



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:49 am BST

PDB ID : 1PAF  
Title : THE 2.5 ANGSTROMS STRUCTURE OF POKEWEED ANTIVIRAL PROTEIN  
Authors : Monzingo, A.F.; Collins, E.J.; Ernst, S.R.; Irvin, J.D.; Robertus, J.D.  
Deposited on : 1992-10-19  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

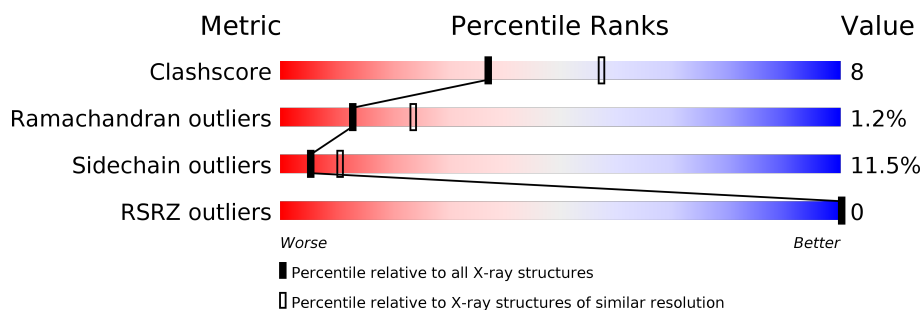
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	262	 63% 27% 8% •
1	B	262	 65% 27% 6% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4207 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 POKEWEEED ANTIVIRAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	262	Total 2060	C 1300	N 355	O 396	S 9	0	0	0
1	B	262	Total 2060	C 1300	N 355	O 396	S 9	0	0	0

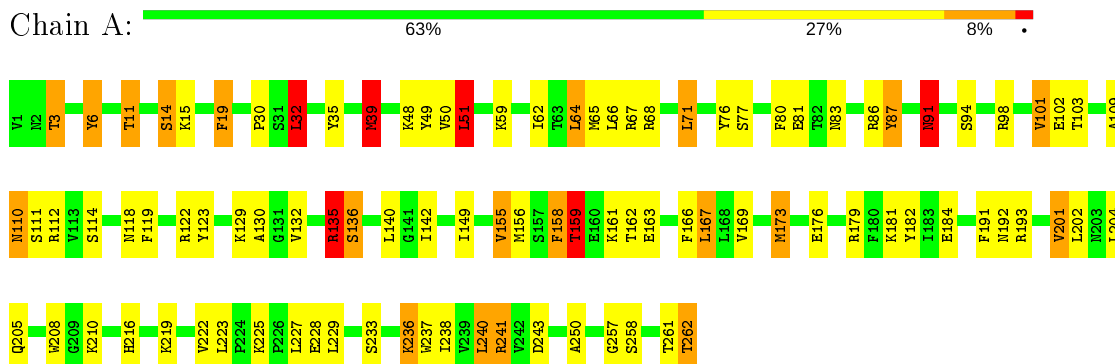
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total 42	O 42	0	0
2	B	45	Total 45	O 45	0	0

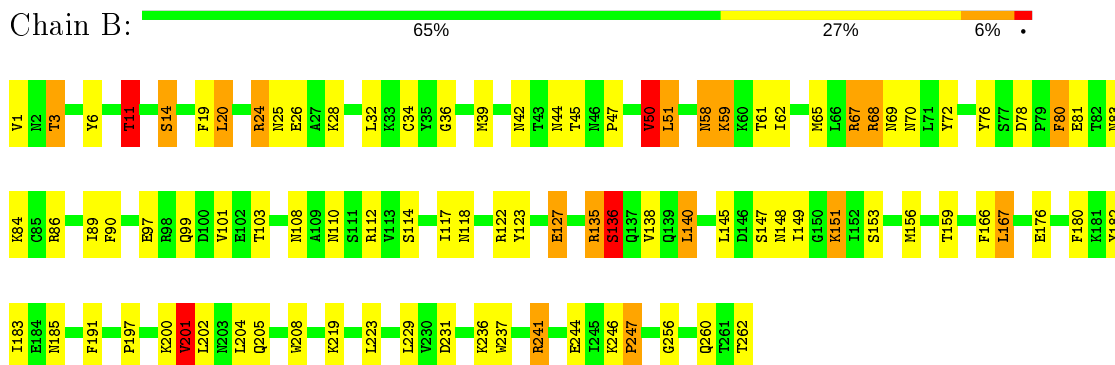
### 3 Residue-property plots [i](#)

