



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2016 – 07:05 PM EDT

PDB ID : 5J96
Title : Crystal structure of Slow Bee Paralysis Virus at 3.4A resolution
Authors : Kalynych, S.; Levdansky, Y.; Palkova, L.; Plevka, P.
Deposited on : 2016-04-08
Resolution : 3.41 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20027939

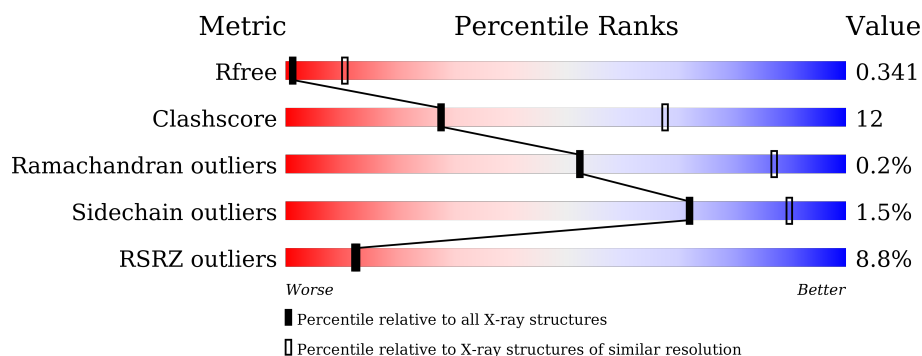
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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 $\leq 5\%$. 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	266	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>31%</div> <div>• 10%</div> </div> </div>
2	B	261	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>
3	C	430	<div> <div>15%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7029 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1896	1216	327	345	8			

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1954	1260	316	364	14			

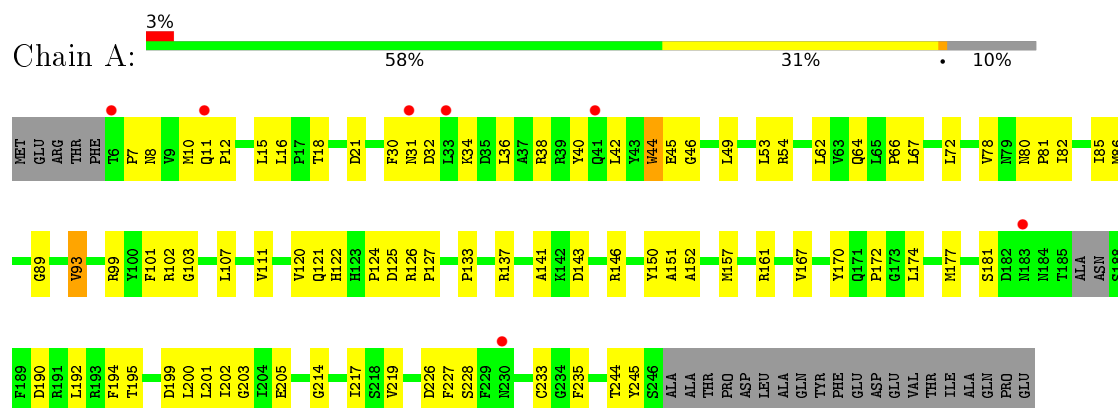
- Molecule 3 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	411	Total	C	N	O	S	0	0	0
			3179	2056	527	588	8			

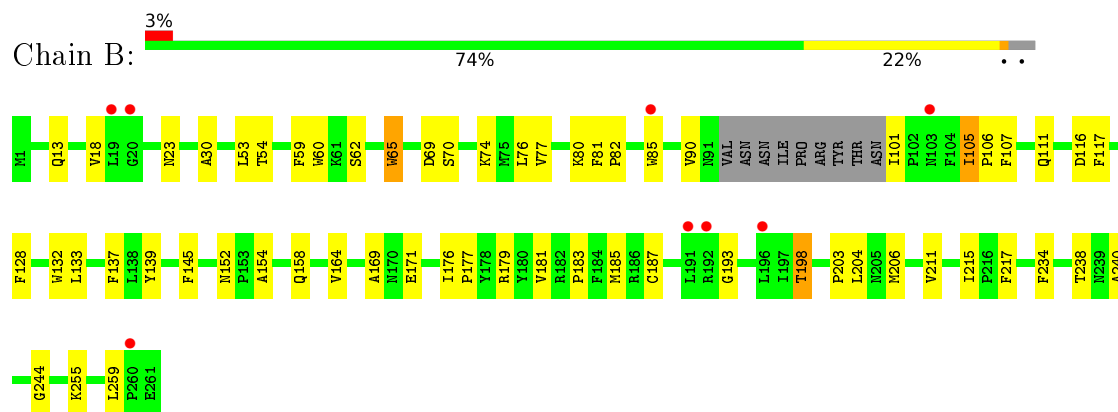
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

