



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:27 PM UTC

PDB ID : 1PAF / pdb_00001paf
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

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

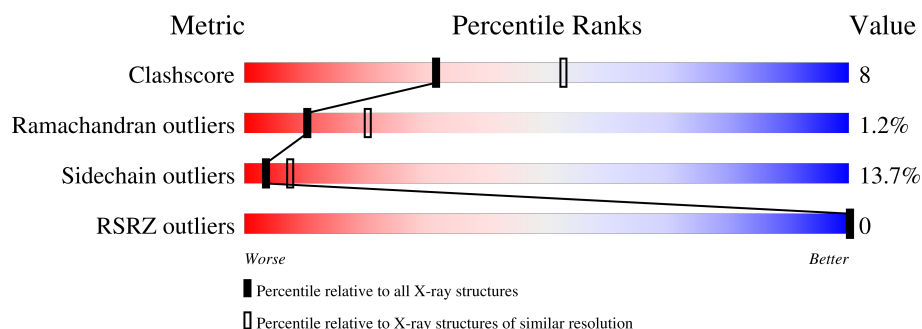
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	262	
1	B	262	

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 POKEWEED ANTIVIRAL PROTEIN.

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

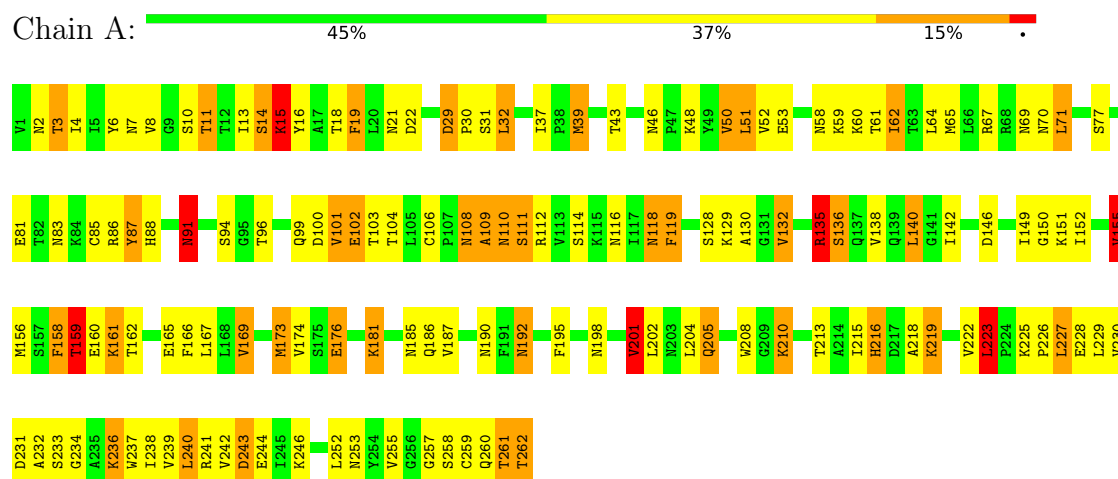
- Molecule 2 is water.