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



- Molecule 1: POKEWEED ANTIVIRAL PROTEIN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.40Å 50.10Å 65.20Å 80.00° 113.20° 116.50°	Depositor
Resolution (Å)	(Not available) – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 99.5 (19.98-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.50Å)	Xtrriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.170 , (Not available) 0.166 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtrriage
Anisotropy	0.308	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,h+1	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	1.45	5/2096 (0.2%)	1.99	54/2840 (1.9%)
1	B	1.49	11/2096 (0.5%)	1.93	58/2840 (2.0%)
All	All	1.47	16/4192 (0.4%)	1.96	112/5680 (2.0%)

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	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	SER	CA-CB	-8.54	1.40	1.52
1	A	208	TRP	CG-CD2	-7.16	1.31	1.43
1	B	244	GLU	CD-OE1	-6.59	1.18	1.25
1	A	123	TYR	CE2-CZ	5.87	1.46	1.38
1	A	163	GLU	CD-OE1	-5.82	1.19	1.25
1	B	237	TRP	CD1-NE1	-5.54	1.28	1.38
1	B	24	ARG	CA-CB	5.53	1.66	1.53
1	B	208	TRP	CD1-NE1	-5.41	1.28	1.38
1	B	208	TRP	CG-CD2	-5.39	1.34	1.43
1	A	208	TRP	CD2-CE2	-5.38	1.34	1.41
1	B	59	LYS	CA-CB	5.26	1.65	1.53
1	B	244	GLU	CA-CB	-5.26	1.42	1.53
1	B	201	VAL	CA-CB	5.18	1.65	1.54
1	B	114	SER	CB-OG	-5.15	1.35	1.42
1	A	241	ARG	CZ-NH1	5.11	1.39	1.33
1	B	14	SER	CA-CB	-5.04	1.45	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	A	208	TRP	CD1-CG-CD2	12.45	116.26	106.30
1	A	112	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	67	ARG	NE-CZ-NH1	11.57	126.08	120.30
1	A	135	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	136	SER	N-CA-CB	11.28	127.42	110.50
1	A	237	TRP	CD1-CG-CD2	11.09	115.17	106.30
1	A	67	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	B	156	MET	CA-CB-CG	9.86	130.06	113.30
1	B	112	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	6	TYR	CB-CG-CD2	-9.36	115.39	121.00
1	A	156	MET	CA-CB-CG	9.35	129.19	113.30
1	A	237	TRP	CE2-CD2-CG	-9.31	99.86	107.30
1	A	112	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	B	122	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	B	156	MET	CG-SD-CE	8.94	114.50	100.20
1	A	237	TRP	CB-CG-CD1	-8.93	115.40	127.00
1	A	35	TYR	CB-CG-CD1	-8.28	116.03	121.00
1	B	127	GLU	CA-CB-CG	8.15	131.33	113.40
1	B	68	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	208	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	237	TRP	CG-CD1-NE1	-7.97	102.13	110.10
1	A	193	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	122	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	237	TRP	CG-CD2-CE3	7.75	140.88	133.90
1	A	208	TRP	CG-CD1-NE1	-7.74	102.36	110.10
1	A	208	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	A	49	TYR	CB-CG-CD2	7.46	125.48	121.00
1	B	24	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	81	GLU	CA-CB-CG	-7.35	97.22	113.40
1	B	86	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	101	VAL	CG1-CB-CG2	-7.25	99.31	110.90
1	A	208	TRP	CB-CG-CD1	-7.03	117.86	127.00
1	B	135	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	136	SER	N-CA-CB	6.97	120.96	110.50
1	B	76	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	B	99	GLN	CA-CB-CG	-6.81	98.43	113.40
1	A	32	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	B	1	VAL	N-CA-C	-6.69	92.94	111.00
1	B	58	ASN	OD1-CG-ND2	-6.68	106.54	121.90
1	B	208	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	A	49	TYR	CB-CG-CD1	-6.64	117.01	121.00
1	B	90	PHE	CB-CG-CD1	-6.59	116.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	LYS	CA-CB-CG	6.50	127.69	113.40