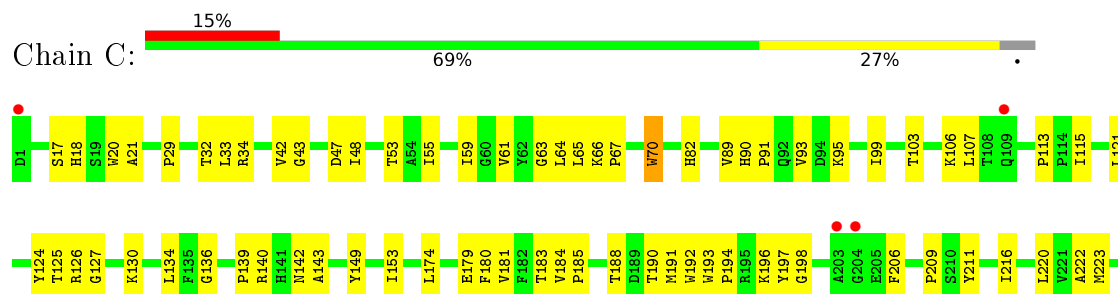
• Molecule 1: VP1

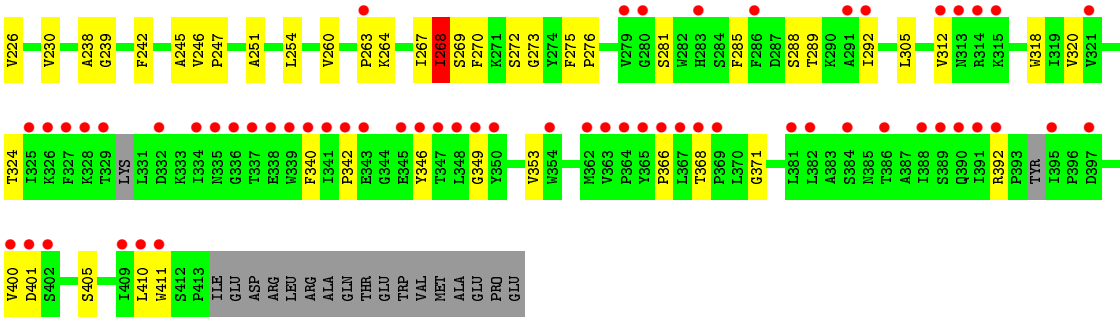


• Molecule 2: VP2



• Molecule 3: Genome polyprotein





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	360.66Å 360.66Å 360.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.70 – 3.41 70.73 – 3.41	Depositor EDS
% Data completeness (in resolution range)	87.4 (70.70-3.41) 87.1 (70.73-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.41Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.339 , 0.339 0.336 , 0.341	Depositor DCC
R_{free} test set	4568 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 6.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	7029	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/1948	0.57	1/2655 (0.0%)
2	B	0.25	0/2004	0.49	0/2733
3	C	0.23	0/3274	0.46	1/4483 (0.0%)
All	All	0.25	0/7226	0.50	2/9871 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	264	LYS	N-CA-C	-5.34	96.57	111.00
1	A	30	PHE	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1896	0	1832	67	0
2	B	1954	0	1865	43	0
3	C	3179	0	3107	89	0
All	All	7029	0	6804	163	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 12.

