Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2017 – 05:55 AM EDT

PDB ID	:	3SEO
Title	:	Crystal structure of VopL C terminal domain
Authors	:	Yu, B.; Rosen, M.K.; Tomchick, D.R.
Deposited on	:	unknown
Resolution	:	2.31 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

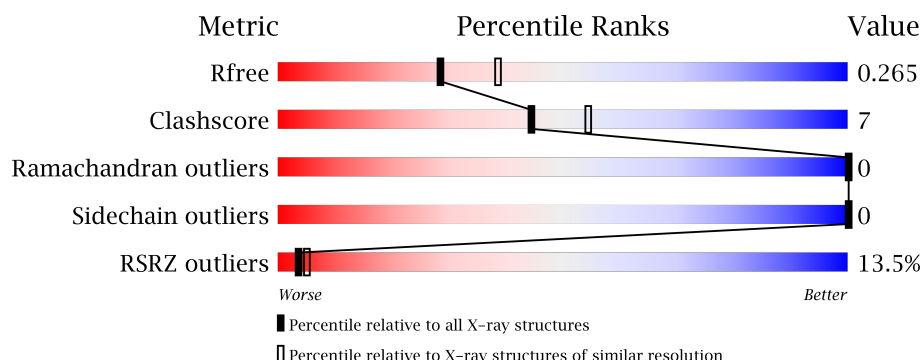|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.31 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		13.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	241	19% 78% 13% 10%
1	B	241	6% 75% 19% 6%

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
2	CL	B	244	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3555 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 VopL C terminal domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total 1723	C 1081	N 294	O 340	S 8	101	0	0
1	B	226	Total 1787	C 1119	N 308	O 351	S 9	58	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q87GE5
A	2	HIS	-	EXPRESSION TAG	UNP Q87GE5
A	3	MET	-	EXPRESSION TAG	UNP Q87GE5
B	1	GLY	-	EXPRESSION TAG	UNP Q87GE5
B	2	HIS	-	EXPRESSION TAG	UNP Q87GE5
B	3	MET	-	EXPRESSION TAG	UNP Q87GE5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total 8	Cl 8	0	0
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	16	Total 16	O 16	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: VopL C terminal domain protein
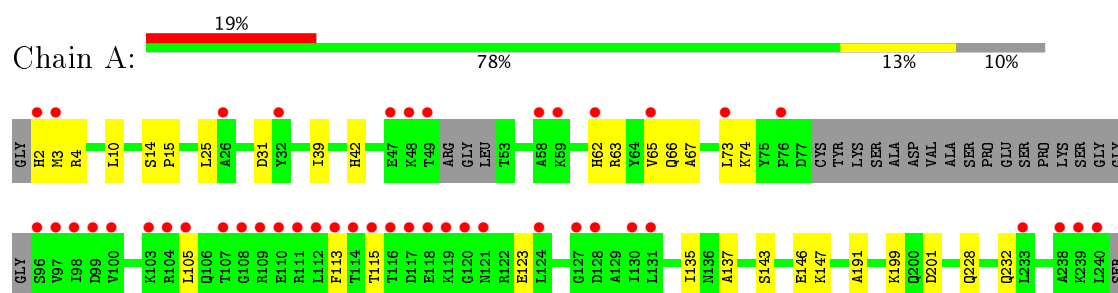
- Molecule 1: VopL C terminal domain protein
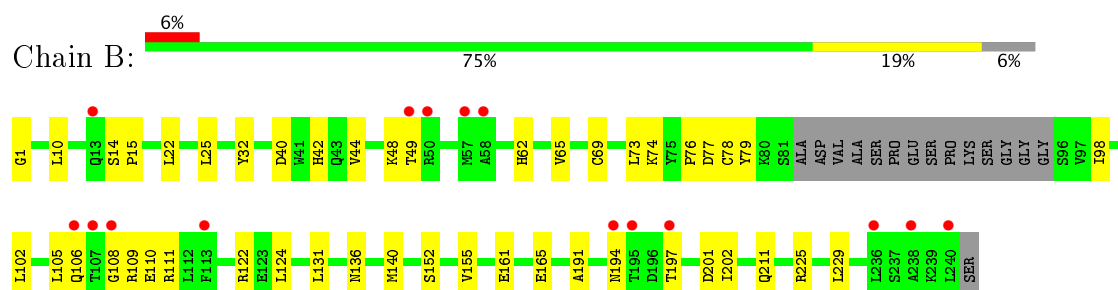
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.18Å 89.85Å 103.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.15 – 2.31 29.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.15-2.31) 98.7 (29.15-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.221 , 0.275 0.207 , 0.265	Depositor DCC
R_{free} test set	1944 reflections (8.47%)	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3555	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 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	0.24	0/1747	0.37	0/2349
1	B	0.24	0/1813	0.36	0/2437
All	All	0.24	0/3560	0.36	0/4786

