	D	23	LEU	2.8
1	C	357	VAL	2.7
1	A	39	ARG	2.7
1	A	440	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	265	THR	2.7
1	A	270	ALA	2.7
2	D	57	GLU	2.6
1	A	502	LEU	2.6
1	C	356	HIS	2.6
1	C	467	PHE	2.6
2	B	58	ALA	2.6
2	D	71	TRP	2.5
1	A	293	GLY	2.5
1	C	447	GLY	2.5
2	D	16	PHE	2.5
1	A	269	ILE	2.5
1	C	422	MET	2.5
1	C	520	GLU	2.5
1	C	364	LEU	2.5
2	D	69	VAL	2.5
2	D	1	MET	2.4
1	C	448	VAL	2.4
1	A	122	ALA	2.4
1	C	398	GLY	2.4
1	C	441	ALA	2.4
1	C	473	PRO	2.4
1	A	430	GLY	2.3
1	C	400	ARG	2.3
2	D	27	ILE	2.3
1	C	502	LEU	2.3
1	A	442	LEU	2.3
1	A	398	GLY	2.3
2	D	74	LEU	2.2
1	A	133	ASP	2.2
2	D	25	GLN	2.2
1	A	508	ARG	2.2
2	B	52	VAL	2.2
1	A	467	PHE	2.2
2	D	73	THR	2.2
1	A	504	LEU	2.2
1	C	126	ASP	2.2
2	D	29	LEU	2.1
2	D	2	TRP	2.1
2	B	55	GLN	2.1
1	A	181	SER	2.1
1	C	414	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	388	ASP	2.1
1	A	264	SER	2.1
1	C	197	HIS	2.1
1	C	122	ALA	2.1
1	C	374	VAL	2.0
1	C	401	TRP	2.0
1	C	474	VAL	2.0
1	A	390	HIS	2.0
2	D	15	PRO	2.0
2	D	26	ASP	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)

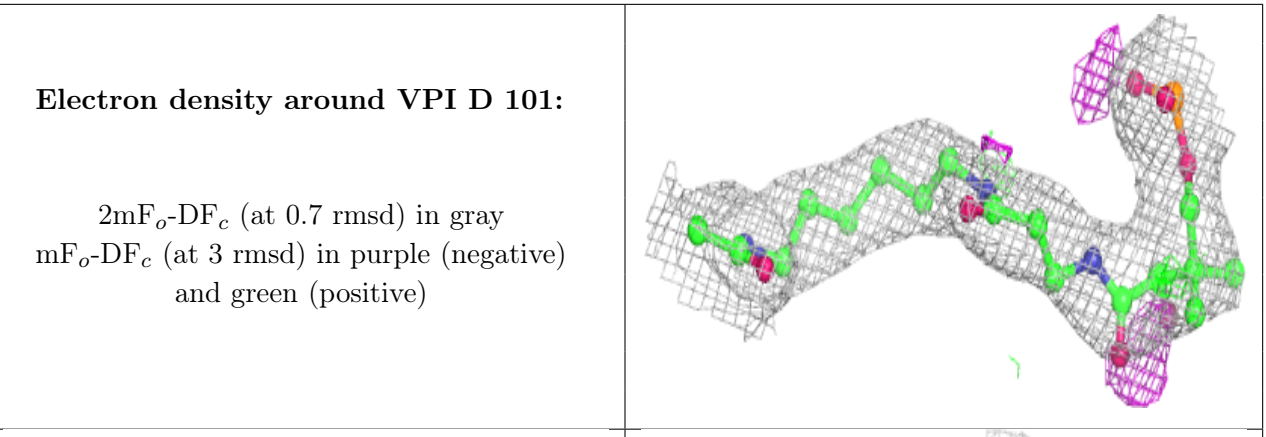
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	NA	C	601	1/1	0.66	0.12	64,64,64,64	0
3	NA	A	601	1/1	0.82	0.10	65,65,65,65	0
4	VPI	D	101	28/29	0.92	0.18	55,65,76,78	0
4	VPI	B	101	28/29	0.95	0.26	54,58,61,61	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.

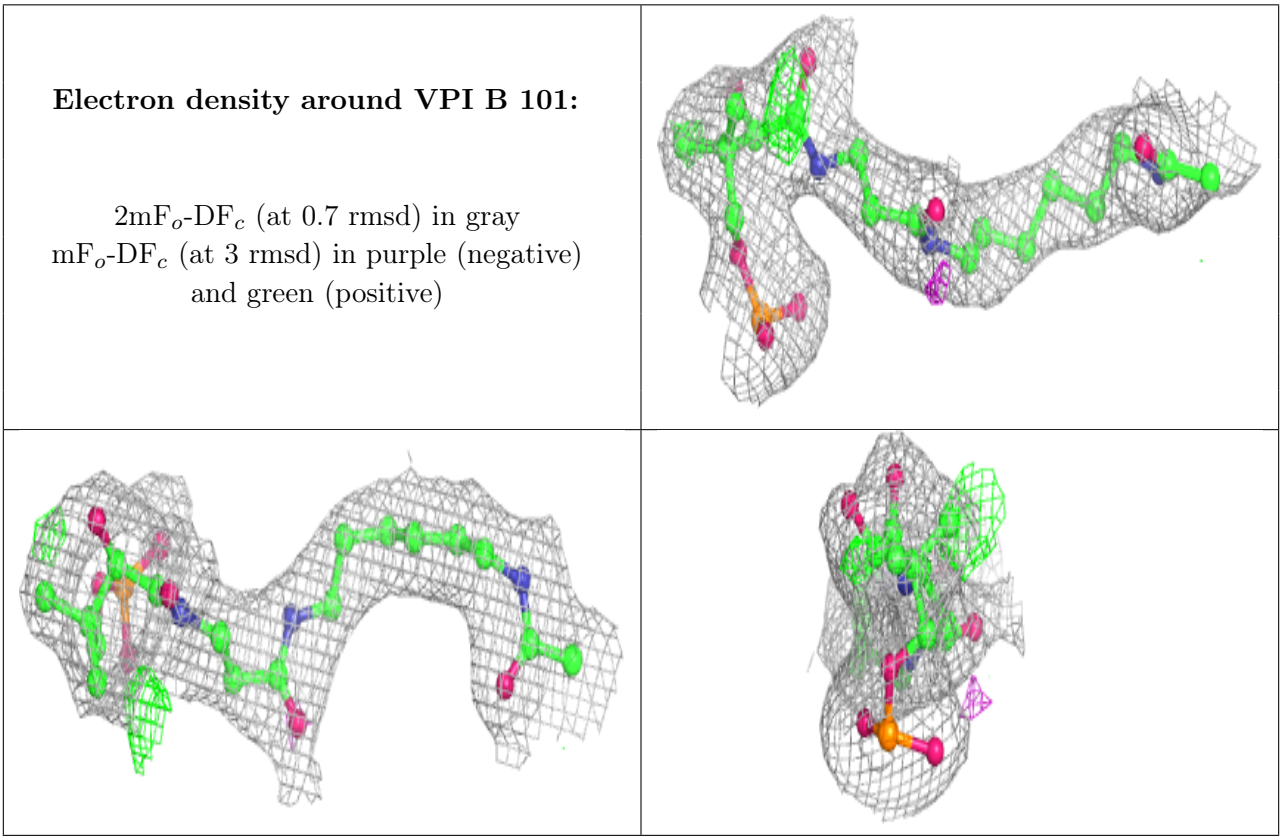
Electron density around VPI D 101:

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



Electron density around VPI B 101:

$2mF_o$-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.