wwPDB X-ray Structure Validation Summary Report (i)

Apr 12, 2023 – 04:13 PM EDT

PDB ID	:	4SBV
Title	:	The REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIPROCAL SPACE
Authors	:	Rossmann, M.G.
Deposited on	:	1985-04-01
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

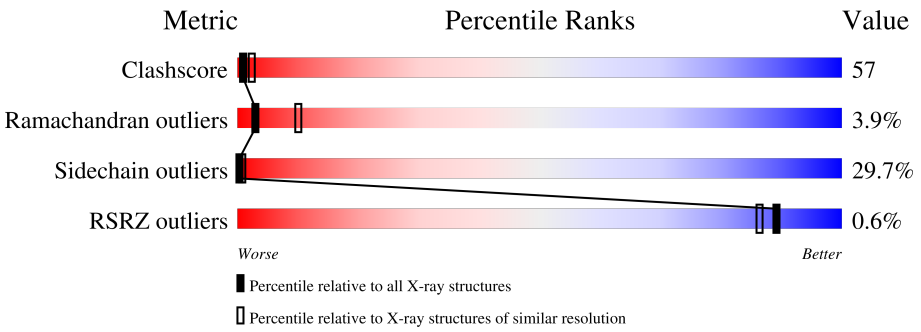
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	260	.% 17% 34% 16% 9% 23%
1	B	260	17% 32% 19% 8% 23%
1	C	260	21% 35% 22% 8% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4723 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 SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1506	956	249	292	9	0	0	0
1	B	199	1506	956	249	292	9	0	0	0
1	C	222	1674	1062	281	319	12	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is water.

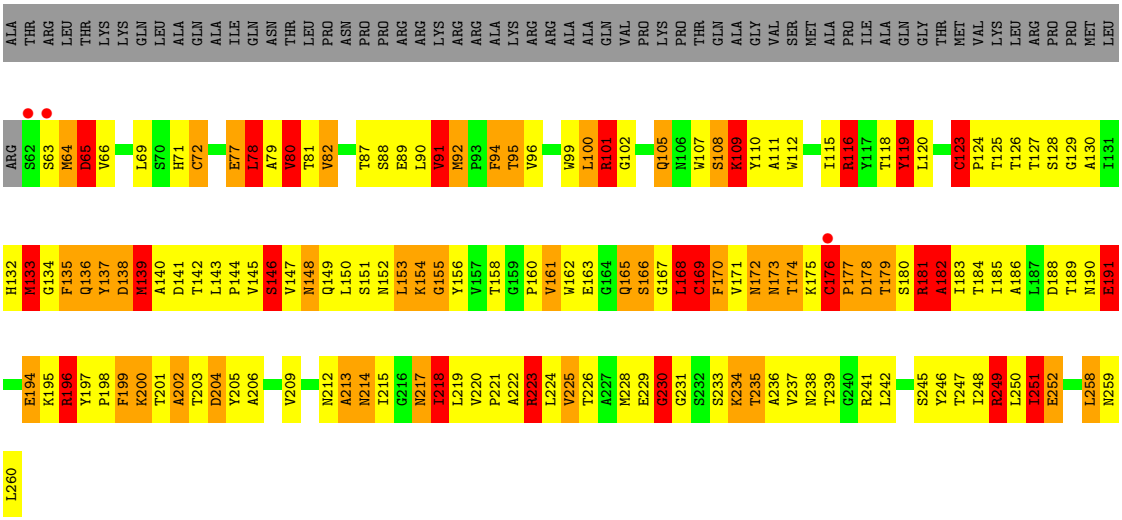
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	15	15	15	0	0
3	B	10	10	10	0	0
3	C	9	9	9	0	0

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.

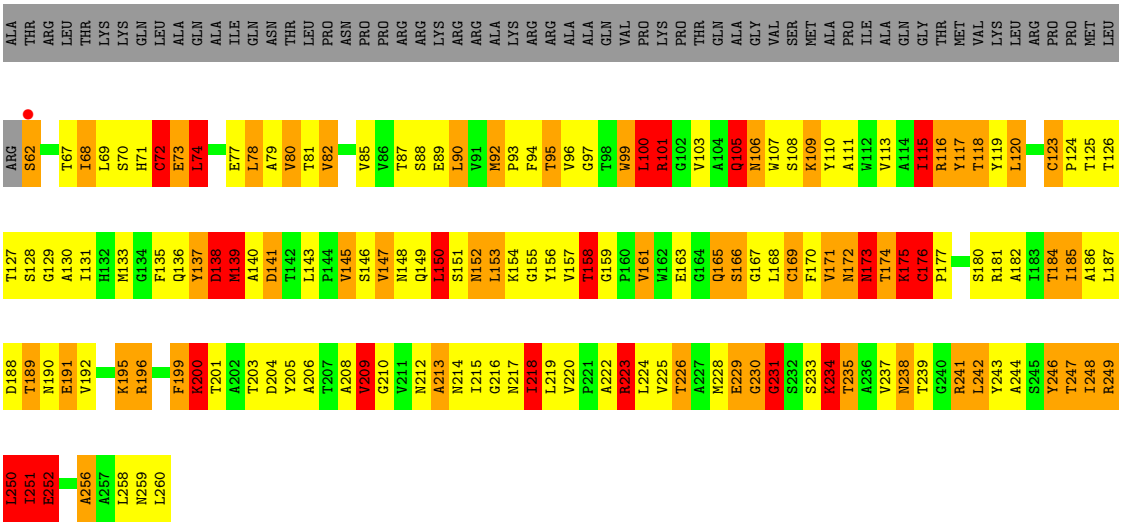
• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain A:



