



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 5J96 / pdb_00005j96
Title : Crystal structure of Slow Bee Paralysis Virus at 3.4Å 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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

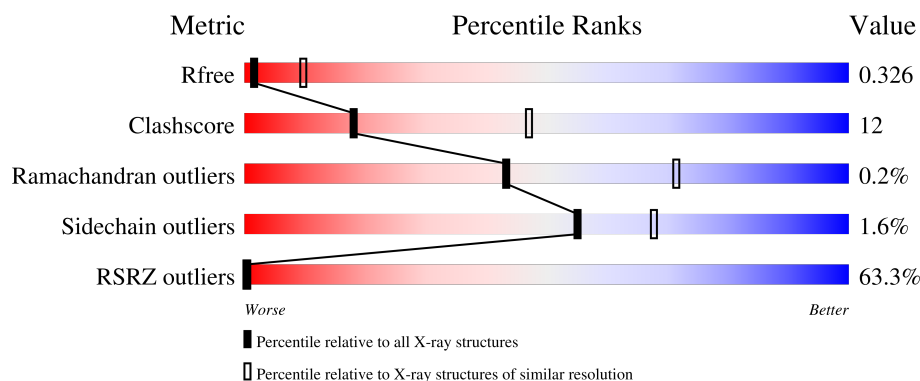
1 Overall quality at a glance

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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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 $\leq 5\%$. 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	60% 54% 34% 10%
2	B	261	61% 72% 24%
3	C	430	59% 68% 27%

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			

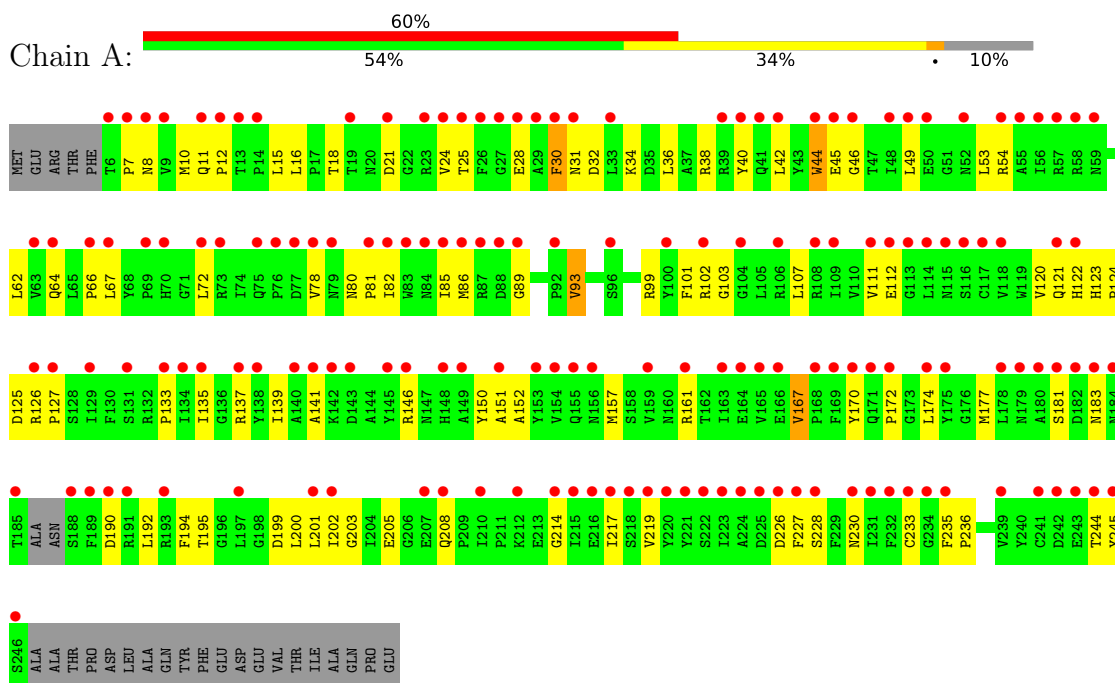
- Molecule 3 is a protein called Genome polyprotein.