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

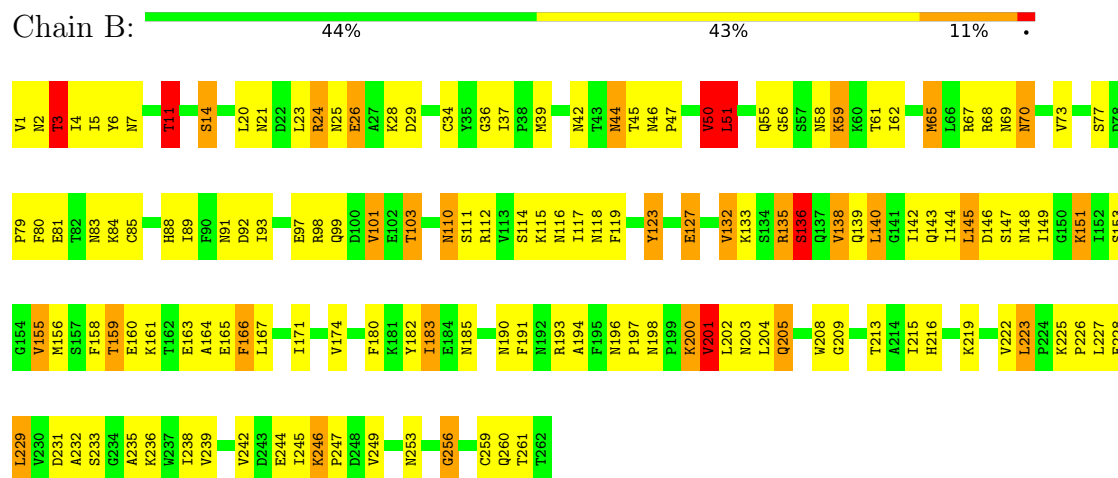
3 Residue-property plots

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: POKEWEED ANTIVIRAL PROTEIN



• Molecule 1: POKEWEED ANTIVIRAL PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.40Å 50.10Å 65.20Å 80.00° 113.20° 116.50°	Depositor
Resolution (Å)	(Not available) – 2.50 59.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 99.3 (59.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.50Å)	Xtriage
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 ²)	20.9	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,h+1	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4207	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	1.93	41/2096 (2.0%)	2.37	121/2840 (4.3%)
1	B	1.98	44/2096 (2.1%)	2.41	135/2840 (4.8%)
All	All	1.96	85/4192 (2.0%)	2.39	256/5680 (4.5%)