1	B	180	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	A	76	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	A	19	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	A	173	MET	CG-SD-CE	-6.26	90.18	100.20
1	B	110	ASN	CA-C-N	6.23	130.90	117.20
1	B	135	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	156	MET	O-C-N	-6.19	112.80	122.70
1	B	19	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	91	ASN	CA-CB-CG	6.17	126.98	113.40
1	B	58	ASN	CB-CG-ND2	6.15	131.47	116.70
1	B	72	TYR	CB-CG-CD2	6.14	124.68	121.00
1	A	241	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	135	ARG	N-CA-C	-6.12	94.48	111.00
1	A	71	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	A	173	MET	CA-CB-CG	-6.06	103.00	113.30
1	B	237	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	A	167	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	80	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	B	136	SER	N-CA-C	-5.91	95.04	111.00
1	B	231	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	241	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	45	THR	CA-CB-CG2	5.84	120.57	112.40
1	A	135	ARG	N-CA-C	-5.78	95.39	111.00
1	A	98	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	110	ASN	N-CA-CB	5.77	120.98	110.60
1	A	250	ALA	CB-CA-C	-5.67	101.60	110.10
1	B	110	ASN	O-C-N	-5.67	113.64	122.70
1	B	237	TRP	CE2-CD2-CG	-5.66	102.78	107.30
1	A	179	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	167	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	182	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	6	TYR	CG-CD1-CE1	-5.52	116.89	121.30
1	A	262	THR	N-CA-C	-5.51	96.12	111.00
1	B	191	PHE	CG-CD2-CE2	-5.46	114.79	120.80
1	A	158	PHE	CA-C-N	5.44	129.16	117.20
1	B	11	THR	CA-CB-CG2	-5.42	104.81	112.40
1	B	237	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	B	42	ASN	CA-CB-CG	5.40	125.28	113.40
1	B	185	ASN	CA-C-N	5.39	129.07	117.20
1	B	260	GLN	CG-CD-NE2	5.39	129.64	116.70
1	B	50	VAL	CA-CB-CG2	5.39	118.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	GLY	CA-C-O	-5.37	110.94	120.60
1	B	151	LYS	CB-CG-CD	-5.34	97.71	111.60
1	A	66	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	20	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	A	68	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	61	THR	OG1-CB-CG2	-5.27	97.87	110.00
1	B	32	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	39	MET	CG-SD-CE	5.25	108.60	100.20
1	A	6	TYR	CD1-CG-CD2	5.18	123.60	117.90
1	B	191	PHE	CB-CG-CD2	-5.18	117.17	120.80
1	A	184	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	B	80	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	64	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	67	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	176	GLU	OE1-CD-OE2	-5.11	117.16	123.30
1	B	237	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	A	51	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	14	SER	CB-CA-C	-5.09	100.43	110.10
1	B	69	ASN	N-CA-CB	-5.07	101.48	110.60
1	B	148	ASN	CA-C-N	5.05	128.32	117.20
1	B	114	SER	CB-CA-C	-5.05	100.50	110.10
1	A	14	SER	O-C-N	5.05	130.78	122.70
1	B	78	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	208	TRP	NE1-CE2-CZ2	-5.04	124.85	130.40
1	B	262	THR	N-CA-C	-5.04	97.38	111.00
1	B	247	PRO	CA-C-N	5.01	128.23	117.20
1	B	117	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	TYR	Sidechain

## 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	2060	0	2083	34	0
1	B	2060	0	2083	32	0
2	A	42	0	0	1	0
2	B	45	0	0	1	0
All	All	4207	0	4166	65	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 8.