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

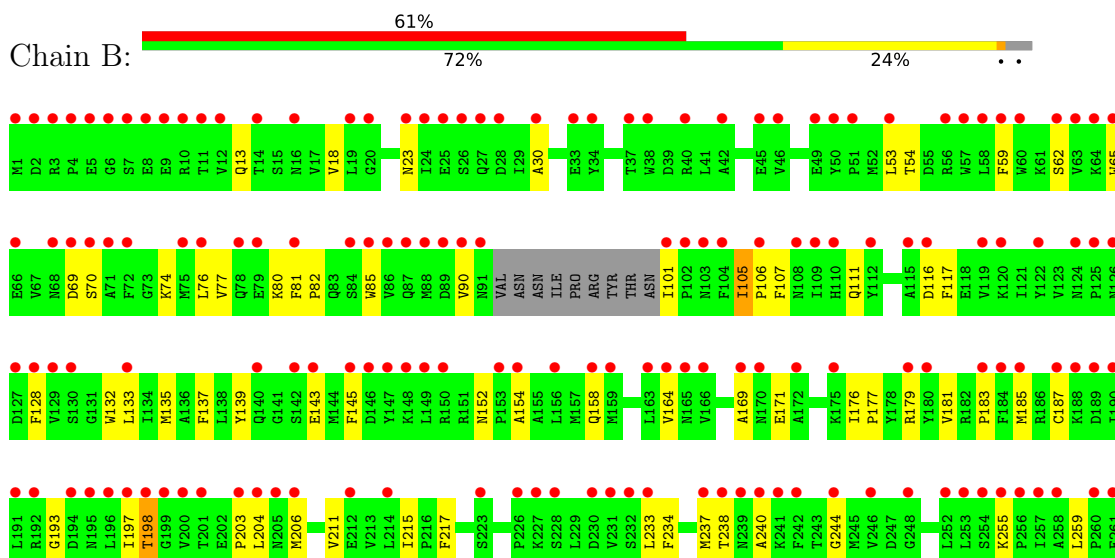
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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 70.70 – 3.41	Depositor EDS
% Data completeness (in resolution range)	87.4 (70.70-3.41) 87.2 (70.70-3.41)	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, CNS 1.3	Depositor
R, R_{free}	0.339 , 0.339 0.322 , 0.326	Depositor DCC
R_{free} test set	4570 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 0.0	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	0.32	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	0.36	0/1948	0.98	13/2655 (0.5%)
2	B	0.31	0/2004	0.80	0/2733
3	C	0.32	0/3274	0.81	5/4483 (0.1%)
All	All	0.33	0/7226	0.86	18/9871 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	PHE	N-CA-C	-7.74	97.29	108.60
1	A	25	THR	N-CA-C	-7.20	99.26	110.42
3	C	264	LYS	N-CA-C	-7.12	96.57	108.75
1	A	167	VAL	CA-C-N	6.42	126.38	120.21
1	A	167	VAL	C-N-CA	6.42	126.38	120.21
1	A	24	VAL	N-CA-C	-6.22	100.45	109.29
3	C	270	PHE	CB-CA-C	-6.18	109.46	116.63
1	A	112	GLU	N-CA-C	5.88	120.73	113.50
3	C	268	ILE	N-CA-C	5.41	120.59	109.34
1	A	183	ASN	N-CA-C	5.40	119.87	113.12
1	A	208	GLN	CA-C-N	5.38	125.38	119.89
1	A	208	GLN	C-N-CA	5.38	125.38	119.89
1	A	123	HIS	CA-C-N	5.23	124.41	118.97
1	A	123	HIS	C-N-CA	5.23	124.41	118.97
1	A	230	ASN	N-CA-C	5.17	117.70	111.40
1	A	236	PRO	O-C-N	5.03	123.51	121.15
3	C	7	THR	CA-C-N	5.02	126.11	119.84
3	C	7	THR	C-N-CA	5.02	126.11	119.84

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	1896	0	1832	70	0
2	B	1954	0	1865	46	0
3	C	3179	0	3107	90	0
All	All	7029	0	6804	169	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 (169) 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
2:B:185:MET:HE1	2:B:206:MET:HB2	1.71	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:LEU:HB3	3:C:53:THR:HB	1.86	0.58
1:A:102:ARG:NH1	3:C:43:GLY:O	2.36	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
1:A:226:ASP:HB2	3:C:42:VAL:H	1.73	0.54
3:C:90:HIS:HB2	3:C:91:PRO:HD2	1.89	0.54
3:C:193:TRP:CD1	3:C:209:PRO:HD3	2.42	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
3:C:87:MET:HE1	3:C:93:VAL:HG13	1.92	0.51