All (163) 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)
3:C:91:PRO:HG3	3:C:125:THR:HG21	1.55	0.86
2:B:105:ILE:HG22	2:B:106:PRO:HD2	1.56	0.85
2:B:53:LEU:HB3	2:B:106:PRO:HB3	1.59	0.84
1:A:18:THR:HG21	3:C:185:PRO:HB3	1.62	0.81
2:B:90:VAL:HG11	2:B:255:LYS:HE3	1.65	0.78
1:A:45:GLU:HG2	1:A:46:GLY:H	1.52	0.75
1:A:78:VAL:HG21	3:C:268:ILE:HA	1.71	0.72
1:A:174:LEU:HD22	2:B:183:PRO:HB3	1.71	0.72
3:C:270:PHE:HA	3:C:305:LEU:HA	1.75	0.68
3:C:82:HIS:HB3	3:C:216:ILE:HD12	1.74	0.67
3:C:272:SER:HA	3:C:275:PHE:HE1	1.61	0.66
3:C:368:THR:HG23	3:C:371:GLY:H	1.60	0.66
1:A:53:LEU:HD21	1:A:62:LEU:HG	1.79	0.65
2:B:187:CYS:HA	2:B:204:LEU:HD13	1.78	0.65
3:C:281:SER:HB2	3:C:288:SER:HB2	1.77	0.65
3:C:91:PRO:HB3	3:C:242:PHE:HZ	1.62	0.64
1:A:174:LEU:HD21	3:C:47:ASP:HB3	1.80	0.64
1:A:21:ASP:OD2	3:C:126:ARG:NH2	2.28	0.63
1:A:8:ASN:HB3	3:C:61:VAL:HG13	1.81	0.62
1:A:62:LEU:HD13	1:A:203:GLY:HA2	1.82	0.62
2:B:111:GLN:HB2	2:B:244:GLY:HA3	1.82	0.62
3:C:103:THR:HB	3:C:106:LYS:HB2	1.82	0.62
1:A:42:LEU:HD22	1:A:89:GLY:HA3	1.81	0.61
1:A:67:LEU:HD13	1:A:167:VAL:HG11	1.83	0.60
1:A:103:GLY:HA3	1:A:227:PHE:HA	1.84	0.60
2:B:30:ALA:HB3	2:B:177:PRO:HD2	1.83	0.60
2:B:65:TRP:HB3	2:B:76:LEU:HD11	1.84	0.59
3:C:269:SER:HB3	3:C:410:LEU:HD23	1.84	0.59
2:B:13:GLN:HG3	2:B:18:VAL:HG22	1.85	0.58
1:A:81:PRO:O	1:A:85:ILE:HG22	2.02	0.58
1:A:102:ARG:NH1	3:C:43:GLY:O	2.36	0.58
1:A:36:LEU:HB3	3:C:53:THR:HB	1.86	0.58
3:C:312:VAL:HG11	3:C:318:TRP:CH2	2.39	0.57
1:A:12:PRO:HG3	3:C:179:GLU:HB3	1.86	0.56
1:A:174:LEU:HD13	2:B:183:PRO:HG3	1.86	0.55
1:A:157:MET:HB3	1:A:161:ARG:HG2	1.88	0.55
1:A:177:MET:HB3	1:A:195:THR:HG22	1.88	0.55
2:B:132:TRP:HE1	3:C:136:GLY:HA2	1.72	0.55
1:A:45:GLU:HG2	1:A:46:GLY:N	2.19	0.55
2:B:77:VAL:HB	2:B:211:VAL:HG12	1.88	0.55
1:A:146:ARG:NH2	1:A:205:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASP:HB2	3:C:42:VAL:H	1.73	0.54
3:C:193:TRP:CD1	3:C:209:PRO:HD3	2.42	0.54
3:C:90:HIS:HB2	3:C:91:PRO:HD2	1.89	0.54
3:C:188:THR:HG22	3:C:190:THR:H	1.72	0.54
1:A:72:LEU:HD13	1:A:133:PRO:HD3	1.90	0.54
1:A:15:LEU:HD13	3:C:180:PHE:HD2	1.74	0.52
1:A:121:GLN:HG3	1:A:152:ALA:HB2	1.91	0.52
1:A:54:ARG:HH22	1:A:141:ALA:HA	1.74	0.52
3:C:320:VAL:HG11	3:C:324:THR:HB	1.92	0.51
1:A:181:SER:HA	2:B:145:PHE:HB3	1.92	0.51
2:B:171:GLU:OE1	2:B:171:GLU:N	2.44	0.51
1:A:11:GLN:NE2	3:C:181:VAL:HG11	2.26	0.51
1:A:11:GLN:HE21	3:C:181:VAL:HG11	1.74	0.50
1:A:7:PRO:HD2	1:A:10:MET:HG3	1.93	0.50
1:A:93:VAL:HG21	3:C:121:LEU:HD21	1.94	0.50