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 (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ILE	CA-CB	9.15	1.65	1.54
1	B	201	VAL	CA-CB	8.69	1.65	1.54
1	A	232	ALA	CA-C	-8.64	1.41	1.52
1	A	201	VAL	CA-CB	8.41	1.65	1.54
1	B	161	LYS	N-CA	8.35	1.55	1.46
1	B	24	ARG	CA-CB	8.09	1.66	1.53
1	B	216	HIS	CD2-NE2	-7.90	1.29	1.37
1	B	153	SER	CA-CB	-7.89	1.40	1.53
1	B	59	LYS	CA-CB	7.71	1.65	1.53
1	B	111	SER	N-CA	7.29	1.54	1.46
1	B	171	ILE	CA-CB	7.27	1.63	1.54
1	B	233	SER	CA-C	-7.21	1.42	1.52
1	B	242	VAL	CA-CB	7.10	1.63	1.54
1	B	245	ILE	CA-CB	7.08	1.63	1.54
1	B	244	GLU	CA-CB	-7.00	1.42	1.53
1	A	215	ILE	CA-CB	-6.99	1.46	1.54
1	A	187	VAL	CA-CB	6.98	1.64	1.54
1	A	208	TRP	CG-CD2	-6.82	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	ILE	CA-CB	6.77	1.62	1.54
1	B	215	ILE	CA-CB	6.76	1.62	1.54
1	A	8	VAL	CA-C	6.74	1.61	1.52
1	B	138	VAL	CA-CB	6.64	1.62	1.54
1	B	239	VAL	C-O	6.64	1.30	1.24
1	B	88	HIS	CD2-NE2	-6.62	1.30	1.37
1	B	70	ASN	CA-C	6.53	1.60	1.52
1	B	249	VAL	N-CA	-6.39	1.38	1.46
1	A	119	PHE	C-O	6.35	1.31	1.23
1	A	15	LYS	CA-C	6.34	1.60	1.52
1	A	226	PRO	CA-CB	-6.14	1.45	1.53
1	B	228	GLU	N-CA	6.12	1.54	1.46
1	A	192	ASN	CA-CB	6.11	1.62	1.53
1	A	88	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	73	VAL	CA-C	5.96	1.60	1.52
1	B	26	GLU	N-CA	-5.92	1.38	1.46
1	A	104	THR	CA-CB	-5.90	1.45	1.53
1	A	242	VAL	CA-C	5.89	1.60	1.52
1	A	156	MET	CA-C	5.88	1.60	1.52
1	B	226	PRO	C-O	5.82	1.30	1.23
1	B	77	SER	C-O	5.79	1.31	1.23
1	B	44	ASN	C-N	5.78	1.41	1.33
1	B	56	GLY	N-CA	-5.77	1.39	1.44
1	A	119	PHE	N-CA	-5.77	1.38	1.46
1	A	52	VAL	CA-CB	5.75	1.61	1.53
1	A	18	THR	CA-CB	5.72	1.62	1.53
1	B	51	LEU	CA-C	-5.71	1.46	1.52
1	B	23	LEU	CA-C	5.69	1.60	1.52
1	A	159	THR	CA-C	5.69	1.60	1.52
1	B	133	LYS	CA-CB	-5.68	1.44	1.53
1	B	228	GLU	C-O	-5.66	1.17	1.24
1	B	259	CYS	N-CA	-5.66	1.38	1.45
1	B	145	LEU	C-O	5.63	1.30	1.24
1	A	227	LEU	C-N	5.60	1.41	1.33
1	A	260	GLN	CD-OE1	5.60	1.34	1.23
1	A	174	VAL	CA-CB	5.58	1.62	1.54
1	A	135	ARG	CA-CB	5.56	1.61	1.53
1	A	246	LYS	CA-C	5.56	1.59	1.52
1	A	96	THR	N-CA	5.50	1.53	1.46
1	B	4	ILE	CA-CB	5.50	1.60	1.54
1	A	85	CYS	CA-C	5.48	1.59	1.52
1	B	226	PRO	C-N	-5.46	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	VAL	CA-CB	5.46	1.61	1.54
1	A	61	THR	CA-C	-5.44	1.46	1.52
1	A	255	VAL	N-CA	5.43	1.52	1.46
1	A	252	LEU	C-N	-5.41	1.26	1.33
1	B	88	HIS	CG-ND1	-5.38	1.32	1.38
1	B	222	VAL	CA-C	5.37	1.59	1.52
1	A	53	GLU	CA-CB	5.37	1.60	1.53
1	A	10	SER	CA-C	-5.36	1.46	1.52
1	B	37	ILE	CA-C	5.33	1.57	1.53
1	A	190	ASN	CA-CB	-5.26	1.45	1.53
1	A	10	SER	C-N	5.25	1.40	1.33
1	A	128	SER	C-N	-5.21	1.26	1.33
1	B	259	CYS	C-N	5.21	1.41	1.33
1	A	100	ASP	CA-C	5.19	1.59	1.52
1	B	110	ASN	CA-CB	5.19	1.62	1.53
1	A	104	THR	C-N	-5.19	1.27	1.33
1	B	208	TRP	CG-CD2	-5.14	1.34	1.43
1	B	14	SER	CA-CB	-5.12	1.45	1.53
1	B	14	SER	CA-C	5.12	1.59	1.52
1	A	195	PHE	C-O	-5.09	1.17	1.23
1	A	230	VAL	C-O	-5.05	1.18	1.24
1	A	215	ILE	CA-C	-5.02	1.46	1.52
1	A	91	ASN	CA-CB	-5.01	1.45	1.53
1	A	112	ARG	NE-CZ	5.01	1.38	1.33
1	B	174	VAL	CA-CB	5.01	1.61	1.54