1:A:181:SER:HA	2:B:145:PHE:HB3	1.92	0.51
2:B:171:GLU:N	2:B:171:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:127:GLY:HA3	3:C:242:PHE:HA	1.95	0.47
3:C:192:TRP:CE3	3:C:245:ALA:HB2	2.48	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:40:TYR:CE1	3:C:21:ALA:HA	2.50	0.47
1:A:122:HIS:NE2	1:A:124:PRO:HG3	2.29	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
1:A:102:ARG:CD	3:C:48:ILE:HD13	2.45	0.46
1:A:86:MET:HE2	3:C:200:PRO:HD2	1.97	0.46
3:C:32:THR:HB	3:C:34:ARG:HG3	1.98	0.46
3:C:267:ILE:CB	3:C:411:TRP:HB2	2.46	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:85:ILE:HG23	1:A:86:MET:HG2	1.98	0.45
1:A:126:ARG:HD2	1:A:199:ASP:HB2	1.98	0.45
2:B:54:THR:HG21	2:B:240:ALA:HB3	1.97	0.45
2:B:135:MET:HE1	2:B:233:LEU:HD22	1.98	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:190:THR:OG1	3:C:191:MET:N	2.49	0.45
1:A:111:VAL:HG22	1:A:217:ILE:HG13	1.99	0.45
1:A:121:GLN:O	1:A:200:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG2	1:A:194:PHE:HE1	1.81	0.45
2:B:179:ARG:NH1	3:C:47:ASP:O	2.50	0.45
3:C:139:PRO:HB2	3:C:140:ARG:NH1	2.32	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
2:B:237:MET:HE2	2:B:240:ALA:HB2	1.99	0.44
3:C:65:LEU:HD22	3:C:93:VAL:HG11	2.00	0.44
3:C:196:LYS:HG3	3:C:206:PHE:O	2.18	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: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
3:C:318:TRP:NE1	3:C:353:VAL:HG23	2.33	0.43
1:A:53:LEU:O	1:A:137:ARG:NE	2.51	0.43
1:A:126:ARG:HH12	1:A:201:LEU:HD21	1.83	0.43
1:A:135:ILE:C	1:A:139:ILE:HG13	2.43	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
1:A:226:ASP:CB	3:C:42:VAL:H	2.32	0.42
2:B:132:TRP:CD1	2:B:215:ILE:HD12	2.54	0.42
1:A:28:GLU:C	1:A:30:PHE:H	2.26	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:91:PRO:HB3	3:C:242:PHE:CZ	2.49	0.41
3:C:153:ILE:O	3:C:211:TYR:HB2	2.20	0.41
1:A:49:LEU:HG	3:C:273:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:TYR:HB2	3:C:245:ALA:CB	2.50	0.41
3:C:193:TRP:HA	3:C:194:PRO:HD3	1.86	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
1:A:44:TRP:HB2	1:A:219:VAL:O	2.20	0.41
3:C:70:TRP:HB3	3:C:230:VAL:O	2.20	0.41
3:C:268:ILE:HD11	3:C:305:LEU:HB3	2.02	0.41
2:B:185:MET:HE2	2:B:185:MET:HB3	1.86	0.40