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain B:



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain C: 21% 35% 22% 8% 15%

ALA THR ARG LEU THR LYS LYS GLN LEU ALA GLN ALA ILE GLN ASN THR LEU PRO ASN PRO PRO ARG ARG LYS ARG ARG ALA LYS ARG ARG ALA ALA GLN VAL PRO LYS PRO THR Q39 I47 A48 Q49 M52 V53 K54 L55 R56 P57 P58 M59 L60 R61 S62 S63 M64 D65 V66 T67

I68 L69 S70 H71 C72 E73 L74 S75 T76 E77 L78 A79 V80 T81 V82 T83 I84 V85 V86 T87 S88 E89 L90 V91 M92 P93 F94 T95 V96 G97 T98 W99 L100 R101 G102 W107 S108 K109 Y110 V113 A114 I115 R116 Y117 T118 Y119 L120 P121 S122 C123 P124 T125 T126 T127 S128 G129 A130 I131

H132 M133 G134 F135 Q136 Y137 D138 M139 A140 L143 P144 V145 S146 Q149 L150 S151 N152 L153 K154 G155 Y156 V157 T158 V161 W162 E163 G164 Q165 S166 G167 L168 C169 F170 V171 N172 N173 T174 K175 C176 P177 D178 T179 S180 R181 A182 I183 T184 I185 A186 L187 D188 T189 N190 E191 V192 S193 E194

K195 R196 Y197 P198 F199 K200 T201 A202 T203 D204 Y205 A206 T207 A208 V209 N212 A213 N214 I215 G216 N217 I218 L219 V220 P221 A222 R223 L224 V225 T226 A227 M228 E229 G230 G231 S232 S233 K234 T235 N238 T239 G240 R241 L242 Y243 A244 S245 Y246 T247 I248 R249 L250 I251 E252 P253 A256 A257

L258 N259 L260

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	334.30Å 334.30Å 757.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80 142.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 75.4 (142.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available) 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.7	EDS
L-test for twinning[1]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.47	8/1537 (0.5%)	2.64	103/2104 (4.9%)
1	B	1.43	7/1537 (0.5%)	2.46	106/2104 (5.0%)
1	C	1.48	11/1708 (0.6%)	2.55	96/2335 (4.1%)
All	All	1.46	26/4782 (0.5%)	2.55	305/6543 (4.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	GLU	N-CA	10.24	1.66	1.46
1	C	155	GLY	N-CA	9.11	1.59	1.46
1	B	231	GLY	N-CA	-8.84	1.32	1.46
1	C	231	GLY	N-CA	-8.78	1.32	1.46
1	A	230	GLY	N-CA	8.31	1.58	1.46

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	ARG	NE-CZ-NH1	31.26	135.93	120.30
1	C	101	ARG	NE-CZ-NH1	26.07	133.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	109	LYS	CA-CB-CG	25.73	170.01	113.40
1	A	196	ARG	NE-CZ-NH2	-18.91	110.84	120.30
1	A	125	THR	N-CA-CB	17.77	144.05	110.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	249	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	241	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1506	0	1504	208	0
1	B	1506	0	1504	180	0
1	C	1674	0	1691	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
3	C	9	0	0	0	0
All	All	4723	0	4699	536	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 57.

The worst 5 of 536 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:C:212:ASN:ND2	1:C:214:ASN:H	1.42	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:VAL:H	1:C:149:GLN:NE2	1.46	1.12
1:C:161:VAL:HG22	1:C:239:THR:CG2	1.82	1.09
1:C:161:VAL:HG22	1:C:239:THR:HG21	1.09	1.08
1:C:131:ILE:HG13	1:C:228:MET:HE2	1.34	1.05

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	197/260 (76%)	160 (81%)	27 (14%)	10 (5%)	2 6
1	B	197/260 (76%)	163 (83%)	29 (15%)	5 (2%)	5 19
1	C	220/260 (85%)	182 (83%)	29 (13%)	9 (4%)	3 9
All	All	614/780 (79%)	505 (82%)	85 (14%)	24 (4%)	3 10

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	B	231	GLY
1	C	219	LEU
1	C	230	GLY
1	C	231	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	167/217 (77%)	121 (72%)	46 (28%)	0 1
1	B	167/217 (77%)	116 (70%)	51 (30%)	0 1
1	C	185/217 (85%)	128 (69%)	57 (31%)	0 0
All	All	519/651 (80%)	365 (70%)	154 (30%)	0 1

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	92	MET
1	C	196	ARG
1	C	121	PRO
1	C	161	VAL
1	C	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	ASN
1	B	214	ASN
1	C	212	ASN
1	B	212	ASN
1	B	217	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 3 ligands modelled in this entry, 3 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(Å^2)	Q<0.9
1	A	199/260 (76%)	0.27	3 (1%)	73	68	12, 22, 60, 83	0
1	B	199/260 (76%)	0.22	1 (0%)	91	88	10, 21, 50, 65	0
1	C	222/260 (85%)	0.15	0	100	100	8, 21, 37, 60	0
All	All	620/780 (79%)	0.21	4 (0%)	89	86	8, 21, 46, 83	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	SER	11.8
1	A	63	SER	8.5
1	A	176	CYS	3.7
1	B	62	SER	3.4

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
2	CA	A	261	1/1	0.95	0.10	27,27,27,27	0
2	CA	C	261	1/1	0.97	0.12	20,20,20,20	0
2	CA	B	261	1/1	0.98	0.12	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.