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	1723	0	1687	19	0
1	B	1787	0	1752	30	0
2	A	1	0	0	0	0
2	B	8	0	0	0	0
3	A	20	0	0	0	0
3	B	16	0	0	0	0
All	All	3555	0	3439	49	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 7.

All (49) 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:161:GLU:O	1:B:165:GLU:HG2	1.88	0.73
1:B:44:VAL:O	1:B:48:LYS:HG2	1.94	0.68
1:B:1:GLY:HA3	1:B:32:TYR:CD1	2.34	0.63
1:B:109:ARG:O	1:B:110:GLU:HB2	2.01	0.61
1:B:78:CYS:SG	1:B:105:LEU:HG	2.42	0.60
1:B:122:ARG:NH2	1:B:124:LEU:HD11	2.18	0.59
1:A:73:LEU:HD12	1:A:74:LYS:N	2.20	0.57
1:B:1:GLY:HA3	1:B:32:TYR:HD1	1.70	0.57
1:B:22:LEU:HD21	1:B:211:GLN:HB2	1.88	0.56
1:A:2:HIS:CG	1:A:3:MET:H	2.23	0.56
1:B:62:HIS:O	1:B:65:VAL:HG22	2.06	0.56
1:A:2:HIS:CD2	1:A:4:ARG:H	2.24	0.54
1:A:62:HIS:O	1:A:65:VAL:HG12	2.08	0.54
1:A:2:HIS:CG	1:A:3:MET:N	2.77	0.53
1:B:74:LYS:O	1:B:76:PRO:HD3	2.08	0.53
1:B:40:ASP:O	1:B:44:VAL:HG13	2.08	0.52
1:B:152:SER:O	1:B:155:VAL:HG23	2.10	0.51
1:B:122:ARG:HH22	1:B:124:LEU:HD11	1.75	0.51
1:A:115:THR:HB	1:A:123:GLU:O	2.10	0.51
1:B:49:THR:OG1	1:B:98:ILE:HG13	2.11	0.50
1:A:228:GLN:O	1:A:232:GLN:HG3	2.13	0.49
1:B:102:LEU:O	1:B:106:GLN:HG3	2.14	0.48
1:B:42:HIS:CE1	1:B:131:LEU:HD21	2.49	0.48
1:B:108:GLY:O	1:B:111:ARG:HB3	2.15	0.47
1:B:14:SER:N	1:B:15:PRO:HD2	2.29	0.46
1:A:67:ALA:HB1	1:A:137:ALA:HB1	1.96	0.46
1:B:225:ARG:NH1	1:B:229:LEU:HG	2.31	0.46
1:A:14:SER:OG	1:A:15:PRO:HD3	2.16	0.46
1:B:62:HIS:HB2	1:B:65:VAL:HG22	1.99	0.45
1:A:191:ALA:O	1:A:201:ASP:HB3	2.17	0.45
1:B:77:ASP:N	1:B:77:ASP:OD1	2.43	0.45
1:A:31:ASP:OD1	1:A:199:LYS:HE3	2.18	0.44
1:B:76:PRO:HA	1:B:79:TYR:CE2	2.53	0.44
1:A:143:SER:OG	1:A:146:GLU:HG3	2.18	0.43
1:A:63:ARG:O	1:A:66:GLN:HG2	2.18	0.43
1:B:136:ASN:O	1:B:140:MET:HG2	2.18	0.43
1:B:191:ALA:O	1:B:201:ASP:HB3	2.18	0.43
1:B:69:CYS:O	1:B:73:LEU:HG	2.19	0.43
1:A:39:ILE:HD11	1:A:147:LYS:HG3	2.01	0.42
1:B:109:ARG:O	1:B:110:GLU:CB	2.67	0.42
1:B:202:ILE:HA	1:B:202:ILE:HD12	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:SER:OG	1:B:15:PRO:HD3	2.19	0.41
1:B:194:ASN:HB2	1:B:197:THR:OG1	2.21	0.41
1:B:10:LEU:HD11	1:B:25:LEU:HD21	2.01	0.41
1:A:14:SER:N	1:A:15:PRO:CD	2.84	0.41
1:A:105:LEU:HD23	1:A:113:PHE:CE1	2.56	0.41
1:A:123:GLU:OE2	1:A:123:GLU:HA	2.21	0.40
1:A:10:LEU:HD11	1:A:25:LEU:HD21	2.03	0.40