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 [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	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%)	24	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	888/957 (93%)	839 (94%)	47 (5%)	2 (0%)	43 71

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%)	200 (98%)	3 (2%)	57 69
2	B	208/234 (89%)	204 (98%)	4 (2%)	50 66
3	C	344/366 (94%)	339 (98%)	5 (2%)	57 69
All	All	755/830 (91%)	743 (98%)	12 (2%)	55 68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	44	TRP
1	A	93	VAL
2	B	105	ILE
2	B	143	GLU
2	B	197	ILE
2	B	198	THR
3	C	70	TRP
3	C	226	VAL
3	C	268	ILE
3	C	321	VAL
3	C	340	PHE

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

Mol	Chain	Res	Type
1	A	11	GLN
1	A	230	ASN
2	B	152	ASN
3	C	100	GLN
3	C	175	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 oligosaccharides 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 [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	239/266 (89%)	2.77	160 (66%) 0 0	45, 68, 91, 112	0
2	B	252/261 (96%)	2.57	158 (62%) 0 0	44, 63, 100, 109	0
3	C	411/430 (95%)	2.76	253 (61%) 0 0	38, 65, 119, 133	0
All	All	902/957 (94%)	2.71	571 (63%) 0 0	38, 65, 114, 133	0

All (571) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	336	GLY	11.6
3	C	259	ASP	10.1
3	C	204	GLY	8.8
3	C	262	TYR	8.6
3	C	402	SER	8.4
2	B	261	GLU	8.1
3	C	291	ALA	7.9
3	C	401	ASP	7.8
1	A	41	GLN	7.7
3	C	321	VAL	7.6
3	C	388	ILE	7.5
2	B	28	ASP	7.5
2	B	191	LEU	7.4
3	C	100	GLN	7.4
3	C	329	THR	7.3
1	A	185	THR	7.3
3	C	406	LYS	7.3
3	C	98	VAL	6.8
3	C	335	ASN	6.8
3	C	1	ASP	6.8
3	C	343	GLU	6.6
3	C	334	ILE	6.6
1	A	8	ASN	6.5

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Mol	Chain	Res	Type	RSRZ
3	C	384	SER	6.5
1	A	55	ALA	6.3
1	A	87	ARG	6.2
3	C	403	ALA	6.1
1	A	40	TYR	6.0
3	C	199	GLY	6.0
2	B	148	LYS	5.9
2	B	190	ILE	5.9
1	A	149	ALA	5.9
3	C	379	ALA	5.9
3	C	205	GLU	5.9
3	C	320	VAL	5.8
3	C	328	LYS	5.8
3	C	25	ASN	5.8
2	B	188	LYS	5.7
2	B	20	GLY	5.6
1	A	7	PRO	5.6
3	C	56	SER	5.6
1	A	189	PHE	5.5
1	A	230	ASN	5.5
3	C	337	THR	5.5
1	A	178	LEU	5.5
3	C	95	LYS	5.4
3	C	317	PHE	5.4
1	A	133	PRO	5.4
1	A	57	ARG	5.4
3	C	263	PRO	5.4
1	A	113	GLY	5.3
3	C	203	ALA	5.3
3	C	198	GLY	5.3
3	C	393	PRO	5.3
1	A	188	SER	5.2