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ASN	OD1-CG-ND2	-16.06	106.54	122.60
1	A	91	ASN	CA-CB-CG	14.38	126.98	112.60
1	B	42	ASN	CA-CB-CG	12.68	125.28	112.60
1	A	192	ASN	OD1-CG-ND2	-11.91	110.69	122.60
1	A	119	PHE	CA-CB-CG	10.86	124.66	113.80
1	B	135	ARG	N-CA-C	-10.68	94.48	110.28
1	B	244	GLU	N-CA-C	10.50	122.72	111.28
1	B	2	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	B	58	ASN	CB-CG-ND2	10.04	131.47	116.40
1	B	136	SER	N-CA-CB	10.02	127.42	110.49
1	A	15	LYS	N-CA-C	-9.88	100.59	111.36
1	A	135	ARG	N-CA-C	-9.78	95.39	109.96
1	B	46	ASN	CA-CB-CG	-9.52	103.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ASN	CA-CB-CG	9.49	122.09	112.60
1	A	243	ASP	CA-CB-CG	8.90	121.50	112.60
1	A	156	MET	O-C-N	-8.88	112.80	122.03
1	B	260	GLN	CG-CD-NE2	8.83	129.64	116.40
1	B	127	GLU	CA-CB-CG	8.62	131.33	114.10
1	A	81	GLU	CA-CB-CG	-8.44	97.22	114.10
1	A	99	GLN	N-CA-C	-8.30	101.77	112.23
1	A	253	ASN	CB-CG-ND2	8.18	128.67	116.40
1	A	58	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	B	92	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	185	ASN	CA-CB-CG	-7.99	104.61	112.60
1	B	156	MET	CA-CB-CG	7.98	130.06	114.10
1	A	158	PHE	CA-C-O	-7.86	110.78	119.34
1	A	253	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	B	99	GLN	CA-CB-CG	-7.84	98.43	114.10
1	A	231	ASP	CA-CB-CG	7.82	120.42	112.60
1	B	260	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	A	21	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	A	69	ASN	N-CA-C	7.75	120.71	111.33
1	A	237	TRP	CB-CG-CD1	-7.67	115.40	126.90
1	B	36	GLY	CA-C-O	-7.64	110.94	119.04
1	B	158	PHE	CA-CB-CG	7.61	121.41	113.80
1	A	108	ASN	CB-CG-ND2	7.56	127.75	116.40
1	A	60	LYS	O-C-N	-7.56	114.73	123.27
1	A	156	MET	CA-CB-CG	7.54	129.19	114.10
1	B	200	LYS	CA-C-O	-7.54	112.43	120.42
1	A	116	ASN	CA-CB-CG	7.51	120.11	112.60
1	A	242	VAL	CA-C-O	-7.45	113.30	121.05
1	B	136	SER	N-CA-C	-7.40	95.04	110.80
1	B	260	GLN	N-CA-C	-7.38	98.52	109.15
1	B	253	ASN	CB-CG-ND2	7.33	127.40	116.40
1	B	223	LEU	CA-C-O	-7.30	112.74	120.70
1	A	7	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	37	ILE	CA-C-O	7.25	123.43	119.15
1	A	70	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	A	108	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	A	46	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	A	15	LYS	CA-C-O	-7.15	112.84	120.42
1	B	253	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	A	260	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	B	7	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	B	2	ASN	CB-CG-ND2	7.06	126.98	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	TRP	CG-CD2-CE3	6.98	140.88	133.90
1	B	46	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	B	166	PHE	N-CA-C	-6.93	103.65	111.07
1	A	14	SER	O-C-N	6.92	130.78	122.27
1	A	29	ASP	CA-C-O	6.90	125.98	120.19
1	A	152	ILE	O-C-N	-6.83	115.90	121.98
1	A	216	HIS	CG-CD2-NE2	-6.81	100.39	107.20
1	A	158	PHE	N-CA-C	6.81	123.16	113.02
1	A	19	PHE	CA-C-N	6.80	129.39	120.28
1	A	19	PHE	C-N-CA	6.80	129.39	120.28
1	B	236	LYS	CA-CB-CG	6.80	127.69	114.10
1	A	158	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	165	GLU	O-C-N	-6.78	114.94	122.12
1	B	235	ALA	N-CA-C	6.76	121.07	110.32
1	B	115	LYS	O-C-N	-6.75	115.77	123.40
1	B	110	ASN	O-C-N	-6.73	113.64	122.59
1	A	223	LEU	CA-C-N	6.71	126.16	118.85
1	A	223	LEU	C-N-CA	6.71	126.16	118.85
1	B	180	PHE	CA-C-N	6.70	129.56	120.38
1	B	180	PHE	C-N-CA	6.70	129.56	120.38
1	B	205	GLN	CG-CD-NE2	6.70	126.45	116.40
1	A	227	LEU	O-C-N	-6.66	114.85	122.84
1	B	4	ILE	CA-C-O	-6.64	113.44	120.48
1	B	127	GLU	CA-C-N	6.60	129.37	120.65
1	B	127	GLU	C-N-CA	6.60	129.37	120.65
1	B	70	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	B	101	VAL	N-CA-C	-6.59	104.33	110.53
1	B	42	ASN	CB-CG-ND2	-6.56	106.56	116.40