1:A:42:HIS:NE2	1:A:135:ILE:HD11	2.37	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	212/241 (88%)	206 (97%)	6 (3%)	0	100	100
1	B	223/241 (92%)	217 (97%)	6 (3%)	0	100	100
All	All	435/482 (90%)	423 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	182/200 (91%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	188/200 (94%)	188 (100%)	0	100	100
All	All	370/400 (92%)	370 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	28	ASN
1	A	228	GLN
1	B	28	ASN
1	B	42	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	218/241 (90%)	1.23	45 (20%)	1	1	40, 82, 173, 191	27 (12%)
1	B	226/241 (93%)	0.58	15 (6%)	19	25	44, 78, 128, 147	18 (7%)
All	All	444/482 (92%)	0.90	60 (13%)	3	5	40, 79, 153, 191	45 (10%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	LYS	7.2
1	A	97	VAL	7.1
1	A	2	HIS	6.8
1	A	110	GLU	6.6
1	A	116	THR	6.5
1	A	114	THR	6.5
1	A	96	SER	6.2
1	A	124	LEU	6.1
1	B	58	ALA	5.8
1	A	113	PHE	5.8
1	A	118	GLU	5.6
1	A	119	LYS	5.6
1	A	100	VAL	5.5
1	A	105	LEU	5.2
1	A	104	ARG	4.9
1	A	112	LEU	4.9
1	A	109	ARG	4.9
1	A	239	LYS	4.7
1	A	240	LEU	4.3
1	B	194	ASN	4.2
1	A	58	ALA	4.0
1	B	107	THR	3.7
1	A	111	ARG	3.6
1	A	98	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	99	ASP	3.6
1	A	3	MET	3.5
1	A	108	GLY	3.3
1	A	128	ASP	3.2
1	A	76	PRO	3.2
1	A	107	THR	3.2
1	A	49	THR	3.1
1	A	117	ASP	3.1
1	A	65	VAL	3.0
1	A	238	ALA	3.0
1	A	131	LEU	2.8
1	A	62	HIS	2.8
1	A	130	ILE	2.8
1	B	197	THR	2.7
1	B	50	ARG	2.6
1	A	47	GLU	2.6
1	A	73	LEU	2.5
1	B	57	MET	2.5
1	B	240	LEU	2.5
1	B	236	LEU	2.5
1	B	195	THR	2.5
1	B	238	ALA	2.4
1	A	48	LYS	2.4
1	A	121	ASN	2.4
1	A	26	ALA	2.3
1	A	115	THR	2.3
1	A	233	LEU	2.2
1	A	103	LYS	2.2
1	B	108	GLY	2.2
1	A	32	TYR	2.1
1	B	49	THR	2.1
1	A	127	GLY	2.1
1	B	13[A]	GLN	2.1
1	B	113	PHE	2.1
1	B	106	GLN	2.0
1	A	120	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	CL	B	244	1/1	0.76	0.20	5.30	94,94,94,94	0
2	CL	B	242	1/1	0.90	0.23	1.62	104,104,104,104	0
2	CL	B	249	1/1	0.90	0.13	-	140,140,140,140	0
2	CL	B	245	1/1	0.94	0.15	-	98,98,98,98	0
2	CL	B	247	1/1	0.19	0.20	-	118,118,118,118	0
2	CL	A	242	1/1	0.15	1.58	-	179,179,179,179	0
2	CL	B	246	1/1	0.87	0.10	-	98,98,98,98	0
2	CL	B	243	1/1	0.86	0.46	-	99,99,99,99	0
2	CL	B	248	1/1	0.91	0.17	-	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.