3	C	345	GLU	5.2
3	C	293	LEU	5.2
1	A	73	ARG	5.2
2	B	63	VAL	5.2
3	C	395	ILE	5.2
3	C	347	THR	5.2
3	C	109	GLN	5.2
2	B	260	PRO	5.1
1	A	142	LYS	5.1
3	C	272	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	TYR	5.1
3	C	314	ARG	5.1
2	B	90	VAL	5.1
3	C	400	VAL	5.0
2	B	255	LYS	5.0
3	C	258	ILE	5.0
2	B	62	SER	5.0
1	A	49	LEU	4.9
3	C	327	PHE	4.9
2	B	75	MET	4.9
3	C	324	THR	4.9
1	A	11	GLN	4.8
1	A	72	LEU	4.8
3	C	350	TYR	4.7
1	A	70	HIS	4.7
3	C	73	ASN	4.7
2	B	146	ASP	4.7
2	B	88	MET	4.7
1	A	242	ASP	4.6
3	C	201	GLN	4.6
2	B	196	LEU	4.6
3	C	344	GLY	4.6
2	B	72	PHE	4.6
3	C	326	LYS	4.6
3	C	389	SER	4.6
2	B	103	ASN	4.6
1	A	86	MET	4.6
1	A	181	SER	4.5
1	A	111	VAL	4.5
3	C	42	VAL	4.5
3	C	30	THR	4.5
3	C	290	LYS	4.5
3	C	297	ALA	4.5
3	C	197	TYR	4.5
2	B	9	GLU	4.5
2	B	204	LEU	4.4
3	C	208	ALA	4.4
1	A	223	ILE	4.4
1	A	88	ASP	4.4
3	C	157	ASN	4.4
1	A	42	LEU	4.4
2	B	142	SER	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	380	SER	4.4
2	B	25	GLU	4.4
3	C	338	GLU	4.4
3	C	99	ILE	4.3
3	C	413	PRO	4.3
3	C	206	PHE	4.3
2	B	26	SER	4.3
2	B	203	PRO	4.3
3	C	281	SER	4.3
2	B	30	ALA	4.2
1	A	143	ASP	4.2
3	C	106	LYS	4.2
2	B	192	ARG	4.2
1	A	159	VAL	4.2
2	B	214	LEU	4.2
3	C	391	ILE	4.2
1	A	19	THR	4.2
1	A	190	ASP	4.2
2	B	129	VAL	4.2
2	B	253	LEU	4.2
3	C	411	TRP	4.2
1	A	66	PRO	4.2
3	C	287	ASP	4.2
3	C	315	LYS	4.2
2	B	91	ASN	4.1
2	B	189	ASP	4.1
3	C	408	ASN	4.1
3	C	101	VAL	4.1
3	C	285	PHE	4.1
1	A	79	ASN	4.1
1	A	25	THR	4.1
1	A	141	ALA	4.1
2	B	143	GLU	4.0
3	C	4	PRO	4.0
2	B	205	ASN	4.0
1	A	26	PHE	4.0
1	A	218	SER	4.0
3	C	255	SER	4.0
3	C	340	PHE	4.0
3	C	392	ARG	4.0
1	A	116	SER	4.0
3	C	94	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	342	PRO	4.0
2	B	170	ASN	4.0
3	C	12	PHE	3.9
1	A	82	ILE	3.9
2	B	104	PHE	3.9
2	B	85	TRP	3.9
1	A	23	ARG	3.9
1	A	54	ARG	3.9
2	B	3	ARG	3.9
3	C	40	VAL	3.9
1	A	182	ASP	3.9
1	A	29	ALA	3.9
3	C	339	TRP	3.9
2	B	10	ARG	3.8
1	A	166	GLU	3.8
3	C	154	SER	3.8
1	A	45	GLU	3.8
2	B	239	ASN	3.8
3	C	387	ALA	3.8
2	B	89	ASP	3.8
2	B	116	ASP	3.8
1	A	129	ILE	3.8
3	C	280	GLY	3.8
3	C	370	LEU	3.8
2	B	232	SER	3.8
3	C	102	MET	3.8
3	C	200	PRO	3.7
1	A	148	HIS	3.7
3	C	128	SER	3.7
2	B	184	PHE	3.7
3	C	292	ILE	3.7
2	B	68	ASN	3.7
3	C	16	PRO	3.7
1	A	175	TYR	3.7
1	A	134	ILE	3.7
1	A	217	ILE	3.7