1:A:32:ASP:HB2	1:A:34:LYS:HE2	1.94	0.49
2:B:154:ALA:HA	3:C:64:LEU:HB3	1.95	0.49
3:C:142:ASN:HA	3:C:174:LEU:O	2.12	0.49
2:B:81:PHE:HB3	2:B:137:PHE:HE1	1.77	0.49
1:A:127:PRO:HA	1:A:192:LEU:O	2.12	0.49
3:C:107:LEU:HD11	3:C:260:VAL:HB	1.95	0.49
1:A:102:ARG:HD3	3:C:48:ILE:HD13	1.94	0.48
1:A:245:TYR:HA	3:C:263:PRO:HD2	1.95	0.48
1:A:16:LEU:HD13	3:C:183:THR:HB	1.95	0.48
3:C:223:MET:HG2	3:C:226:VAL:HB	1.95	0.48
3:C:124:TYR:HB2	3:C:245:ALA:HB3	1.96	0.48
1:A:64:GLN:O	1:A:66:PRO:HD3	2.13	0.48
3:C:130:LYS:HD3	3:C:239:GLY:HA2	1.95	0.48
3:C:285:PHE:CG	3:C:292:ILE:HD11	2.48	0.48
3:C:192:TRP:CE3	3:C:245:ALA:HB2	2.48	0.47
3:C:127:GLY:HA3	3:C:242:PHE:HA	1.95	0.47
3:C:289:THR:HG21	3:C:392:ARG:NH2	2.29	0.47
2:B:70:SER:HB3	2:B:217:PHE:H	1.79	0.47
1:A:120:VAL:HG12	1:A:202:ILE:HG13	1.96	0.47
1:A:122:HIS:NE2	1:A:124:PRO:HG3	2.29	0.47
1:A:40:TYR:CE1	3:C:21:ALA:HA	2.50	0.47
2:B:139:TYR:CE1	2:B:179:ARG:HB2	2.49	0.47
1:A:78:VAL:HG21	3:C:268:ILE:CA	2.43	0.47
2:B:152:ASN:HD21	3:C:99:ILE:HG21	1.80	0.47
2:B:76:LEU:HD12	2:B:76:LEU:HA	1.75	0.47
2:B:80:LYS:HD3	2:B:259:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:CD	3:C:48:ILE:HD13	2.45	0.46
3:C:267:ILE:CB	3:C:411:TRP:HB2	2.46	0.46
3:C:32:THR:HB	3:C:34:ARG:HG3	1.98	0.46
2:B:133:LEU:HB2	2:B:164:VAL:HB	1.98	0.46
1:A:99:ARG:HB2	1:A:233:CYS:SG	2.55	0.46
2:B:132:TRP:CD2	3:C:134:LEU:HD21	2.51	0.46
2:B:193:GLY:HA3	2:B:198:THR:O	2.15	0.46
3:C:55:ILE:O	3:C:59:ILE:HG12	2.14	0.46
2:B:23:ASN:ND2	2:B:169:ALA:O	2.48	0.46
3:C:270:PHE:HA	3:C:305:LEU:HD23	1.98	0.45
1:A:126:ARG:HD2	1:A:199:ASP:HB2	1.98	0.45
1:A:85:ILE:HG23	1:A:86:MET:HG2	1.98	0.45
2:B:54:THR:HG21	2:B:240:ALA:HB3	1.97	0.45
3:C:95:LYS:HE3	3:C:197:TYR:CE1	2.51	0.45
1:A:49:LEU:HD23	1:A:214:GLY:HA3	1.98	0.45
2:B:128:PHE:HD1	3:C:226:VAL:HG23	1.81	0.45
3:C:272:SER:HA	3:C:275:PHE:CE1	2.46	0.45
3:C:17:SER:HG	3:C:20:TRP:HE1	1.63	0.45
3:C:190:THR:OG1	3:C:191:MET:N	2.49	0.45
1:A:121:GLN:O	1:A:200:LEU:HD12	2.17	0.45
1:A:111:VAL:HG22	1:A:217:ILE:HG13	1.99	0.45
1:A:172:PRO:HG2	1:A:194:PHE:HE1	1.81	0.45
3:C:139:PRO:HB2	3:C:140:ARG:NH1	2.32	0.45
2:B:179:ARG:NH1	3:C:47:ASP:O	2.50	0.45
1:A:38:ARG:HG3	1:A:40:TYR:HB2	1.98	0.44
1:A:194:PHE:HB3	2:B:181:VAL:HG21	1.99	0.44
1:A:190:ASP:O	1:A:195:THR:HG23	2.17	0.44
3:C:196:LYS:HG3	3:C:206:PHE:O	2.18	0.44
3:C:65:LEU:HD22	3:C:93:VAL:HG11	2.00	0.44
2:B:132:TRP:NE1	3:C:136:GLY:HA2	2.33	0.44
2:B:59:PHE:HB2	2:B:234:PHE:CE2	2.53	0.44