1	B	231	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	1	VAL	N-CA-C	-6.45	92.94	111.00
1	A	7	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	111	SER	N-CA-C	6.38	121.07	113.16
1	A	70	ASN	CA-CB-CG	6.36	118.96	112.60
1	B	65	MET	O-C-N	-6.36	115.97	123.22
1	B	55	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	A	261	THR	N-CA-C	6.33	118.05	111.03
1	B	198	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	101	VAL	N-CA-C	-6.28	104.15	111.00
1	A	14	SER	N-CA-C	6.24	119.06	111.82
1	A	208	TRP	CD1-CG-CD2	6.23	116.26	106.30
1	A	237	TRP	CG-CD1-NE1	-6.21	102.13	110.20
1	A	110	ASN	N-CA-CB	6.21	120.98	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	THR	CA-C-O	-6.20	113.85	120.42
1	A	232	ALA	N-CA-C	6.20	124.00	110.80
1	B	196	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	B	198	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	190	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	A	136	SER	N-CA-CB	6.19	120.96	110.49
1	B	156	MET	CG-SD-CE	6.18	114.50	100.90
1	B	117	ILE	N-CA-C	-6.18	97.49	106.88
1	B	148	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	37	ILE	O-C-N	-6.18	116.20	121.57
1	B	183	ILE	O-C-N	6.18	128.78	121.80
1	B	232	ALA	N-CA-C	6.17	120.07	112.54
1	A	2	ASN	CA-C-N	-6.16	113.70	122.94
1	A	2	ASN	C-N-CA	-6.16	113.70	122.94
1	A	109	ALA	O-C-N	-6.14	115.79	122.79
1	A	201	VAL	N-CA-CB	6.14	118.89	110.54
1	A	237	TRP	CE2-CD2-CG	-6.12	99.86	107.20
1	B	238	ILE	CA-C-N	-6.11	114.64	123.06
1	B	238	ILE	C-N-CA	-6.11	114.64	123.06
1	A	118	ASN	CA-CB-CG	-6.10	106.50	112.60
1	A	176	GLU	CB-CG-CD	6.10	122.97	112.60
1	A	216	HIS	CE1-NE2-CD2	6.09	115.09	109.00
1	A	255	VAL	N-CA-C	-6.07	99.47	108.45
1	B	111	SER	CA-CB-OG	6.06	123.22	111.10
1	A	244	GLU	N-CA-C	6.06	117.96	111.36
1	B	259	CYS	O-C-N	-6.05	116.14	123.10
1	A	22	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	99	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	B	143	GLN	N-CA-CB	6.03	119.59	110.30
1	A	208	TRP	CG-CD1-NE1	-6.03	102.36	110.20
1	A	208	TRP	CB-CG-CD1	-6.03	117.86	126.90
1	B	146	ASP	CA-C-O	-6.02	114.46	120.90
1	B	185	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	B	193	ARG	O-C-N	5.96	130.04	123.25
1	B	194	ALA	N-CA-C	-5.95	101.47	110.28
1	B	3	THR	CB-CA-C	5.94	120.72	109.37
1	B	228	GLU	CA-C-O	5.93	126.81	120.46
1	B	45	THR	CA-CB-CG2	5.92	120.57	110.50
1	A	198	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	151	LYS	CB-CG-CD	-5.91	97.71	111.30
1	B	7	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	21	ASN	CB-CG-ND2	5.90	125.25	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	GLU	N-CA-C	5.87	118.46	111.71
1	B	11	THR	CA-C-N	5.85	131.88	121.75
1	B	11	THR	C-N-CA	5.85	131.88	121.75
1	A	218	ALA	N-CA-C	5.83	118.79	110.10
1	B	216	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	B	2	ASN	N-CA-C	-5.79	101.95	110.52
1	A	234	GLY	CA-C-O	5.79	125.39	118.97
1	B	205	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	B	165	GLU	CA-C-O	-5.77	114.31	120.42
1	B	180	PHE	N-CA-C	5.77	118.28	108.02
1	A	181	LYS	CA-C-O	5.76	126.61	120.10
1	A	205	GLN	CG-CD-NE2	5.72	124.98	116.40
1	B	69	ASN	N-CA-CB	-5.72	101.48	110.06
1	B	61	THR	OG1-CB-CG2	-5.71	97.87	109.30
1	A	15	LYS	N-CA-CB	-5.69	101.74	110.16
1	B	45	THR	CA-CB-OG1	-5.68	101.08	109.60
1	B	148	ASN	O-C-N	-5.68	115.67	122.15
1	B	155	VAL	CA-C-N	5.65	128.65	120.79
1	B	155	VAL	C-N-CA	5.65	128.65	120.79
1	A	70	ASN	CB-CG-ND2	5.63	124.84	116.40
1	B	14	SER	N-CA-C	5.62	117.88	111.02
1	B	209	GLY	O-C-N	5.61	127.58	122.19
1	B	148	ASN	N-CA-C	-5.61	105.25	111.36
1	B	203	ASN	CA-C-N	5.60	128.24	120.29
1	B	203	ASN	C-N-CA	5.60	128.24	120.29
1	B	14	SER	CA-C-O	5.59	127.22	121.07
1	A	216	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	198	ASN	CA-C-N	5.57	125.67	119.32
