



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:50 PM UTC

PDB ID : 3V42 / pdb_00003v42
Title : Crystal structure of renal tumor suppressor protein, folliculin
Authors : Nookala, R.K.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2011-12-14
Resolution : 2.00 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

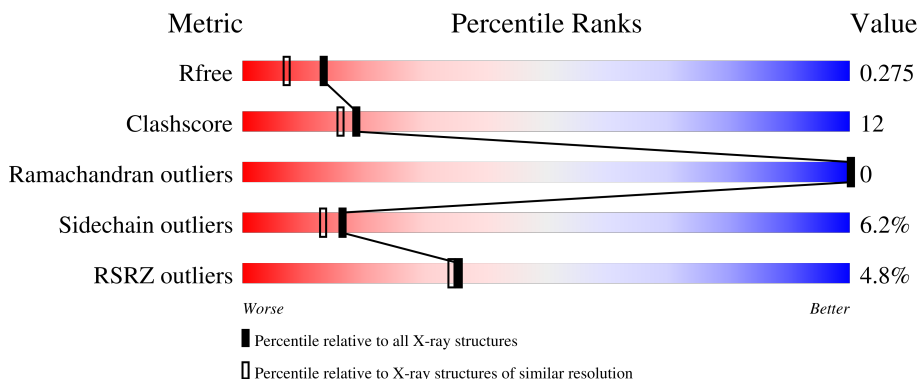
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	226	5% 44% 35% 7% 13%
1	B	226	3% 40% 42% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3308 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 Folliculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1540	998	261	273	8			
1	B	199	Total	C	N	O	S	0	1	0
			1544	1000	261	275	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	ALA	CYS	engineered mutation	UNP Q8NFG4
A	503	ALA	CYS	engineered mutation	UNP Q8NFG4
A	506	ALA	CYS	engineered mutation	UNP Q8NFG4
B	454	ALA	CYS	engineered mutation	UNP Q8NFG4
B	503	ALA	CYS	engineered mutation	UNP Q8NFG4
B	506	ALA	CYS	engineered mutation	UNP Q8NFG4

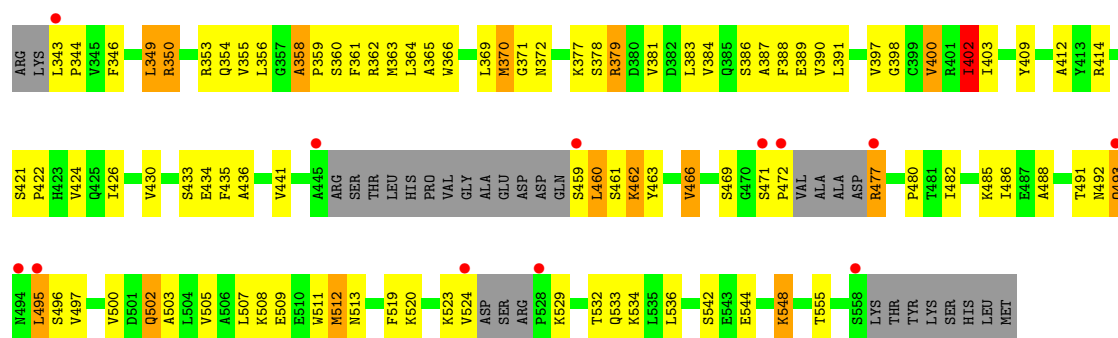
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	119	Total	O	0	0
			119	119		