2:B:85:TRP:HH2	2:B:203:PRO:HB2	1.82	0.44
3:C:149:TYR:CD1	3:C:184:VAL:HB	2.52	0.43
2:B:59:PHE:HZ	2:B:62:SER:HB3	1.83	0.43
2:B:185:MET:HE3	2:B:206:MET:HB2	2.00	0.43
2:B:65:TRP:CZ3	2:B:217:PHE:HB2	2.54	0.43
1:A:80:ASN:OD1	1:A:82:ILE:HG22	2.18	0.43
2:B:105:ILE:O	2:B:107:PHE:N	2.49	0.43
1:A:34:LYS:HE3	3:C:245:ALA:O	2.18	0.43
1:A:101:PHE:HA	1:A:228:SER:O	2.19	0.43
2:B:69:ASP:OD2	2:B:74:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:318:TRP:NE1	3:C:353:VAL:HG23	2.33	0.43
1:A:126:ARG:HH12	1:A:201:LEU:HD21	1.83	0.43
1:A:53:LEU:O	1:A:137:ARG:NE	2.51	0.43
1:A:245:TYR:CD2	3:C:263:PRO:HG3	2.53	0.43
1:A:235:PHE:HB2	2:B:158:GLN:OE1	2.18	0.43
3:C:222:ALA:HB1	3:C:226:VAL:HG12	2.01	0.42
2:B:132:TRP:CD1	2:B:215:ILE:HD12	2.54	0.42
1:A:226:ASP:CB	3:C:42:VAL:H	2.32	0.42
3:C:115:ILE:HD12	3:C:238:ALA:HB2	2.01	0.42
1:A:124:PRO:HB3	1:A:170:TYR:HB2	2.02	0.42
1:A:107:LEU:HD13	1:A:200:LEU:HD22	2.01	0.42
3:C:66:LYS:HA	3:C:67:PRO:HD3	1.89	0.42
3:C:63:GLY:HA3	3:C:113:PRO:HB3	2.02	0.42
3:C:193:TRP:NE1	3:C:209:PRO:HD3	2.35	0.41
1:A:151:ALA:HB1	3:C:33:LEU:HB3	2.02	0.41
1:A:85:ILE:HG13	1:A:244:THR:HG21	2.02	0.41
3:C:153:ILE:O	3:C:211:TYR:HB2	2.20	0.41
3:C:91:PRO:HB3	3:C:242:PHE:CZ	2.49	0.41
1:A:49:LEU:HG	3:C:273:GLY:HA3	2.01	0.41
3:C:193:TRP:HA	3:C:194:PRO:HD3	1.86	0.41
3:C:124:TYR:HB2	3:C:245:ALA:CB	2.50	0.41
3:C:312:VAL:HG11	3:C:318:TRP:HH2	1.83	0.41
2:B:82:PRO:HG3	2:B:117:PHE:CZ	2.55	0.41
3:C:254:LEU:HD23	3:C:254:LEU:HA	1.90	0.41
2:B:101:ILE:HD12	2:B:101:ILE:N	2.35	0.41
3:C:18:HIS:CD2	3:C:29:PRO:HD2	2.56	0.41
3:C:70:TRP:HB3	3:C:230:VAL:O	2.20	0.41
1:A:44:TRP:HB2	1:A:219:VAL:O	2.20	0.41
3:C:268:ILE:HD11	3:C:305:LEU:HB3	2.02	0.41
3:C:89:VAL:HG11	3:C:149:TYR:HE1	1.86	0.40
2:B:116:ASP:HB2	2:B:238:THR:OG1	2.21	0.40
2:B:176:ILE:HA	2:B:177:PRO:HD2	1.96	0.40
3:C:143:ALA:HB2	3:C:220:LEU:HA	2.03	0.40
3:C:198:GLY:HA2	3:C:251:ALA:HB2	2.03	0.40
3:C:276:PRO:HB3	3:C:405:SER:O	2.21	0.40
3:C:342:PRO:HG2	3:C:346:TYR:OH	2.21	0.40
3:C:400:VAL:HG22	3:C:401:ASP:H	1.86	0.40
3:C:246:VAL:HA	3:C:247:PRO:HD3	1.93	0.40
3:C:366:PRO:HB2	3:C:368:THR:HG22	2.04	0.40
1:A:125:ASP:OD1	1:A:150:TYR:OH	2.25	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	235/266 (88%)	225 (96%)	10 (4%)	0	100	100
2	B	248/261 (95%)	236 (95%)	12 (5%)	0	100	100
3	C	405/430 (94%)	378 (93%)	25 (6%)	2 (0%)	34	75
All	All	888/957 (93%)	839 (94%)	47 (5%)	2 (0%)	52	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	268	ILE
3	C	349	GLY