1	B	198	ASN	C-N-CA	5.57	125.67	119.32
1	B	116	ASN	N-CA-C	5.57	118.07	110.55
1	A	132	VAL	CA-C-O	-5.57	116.12	121.63
1	A	112	ARG	N-CA-C	5.57	118.31	109.96
1	A	173	MET	CA-CB-CG	-5.55	103.00	114.10
1	A	237	TRP	CD1-CG-CD2	5.55	115.17	106.30
1	A	37	ILE	CA-C-N	5.53	125.54	119.90
1	A	37	ILE	C-N-CA	5.53	125.54	119.90
1	A	156	MET	N-CA-CB	-5.52	101.86	109.91
1	B	119	PHE	CA-C-O	-5.51	115.52	121.36
1	B	225	LYS	CA-C-N	5.50	125.50	119.89
1	B	225	LYS	C-N-CA	5.50	125.50	119.89
1	B	7	ASN	CA-C-O	5.49	126.25	120.54
1	B	160	GLU	N-CA-C	5.49	116.94	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	VAL	N-CA-CB	-5.49	100.56	111.91
1	B	163	GLU	CA-C-O	-5.45	114.78	120.55
1	B	139	GLN	N-CA-C	5.45	117.72	110.53
1	B	213	THR	O-C-N	5.42	128.33	122.15
1	B	242	VAL	N-CA-C	-5.40	105.26	110.72
1	A	31	SER	CA-C-O	5.39	124.76	118.77
1	B	93	ILE	CA-C-O	-5.37	114.61	120.84
1	A	91	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	144	ILE	O-C-N	5.37	127.08	121.87
1	A	253	ASN	O-C-N	-5.37	116.67	122.79
1	B	261	THR	N-CA-CB	-5.35	102.31	110.07
1	A	136	SER	N-CA-C	-5.34	99.42	110.80
1	B	166	PHE	CA-C-O	-5.34	115.21	120.82
1	A	14	SER	CB-CA-C	-5.34	100.43	110.67
1	A	21	ASN	N-CA-C	-5.33	106.28	112.89
1	A	259	CYS	N-CA-C	-5.33	99.60	108.07
1	A	169	VAL	CA-C-O	-5.32	115.14	121.05
1	B	261	THR	O-C-N	5.32	127.84	122.09
1	A	262	THR	N-CA-C	-5.32	96.12	111.00
1	A	192	ASN	CB-CG-ND2	5.31	124.37	116.40
1	A	37	ILE	N-CA-C	5.31	113.12	107.76
1	B	29	ASP	N-CA-C	-5.29	103.37	109.93
1	B	191	PHE	N-CA-C	5.27	118.50	111.75
1	B	114	SER	CB-CA-C	-5.27	100.50	109.51
1	B	229	LEU	N-CA-CB	-5.25	102.94	110.87
1	A	174	VAL	CA-C-O	-5.24	114.23	120.78
1	B	246	LYS	CA-C-O	-5.23	113.27	118.34
1	A	205	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	101	VAL	CG1-CB-CG2	-5.22	99.31	110.80
1	B	88	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	B	216	HIS	CB-CG-ND1	5.21	130.51	122.70
1	B	42	ASN	CA-C-O	-5.21	115.66	121.81
1	A	106	CYS	O-C-N	-5.20	115.34	121.32
1	B	261	THR	N-CA-C	5.20	116.75	111.14
1	B	79	PRO	N-CA-CB	5.20	107.94	103.31
1	B	110	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	102	GLU	CA-C-N	5.19	127.76	120.28
1	A	102	GLU	C-N-CA	5.19	127.76	120.28
1	A	71	LEU	N-CA-C	5.18	121.82	110.80
1	A	151	LYS	CG-CD-CE	-5.17	99.41	111.30
1	A	110	ASN	CA-CB-CG	-5.17	107.43	112.60
1	A	135	ARG	NE-CZ-NH2	-5.17	114.55	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	CYS	CA-C-N	-5.17	115.87	123.00
1	B	85	CYS	C-N-CA	-5.17	115.87	123.00
1	B	159	THR	CA-C-N	5.16	127.15	120.44
1	B	159	THR	C-N-CA	5.16	127.15	120.44
1	A	4	ILE	O-C-N	-5.16	117.30	123.03
1	B	123	TYR	CA-C-N	5.15	125.20	119.32
1	B	123	TYR	C-N-CA	5.15	125.20	119.32
1	A	155	VAL	N-CA-C	-5.15	101.07	108.53
1	A	43	THR	CA-C-N	5.15	130.15	121.14
1	A	43	THR	C-N-CA	5.15	130.15	121.14
1	B	11	THR	OG1-CB-CG2	5.14	119.59	109.30
1	A	146	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	112	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	262	THR	CB-CA-C	5.13	120.39	109.10
1	A	52	VAL	O-C-N	-5.12	117.51	122.99
1	B	98	ARG	CA-C-N	-5.12	111.97	120.68
1	B	98	ARG	C-N-CA	-5.12	111.97	120.68
1	A	195	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	103	THR	N-CA-CB	-5.10	102.44	110.30
1	A	186	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	16	TYR	O-C-N	-5.09	116.59	122.09
1	B	194	ALA	O-C-N	-5.09	116.68	122.89
1	A	150	GLY	O-C-N	-5.08	116.94	122.68
1	B	245	ILE	N-CA-CB	-5.06	105.37	112.35
1	A	67	ARG	CA-C-O	-5.05	115.11	120.92
1	B	50	VAL	CA-CB-CG2	5.05	118.99	110.40
1	B	256	GLY	N-CA-C	5.05	118.41	111.54
1	B	227	LEU	N-CA-CB	-5.05	102.20	110.68
1	B	174	VAL	CA-C-O	-5.05	114.47	120.78
1	A	260	GLN	CA-C-N	5.04	127.49	120.63
1	A	260	GLN	C-N-CA	5.04	127.49	120.63
1	B	164	ALA	N-CA-C	5.03	116.76	111.28
1	A	50	VAL	CB-CA-C	-5.02	103.09	110.82