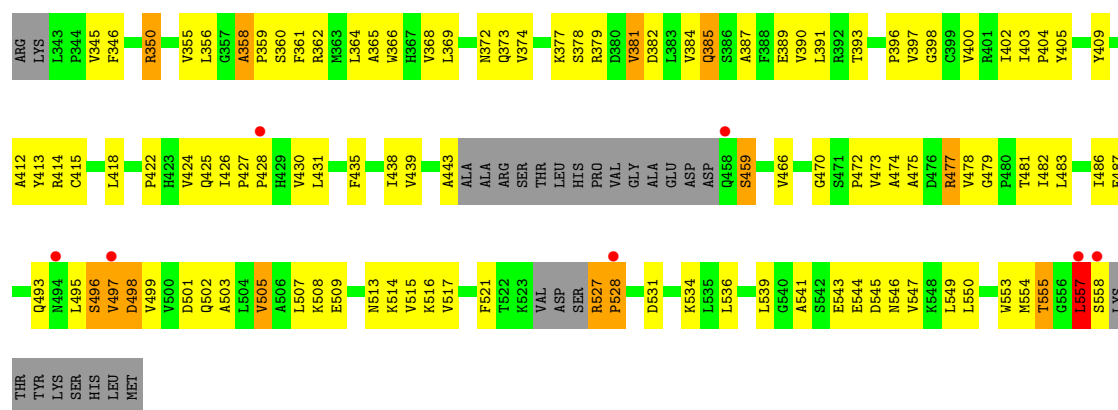
3 Residue-property plots

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: Folliculin



• Molecule 1: Folliculin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	86.05Å 99.95Å 107.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 2.00 29.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.14-2.00) 98.9 (29.14-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.268 0.215 , 0.275	Depositor DCC
R_{free} test set	1570 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3308	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5627e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	2.08	58/1572 (3.7%)	1.20	12/2130 (0.6%)
1	B	2.16	65/1580 (4.1%)	1.27	20/2149 (0.9%)
All	All	2.12	123/3152 (3.9%)	1.23	32/4279 (0.7%)