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	203/230 (88%)	199 (98%)	4 (2%)	63	87
2	B	208/234 (89%)	204 (98%)	4 (2%)	65	87
3	C	344/366 (94%)	341 (99%)	3 (1%)	84	94
All	All	755/830 (91%)	744 (98%)	11 (2%)	72	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN

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Mol	Chain	Res	Type
1	A	44	TRP
1	A	93	VAL
1	A	143	ASP
2	B	60	TRP
2	B	65	TRP
2	B	105	ILE
2	B	198	THR
3	C	70	TRP
3	C	268	ILE
3	C	340	PHE

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	11	GLN
2	B	152	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	239/266 (89%)	0.38	7 (2%) 55 49	45, 68, 91, 112	0
2	B	252/261 (96%)	0.38	8 (3%) 51 46	44, 63, 100, 109	0
3	C	411/430 (95%)	0.77	64 (15%) 3 3	38, 65, 119, 133	0
All	All	902/957 (94%)	0.56	79 (8%) 12 13	38, 65, 114, 133	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	291	ALA	6.1
3	C	340	PHE	5.5
3	C	335	ASN	4.9
3	C	279	VAL	4.7
2	B	103	ASN	4.6
3	C	400	VAL	4.4
3	C	401	ASP	4.1
3	C	336	GLY	4.1
3	C	313	ASN	3.9
2	B	191	LEU	3.8
3	C	411	TRP	3.7
3	C	346	TYR	3.7
3	C	366	PRO	3.6
3	C	339	TRP	3.6
3	C	402	SER	3.6
3	C	369	PRO	3.6
3	C	337	THR	3.6
3	C	367	LEU	3.6
3	C	349	GLY	3.5
3	C	327	PHE	3.5
3	C	354	TRP	3.5
3	C	326	LYS	3.4
2	B	85	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	292	ILE	3.4
3	C	203	ALA	3.3
3	C	391	ILE	3.2
3	C	362	MET	3.1
3	C	345	GLU	3.0
2	B	192	ARG	3.0
3	C	381	LEU	3.0
3	C	312	VAL	2.9
3	C	341	ILE	2.9
3	C	395	ILE	2.9
3	C	364	PRO	2.8
3	C	390	GLN	2.8
3	C	388	ILE	2.8
3	C	328	LYS	2.7
3	C	409	ILE	2.7
3	C	389	SER	2.7
3	C	397	ASP	2.7
2	B	196	LEU	2.7
3	C	384	SER	2.6
2	B	19	LEU	2.5
3	C	325	ILE	2.5
3	C	347	THR	2.5
3	C	386	THR	2.5
3	C	332	ASP	2.5
1	A	41	GLN	2.5
3	C	1	ASP	2.5
3	C	315	LYS	2.4
3	C	410	LEU	2.4
3	C	350	TYR	2.4
3	C	314	ARG	2.4
3	C	368	THR	2.4
3	C	363	VAL	2.4
3	C	365	TYR	2.3
3	C	348	LEU	2.3
3	C	342	PRO	2.3
1	A	31	ASN	2.3
2	B	260	PRO	2.3
3	C	204	GLY	2.2
3	C	263	PRO	2.2
3	C	109	GLN	2.2
1	A	183	ASN	2.2
3	C	321	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	6	THR	2.2
3	C	283	HIS	2.2
1	A	11	GLN	2.2
3	C	338	GLU	2.2
1	A	230	ASN	2.2
3	C	392	ARG	2.2
2	B	20	GLY	2.1
1	A	33	LEU	2.1
3	C	329	THR	2.1
3	C	343	GLU	2.1
3	C	280	GLY	2.1
3	C	382	LEU	2.0
3	C	286	PHE	2.0
3	C	334	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.