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	36	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	67	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 (67) 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:B:34:CYS:SG	1:B:39:MET:HE3	2.49	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:A:261:THR:HG22	1:A:262:THR:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:CYS:SG	1:B:39:MET:CE	3.01	0.48
1:B:127:GLU:OE1	1:B:135:ARG:HB3	2.14	0.48
1:A:3:THR:HA	1:A:51:LEU:O	2.14	0.48
1:A:142:ILE:HD13	1:A:173:MET:HE1	1.96	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
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:HG3	1:A:241:ARG:HH11	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:OD1	1:B:83:ASN:N	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:29:ASP:CG	1:A:32:LEU:HD22	2.43	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:HB2	1:A:236:LYS:HE2	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:87:TYR:CZ	1:A:102:GLU:HG3	2.56	0.41
1:A:142:ILE:HD13	1:A:173:MET:CE	2.51	0.41
1:B:26:GLU:HG3	1:B:50:VAL:CG1	2.51	0.41
1:B:62:ILE:HG21	1:B:166:PHE:CZ	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	8	16
1	B	260/262 (99%)	244 (94%)	14 (5%)	2 (1%)	16	31
All	All	520/524 (99%)	489 (94%)	25 (5%)	6 (1%)	10	20

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%)	192 (82%)	42 (18%)	2	3
1	B	234/234 (100%)	212 (91%)	22 (9%)	8	18
All	All	468/468 (100%)	404 (86%)	64 (14%)	3	7