All (65) 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:62:ILE:HD12	1:A:149:ILE:HG23	1.70	0.74
1:B:135:ARG:HH11	1:B:205:GLN:NE2	1.93	0.66
1:B:136:SER:HA	1:B:197:PRO:HG2	1.78	0.65
1:A:135:ARG:HH11	1:A:205:GLN:HE21	1.47	0.63
1:A:65:MET:SD	1:A:101:VAL:HA	2.38	0.62
1:A:135:ARG:HH11	1:A:205:GLN:NE2	1.97	0.61
1:A:223:LEU:HB2	1:A:240:LEU:O	2.02	0.60
1:B:80:PHE:O	1:B:84:LYS:HB2	2.01	0.60
1:B:89:ILE:HG23	1:B:101:VAL:HG11	1.84	0.59
1:A:135:ARG:HD2	1:A:205:GLN:HE22	1.68	0.58
1:A:140:LEU:HD12	1:A:169:VAL:HG22	1.87	0.57
1:B:123:TYR:O	1:B:127:GLU:HG2	2.04	0.57
1:A:6:TYR:OH	1:A:11:THR:HG21	2.06	0.55
1:B:65:MET:SD	1:B:101:VAL:HA	2.47	0.55
1:B:183:ILE:HG12	1:B:201:VAL:HB	1.89	0.53
1:B:67:ARG:HH21	1:B:70:ASN:HD21	1.56	0.53
1:B:200:LYS:O	1:B:204:LEU:HB2	2.09	0.53
1:A:11:THR:HG22	1:A:15:LYS:HB3	1.91	0.52
1:A:201:VAL:O	1:A:205:GLN:HG3	2.10	0.51
1:B:135:ARG:HH11	1:B:205:GLN:HE21	1.58	0.51
1:B:182:TYR:HE2	1:B:201:VAL:HG12	1.75	0.51
1:B:34:CYS:SG	1:B:39:MET:HE1	2.50	0.51
1:A:261:THR:HG22	1:A:262:THR:HG23	1.92	0.50
1:A:155:VAL:HG22	1:A:158:PHE:HD2	1.78	0.49
1:A:228:GLU:HG2	1:A:238:ILE:HG12	1.96	0.48
1:B:127:GLU:OE1	1:B:135:ARG:HB3	2.14	0.48
1:B:34:CYS:SG	1:B:39:MET:CE	3.01	0.48
1:A:3:THR:HA	1:A:51:LEU:O	2.14	0.48
1:A:119:PHE:CD2	1:A:129:LYS:HE3	2.49	0.47
1:B:135:ARG:HD2	1:B:205:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:O	1:B:24:ARG:HG3	2.15	0.47
1:A:219:LYS:O	1:A:222:VAL:HG12	2.15	0.46
1:B:25:ASN:HA	1:B:28:LYS:HE2	1.97	0.46
1:B:136:SER:HB3	1:B:202:LEU:HD11	1.97	0.46
1:B:47:PRO:O	1:B:68:ARG:HD3	2.15	0.46
1:A:241:ARG:HH11	1:A:241:ARG:HG3	1.81	0.45
1:A:109:ALA:O	1:A:110:ASN:HB2	2.16	0.45
1:B:6:TYR:OH	1:B:11:THR:HG21	2.17	0.45
1:A:77:SER:HA	1:A:86:ARG:O	2.17	0.44
1:B:256:GLY:HA3	2:B:822:HOH:O	2.16	0.44
1:B:83:ASN:N	1:B:83:ASN:OD1	2.50	0.44
1:A:130:ALA:HA	1:A:161:LYS:HG2	2.00	0.44
1:A:159:THR:HG22	1:A:162:THR:H	1.83	0.43
1:B:182:TYR:CE2	1:B:201:VAL:HG12	2.53	0.43
1:A:176:GLU:HA	1:A:176:GLU:OE1	2.17	0.43
1:A:62:ILE:HD13	1:A:166:PHE:CZ	2.53	0.43
1:B:140:LEU:HD22	1:B:197:PRO:HD3	2.00	0.43
1:A:118:ASN:HB2	2:A:807:HOH:O	2.17	0.43
1:A:216:HIS:HE1	1:A:257:GLY:O	2.02	0.43
1:A:236:LYS:HE2	1:A:236:LYS:HB2	1.63	0.43
1:B:246:LYS:N	1:B:247:PRO:HD2	2.34	0.43
1:B:3:THR:HA	1:B:51:LEU:O	2.20	0.42
1:A:32:LEU:HB3	1:A:39:MET:HG2	2.01	0.42
1:A:94:SER:CB	1:B:44:ASN:HD21	2.33	0.41
1:A:91:ASN:HB3	1:A:119:PHE:O	2.20	0.41
1:A:83:ASN:OD1	1:A:83:ASN:N	2.53	0.41
1:A:142:ILE:HD13	1:A:173:MET:CE	2.51	0.41
1:B:62:ILE:HG21	1:B:166:PHE:CZ	2.55	0.41
1:B:26:GLU:HG3	1:B:50:VAL:CG1	2.51	0.41
1:A:87:TYR:CZ	1:A:102:GLU:HG3	2.56	0.41
1:A:210:LYS:HD3	1:A:227:LEU:HD11	2.02	0.41
1:A:241:ARG:NH2	1:A:243:ASP:HB2	2.36	0.41
1:B:97:GLU:O	1:B:101:VAL:HG23	2.21	0.41
1:B:135:ARG:NH1	1:B:205:GLN:HE21	2.19	0.40
1:B:145:LEU:O	1:B:149:ILE:HG13	2.22	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	260/262 (99%)	245 (94%)	11 (4%)	4 (2%)	10	18
1	B	260/262 (99%)	244 (94%)	14 (5%)	2 (1%)	19	35
All	All	520/524 (99%)	489 (94%)	25 (5%)	6 (1%)	13	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	91	ASN
1	A	136	SER
1	B	136	SER
1	A	159	THR
1	B	118	ASN