1	A	220	TYR	3.6
2	B	79	GLU	3.6
3	C	355	ARG	3.6
2	B	198	THR	3.6
1	A	127	PRO	3.6
2	B	183	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	58	ARG	3.6
2	B	8	GLU	3.6
2	B	195	ASN	3.6
2	B	169	ALA	3.6
3	C	278	TYR	3.6
2	B	70	SER	3.6
3	C	96	ASP	3.6
1	A	64	GLN	3.6
2	B	6	GLY	3.6
2	B	115	ALA	3.6
3	C	358	ALA	3.6
3	C	196	LYS	3.6
3	C	385	ASN	3.6
3	C	110	TYR	3.6
3	C	398	TYR	3.6
1	A	222	SER	3.5
3	C	27	SER	3.5
2	B	24	ILE	3.5
2	B	122	TYR	3.5
3	C	71	ASN	3.5
2	B	242	PHE	3.5
2	B	7	SER	3.5
3	C	19	SER	3.5
3	C	390	GLN	3.5
3	C	176	GLU	3.5
3	C	386	THR	3.5
3	C	298	VAL	3.5
1	A	44	TRP	3.5
3	C	75	THR	3.5
3	C	35	LEU	3.5
1	A	39	ARG	3.5
3	C	333	LYS	3.4
1	A	235	PHE	3.4
2	B	86	VAL	3.4
3	C	279	VAL	3.4
1	A	33	LEU	3.4
2	B	87	GLN	3.4
3	C	120	SER	3.4
3	C	194	PRO	3.4
1	A	30	PHE	3.4
2	B	59	PHE	3.4
3	C	289	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	33	GLU	3.4
1	A	210	ILE	3.4
1	A	76	PRO	3.4
2	B	223	SER	3.4
1	A	225	ASP	3.4
2	B	147	TYR	3.4
3	C	111	TYR	3.4
3	C	346	TYR	3.4
3	C	164	ALA	3.4
3	C	397	ASP	3.4
1	A	48	ILE	3.4
3	C	142	ASN	3.3
1	A	246	SER	3.3
3	C	381	LEU	3.3
3	C	63	GLY	3.3
3	C	72	ALA	3.3
3	C	295	TYR	3.3
1	A	69	PRO	3.3
1	A	191	ARG	3.3
3	C	270	PHE	3.3
3	C	260	VAL	3.3
1	A	245	TYR	3.3
2	B	71	ALA	3.3
3	C	359	TYR	3.3
1	A	92	PRO	3.3
2	B	194	ASP	3.3
1	A	146	ARG	3.3
2	B	206	MET	3.3
1	A	233	CYS	3.3
2	B	69	ASP	3.3
1	A	13	THR	3.3
1	A	244	THR	3.3
2	B	58	LEU	3.3
2	B	163	LEU	3.3
3	C	405	SER	3.2
3	C	407	ASP	3.2
3	C	13	VAL	3.2
1	A	183	ASN	3.2
3	C	268	ILE	3.2
1	A	114	LEU	3.2
2	B	153	PRO	3.2
2	B	175	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	288	SER	3.2
3	C	22	HIS	3.2
3	C	368	THR	3.2
2	B	57	TRP	3.2
1	A	184	ASN	3.2
3	C	296	GLY	3.2
2	B	200	VAL	3.2
3	C	138	ASN	3.2
1	A	201	LEU	3.2
2	B	133	LEU	3.2
2	B	110	HIS	3.2
3	C	283	HIS	3.2
1	A	67	LEU	3.2
1	A	138	TYR	3.2
3	C	29	PRO	3.2
3	C	266	SER	3.2
1	A	6	THR	3.2
3	C	37	GLY	3.1
3	C	276	PRO	3.1
3	C	369	PRO	3.1
3	C	341	ILE	3.1
3	C	305	LEU	3.1
2	B	49	GLU	3.1
3	C	68	PHE	3.1
3	C	264	LYS	3.1
3	C	356	ASP	3.1
1	A	102	ARG	3.1
3	C	239	GLY	3.1
3	C	11	PHE	3.1
1	A	109	ILE	3.1
1	A	163	ILE	3.1
1	A	115	ASN	3.1
2	B	126	ASN	3.1
3	C	383	ALA	3.1
2	B	252	LEU	3.1
2	B	201	THR	3.1
3	C	372	GLU	3.1
1	A	12	PRO	3.1
1	A	75	GLN	3.0
3	C	256	ARG	3.0
2	B	84	SER	3.0