All (64) 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	15	LYS
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	62	ILE
1	A	64	LEU
1	A	91	ASN
1	A	103	THR
1	A	108	ASN
1	A	111	SER
1	A	114	SER
1	A	132	VAL
1	A	135	ARG
1	A	138	VAL
1	A	140	LEU
1	A	155	VAL
1	A	159	THR
1	A	161	LYS
1	A	167	LEU
1	A	181	LYS
1	A	192	ASN
1	A	201	VAL
1	A	202	LEU
1	A	204	LEU
1	A	210	LYS
1	A	219	LYS
1	A	223	LEU

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Mol	Chain	Res	Type
1	A	225	LYS
1	A	229	LEU
1	A	233	SER
1	A	236	LYS
1	A	239	VAL
1	A	240	LEU
1	A	258	SER
1	B	3	THR
1	B	5	ILE
1	B	11	THR
1	B	14	SER
1	B	50	VAL
1	B	51	LEU
1	B	59	LYS
1	B	81	GLU
1	B	103	THR
1	B	110	ASN
1	B	132	VAL
1	B	138	VAL
1	B	140	LEU
1	B	147	SER
1	B	151	LYS
1	B	155	VAL
1	B	159	THR
1	B	167	LEU
1	B	201	VAL
1	B	219	LYS
1	B	223	LEU
1	B	229	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	25	ASN
1	A	46	ASN
1	A	69	ASN
1	A	99	GLN
1	A	108	ASN
1	A	186	GLN
1	A	192	ASN
1	A	205	GLN

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Mol	Chain	Res	Type
1	B	7	ASN
1	B	70	ASN
1	B	108	ASN
1	B	185	ASN
1	B	205	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 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 [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	262/262 (100%)	-0.52	0 100 100	9, 19, 29, 33	0
1	B	262/262 (100%)	-0.57	0 100 100	10, 18, 27, 34	0
All	All	524/524 (100%)	-0.54	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 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.