### 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	234/234 (100%)	201 (86%)	33 (14%)	3	6
1	B	234/234 (100%)	213 (91%)	21 (9%)	9	19
All	All	468/468 (100%)	414 (88%)	54 (12%)	5	11

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	11	THR
1	A	14	SER
1	A	19	PHE
1	A	30	PRO
1	A	32	LEU
1	A	39	MET
1	A	48	LYS
1	A	50	VAL
1	A	51	LEU
1	A	59	LYS
1	A	64	LEU
1	A	91	ASN
1	A	103	THR
1	A	111	SER
1	A	114	SER
1	A	132	VAL
1	A	135	ARG
1	A	155	VAL
1	A	159	THR
1	A	167	LEU
1	A	181	LYS
1	A	191	PHE
1	A	192	ASN
1	A	201	VAL
1	A	202	LEU
1	A	204	LEU
1	A	225	LYS
1	A	229	LEU
1	A	233	SER
1	A	236	LYS
1	A	240	LEU
1	A	258	SER
1	B	3	THR
1	B	11	THR
1	B	14	SER
1	B	50	VAL
1	B	51	LEU
1	B	58	ASN
1	B	59	LYS
1	B	81	GLU
1	B	103	THR
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	138	VAL
1	B	140	LEU
1	B	147	SER
1	B	151	LYS
1	B	159	THR
1	B	167	LEU
1	B	201	VAL
1	B	219	LYS
1	B	223	LEU
1	B	229	LEU
1	B	241	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	148	ASN
1	A	205	GLN
1	B	108	ASN
1	B	185	ASN
1	B	196	ASN
1	B	205	GLN
1	B	260	GLN

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	262/262 (100%)	-0.69	0 100 100	9, 19, 29, 33	0
1	B	262/262 (100%)	-0.73	0 100 100	10, 19, 27, 34	0
All	All	524/524 (100%)	-0.71	0 100 100	9, 19, 28, 34	0

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.