2	B	212	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	55	ILE	3.0
3	C	313	ASN	3.0
2	B	1	MET	3.0
1	A	104	GLY	3.0
2	B	101	ILE	3.0
1	A	151	ALA	3.0
3	C	44	ARG	3.0
1	A	27	GLY	3.0
1	A	117	CYS	3.0
1	A	171	GLN	3.0
1	A	169	PHE	3.0
2	B	150	ARG	2.9
3	C	354	TRP	2.9
3	C	303	ALA	2.9
1	A	96	SER	2.9
2	B	119	VAL	2.9
2	B	166	VAL	2.9
3	C	226	VAL	2.9
2	B	109	ILE	2.9
1	A	179	ASN	2.9
1	A	126	ARG	2.9
2	B	51	PRO	2.9
3	C	404	ALA	2.9
1	A	241	CYS	2.9
3	C	271	LYS	2.9
2	B	228	SER	2.9
3	C	104	GLN	2.9
1	A	59	ASN	2.9
2	B	14	THR	2.9
2	B	23	ASN	2.9
2	B	256	PRO	2.9
1	A	232	PHE	2.9
2	B	78	GLN	2.9
2	B	34	TYR	2.9
2	B	145	PHE	2.9
2	B	120	LYS	2.9
3	C	18	HIS	2.8
1	A	168	PRO	2.8
1	A	112	GLU	2.8
2	B	240	ALA	2.8
3	C	238	ALA	2.8
2	B	60	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	49	GLY	2.8
3	C	129	ILE	2.8
3	C	174	LEU	2.8
1	A	118	VAL	2.8
3	C	177	VAL	2.8
3	C	5	ASP	2.8
1	A	31	ASN	2.8
2	B	128	PHE	2.8
3	C	218	ASN	2.8
3	C	294	ARG	2.8
1	A	14	PRO	2.8
1	A	216	GLU	2.8
3	C	331	LEU	2.8
1	A	121	GLN	2.8
3	C	97	GLN	2.8
3	C	28	GLU	2.8
3	C	108	THR	2.8
3	C	160	THR	2.8
3	C	382	LEU	2.7
1	A	243	GLU	2.7
2	B	45	GLU	2.7
3	C	325	ILE	2.7
1	A	226	ASP	2.7
2	B	2	ASP	2.7
2	B	124	ASN	2.7
1	A	122	HIS	2.7
1	A	56	ILE	2.7
3	C	399	ILE	2.7
3	C	178	SER	2.7
2	B	241	LYS	2.7
1	A	21	ASP	2.7
2	B	165	ASN	2.7
3	C	43	GLY	2.7
3	C	274	TYR	2.7
3	C	323	ASP	2.7
3	C	360	ALA	2.7
3	C	375	ALA	2.7
1	A	239	VAL	2.7
2	B	159	MET	2.7
2	B	56	ARG	2.7
2	B	254	SER	2.7
3	C	202	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	311	ASN	2.7
1	A	85	ILE	2.6
1	A	137	ARG	2.6
2	B	64	LYS	2.6
1	A	234	GLY	2.6
3	C	322	GLY	2.6
2	B	11	THR	2.6
1	A	207	GLU	2.6
3	C	192	TRP	2.6
1	A	219	VAL	2.6
1	A	228	SER	2.6
2	B	227	LYS	2.6
3	C	261	ILE	2.6
3	C	180	PHE	2.6
1	A	108	ARG	2.6
3	C	105	SER	2.6
1	A	89	GLY	2.6
1	A	50	GLU	2.6
1	A	164	GLU	2.6
2	B	42	ALA	2.6
3	C	361	TYR	2.6
3	C	227	PRO	2.6
3	C	284	SER	2.6
1	A	155	GLN	2.6
2	B	27	GLN	2.6
1	A	77	ASP	2.6
2	B	230	ASP	2.6
3	C	240	ASP	2.6
2	B	106	PRO	2.5
3	C	357	GLY	2.5
3	C	137	ASN	2.5
3	C	156	ASP	2.5
3	C	282	TRP	2.5
3	C	125	THR	2.5
2	B	50	TYR	2.5
3	C	377	TYR	2.5
1	A	24	VAL	2.5
3	C	207	VAL	2.5
3	C	409	ILE	2.5
1	A	197	LEU	2.5
2	B	149	LEU	2.5
2	B	130	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	9	ALA	2.5
1	A	215	ILE	2.5
2	B	16	ASN	2.5
3	C	265	ASP	2.5
3	C	307	ASN	2.5
2	B	156	LEU	2.5
3	C	65	LEU	2.5
3	C	376	GLN	2.5
2	B	37	THR	2.4
1	A	153	TYR	2.4
2	B	112	TYR	2.4
2	B	248	GLY	2.4
2	B	185	MET	2.4
1	A	212	LYS	2.4
1	A	83	TRP	2.4
3	C	69	ASP	2.4
2	B	12	VAL	2.4
3	C	286	PHE	2.4
1	A	131	SER	2.4
2	B	233	LEU	2.4
1	A	81	PRO	2.4
2	B	102	PRO	2.4
3	C	312	VAL	2.4
1	A	46	GLY	2.4
1	A	135	ILE	2.4
1	A	174	LEU	2.4
2	B	231	VAL	2.4
3	C	366	PRO	2.4
3	C	237	ALA	2.4
2	B	237	MET	2.4
3	C	412	SER	2.4
2	B	4	PRO	2.4
2	B	38	TRP	2.4
3	C	20	TRP	2.4
3	C	139	PRO	2.4
1	A	221	TYR	2.3
2	B	197	ILE	2.3
2	B	158	GLN	2.3
3	C	107	LEU	2.3
3	C	23	GLY	2.3
3	C	34	ARG	2.3
1	A	100	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	127	ASP	2.3
3	C	85	TRP	2.3
3	C	24	THR	2.3
3	C	269	SER	2.3
1	A	170	TYR	2.3
2	B	180	TYR	2.3
3	C	124	TYR	2.3
3	C	83	LEU	2.3
1	A	9	VAL	2.3
2	B	40	ARG	2.3
3	C	219	PRO	2.3
3	C	234	PRO	2.3
3	C	70	TRP	2.3
3	C	222	ALA	2.3
3	C	62	TYR	2.3
3	C	319	ILE	2.3
1	A	224	ALA	2.3
3	C	191	MET	2.3
3	C	299	SER	2.3
2	B	108	ASN	2.3
2	B	179	ARG	2.3
2	B	257	ILE	2.2
3	C	245	ALA	2.2
1	A	180	ALA	2.2
2	B	164	VAL	2.2
1	A	140	ALA	2.2
1	A	172	PRO	2.2
2	B	19	LEU	2.2
2	B	244	GLY	2.2
3	C	33	LEU	2.2
3	C	332	ASP	2.2
2	B	154	ALA	2.2
3	C	10	LYS	2.2
1	A	227	PHE	2.2
3	C	90	HIS	2.2
1	A	165	VAL	2.2
1	A	84	ASN	2.2
2	B	5	GLU	2.2
3	C	84	LEU	2.2
1	A	214	GLY	2.2
2	B	125	PRO	2.2
1	A	161	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	77	ARG	2.2
1	A	63	VAL	2.2
3	C	14	PRO	2.2
2	B	187	CYS	2.2
2	B	66	GLU	2.1
2	B	172	ALA	2.1
3	C	310	ALA	2.1
2	B	199	GLY	2.1
2	B	246	VAL	2.1
2	B	238	THR	2.1
3	C	190	THR	2.1
2	B	53	LEU	2.1
1	A	28	GLU	2.1
2	B	46	VAL	2.1
3	C	15	ILE	2.1
2	B	226	PRO	2.1
1	A	156	ASN	2.1
3	C	78	ASN	2.1
1	A	78	VAL	2.1
1	A	154	VAL	2.1
2	B	76	LEU	2.1
3	C	187	ILE	2.1
1	A	193	ARG	2.1
3	C	81	GLY	2.1
2	B	81	PHE	2.1
3	C	215	PHE	2.1
3	C	396	PRO	2.1
1	A	106	ARG	2.0
2	B	258	ALA	2.0
2	B	140	GLN	2.0
3	C	112	LEU	2.0
3	C	348	LEU	2.0
3	C	155	SER	2.0
1	A	52	ASN	2.0
2	B	65	TRP	2.0
3	C	74	ASP	2.0
3	C	135	PHE	2.0
3	C	275	PHE	2.0
1	A	208	GLN	2.0
3	C	3	PRO	2.0
3	C	161	LEU	2.0
1	A	202	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	2.0
3	C	308	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.