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	GLU	C-O	-8.02	1.14	1.24
1	B	369	LEU	C-O	-7.85	1.15	1.24
1	A	400	VAL	C-O	-7.75	1.15	1.24
1	B	505	VAL	C-O	-7.56	1.15	1.24
1	B	466	VAL	C-O	-7.50	1.16	1.24
1	A	366	TRP	C-O	-7.29	1.15	1.24
1	A	397	VAL	C-O	-6.85	1.15	1.24
1	B	550	LEU	C-O	-6.75	1.16	1.24
1	B	362	ARG	C-O	-6.71	1.16	1.24
1	A	402	ILE	C-O	-6.68	1.17	1.24
1	B	365	ALA	C-O	-6.65	1.16	1.24
1	A	503	ALA	CA-CB	-6.64	1.43	1.53
1	A	485	LYS	C-O	-6.57	1.16	1.24
1	A	482	ILE	C-O	-6.56	1.16	1.24
1	A	391	LEU	C-O	-6.51	1.16	1.24
1	B	553	TRP	C-O	-6.43	1.15	1.24
1	B	364	LEU	C-O	-6.41	1.16	1.24
1	A	350	ARG	C-O	-6.34	1.16	1.24
1	B	487	GLU	C-O	-6.31	1.16	1.24
1	B	482	ILE	C-O	-6.26	1.16	1.24
1	B	555	THR	C-O	-6.23	1.16	1.24
1	A	508	LYS	C-O	-6.19	1.16	1.24
1	A	383	LEU	C-O	-6.18	1.17	1.24
1	B	385	GLN	C-O	-6.08	1.17	1.24
1	A	466	VAL	C-O	-6.07	1.17	1.24
1	A	365	ALA	C-O	-6.03	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	SER	C-O	-6.03	1.17	1.24
1	A	362	ARG	C-O	-6.00	1.17	1.24
1	A	369	LEU	C-O	-6.00	1.17	1.24
1	B	400	VAL	C-O	-5.92	1.17	1.24
1	A	358	ALA	C-O	-5.90	1.19	1.24
1	B	397	VAL	C-O	-5.89	1.17	1.24
1	A	548	LYS	C-O	-5.86	1.17	1.24
1	B	346	PHE	C-O	-5.86	1.16	1.23
1	B	547	VAL	C-O	-5.86	1.17	1.24
1	B	486	ILE	C-O	-5.81	1.17	1.24
1	A	544	GLU	C-O	-5.80	1.17	1.24
1	A	390	VAL	C-O	-5.79	1.17	1.24
1	A	388	PHE	C-O	-5.76	1.17	1.24
1	B	356	LEU	C-O	-5.75	1.16	1.24
1	B	384	VAL	C-O	-5.74	1.17	1.24
1	B	418	LEU	C-O	-5.73	1.17	1.24
1	B	404	PRO	C-O	-5.66	1.17	1.24
1	B	513	ASN	C-O	-5.64	1.17	1.24
1	B	413	TYR	C-O	-5.63	1.17	1.24
1	B	545	ASP	C-O	-5.61	1.17	1.24
1	A	356	LEU	C-O	-5.60	1.17	1.24
1	A	384	VAL	C-O	-5.59	1.17	1.24
1	B	390	VAL	C-O	-5.59	1.17	1.24
1	A	505	VAL	C-O	-5.57	1.17	1.24
1	A	361	PHE	C-O	-5.57	1.17	1.24
1	A	370	MET	C-O	-5.54	1.16	1.24
1	B	544	GLU	C-O	-5.54	1.17	1.24
1	B	387	ALA	C-O	-5.53	1.17	1.24
1	A	507	LEU	C-O	-5.49	1.17	1.24
1	A	355	VAL	C-O	-5.49	1.18	1.24
1	B	368	VAL	C-O	-5.49	1.18	1.24
1	A	386	SER	C-O	-5.48	1.17	1.24
1	B	393	THR	C-O	-5.45	1.17	1.24
1	B	502	GLN	C-O	-5.44	1.17	1.24
1	B	516	LYS	C-O	-5.44	1.17	1.24
1	B	350	ARG	C-O	-5.44	1.17	1.24
1	B	361	PHE	C-O	-5.44	1.17	1.24
1	A	509	GLU	C-O	-5.43	1.17	1.24
1	B	536	LEU	C-O	-5.43	1.17	1.24
1	B	358	ALA	C-O	-5.41	1.19	1.24
1	A	381	VAL	C-O	-5.39	1.17	1.24
1	B	470	GLY	C-O	-5.38	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	LEU	C-O	-5.38	1.17	1.24
1	B	472	PRO	C-O	-5.38	1.17	1.23
1	B	345	VAL	C-O	-5.38	1.18	1.23
1	A	354	GLN	C-O	-5.38	1.18	1.24
1	B	478	VAL	C-O	-5.37	1.17	1.24
1	A	533	GLN	C-O	-5.36	1.17	1.24
1	B	426	ILE	C-O	-5.34	1.18	1.24
1	B	382	ASP	C-O	-5.34	1.17	1.24
1	B	374	VAL	C-O	-5.34	1.18	1.24
1	A	436	ALA	C-O	-5.33	1.17	1.23
1	A	441	VAL	C-O	-5.33	1.18	1.24
1	B	546	ASN	C-O	-5.33	1.17	1.24
1	A	512	MET	C-O	-5.31	1.18	1.24
1	B	409	TYR	C-O	-5.30	1.17	1.23
1	A	488	ALA	C-O	-5.29	1.18	1.24
1	B	503	ALA	CA-CB	-5.29	1.45	1.53
1	A	371	GLY	C-O	-5.29	1.17	1.24
1	A	519	PHE	C-O	-5.28	1.18	1.24
1	A	353	ARG	C-O	-5.28	1.18	1.24
1	A	433	SER	C-O	-5.28	1.17	1.23
1	A	534	LYS	C-O	-5.26	1.18	1.24
1	B	438	ILE	C-O	-5.26	1.18	1.24
1	B	501	ASP	C-O	-5.25	1.18	1.24
1	A	555	THR	C-O	-5.25	1.17	1.24
1	B	541	ALA	CA-CB	-5.23	1.45	1.53
1	B	483	LEU	C-O	-5.22	1.18	1.24
1	B	439	VAL	C-O	-5.21	1.18	1.24
1	B	412	ALA	C-O	-5.19	1.17	1.24
1	A	486	ILE	C-O	-5.19	1.18	1.24
1	B	373	GLN	C-O	-5.17	1.17	1.23
1	A	349	LEU	C-O	-5.17	1.18	1.24
1	B	534	LYS	C-O	-5.17	1.18	1.24
1	B	507	LEU	C-O	-5.15	1.18	1.24
1	B	481	THR	C-O	-5.15	1.18	1.24
1	A	500	VAL	C-O	-5.14	1.18	1.24
1	B	479	GLY	C-O	-5.14	1.17	1.24
1	A	536	LEU	C-O	-5.14	1.18	1.24
1	A	364	LEU	C-O	-5.13	1.18	1.24
1	A	426	ILE	C-O	-5.12	1.18	1.24
1	B	366	TRP	C-O	-5.11	1.18	1.24
1	B	517	VAL	C-O	-5.11	1.18	1.24
1	A	398	GLY	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	ALA	C-O	-5.10	1.18	1.24
1	A	469	SER	C-O	-5.09	1.17	1.23
1	B	398	GLY	C-O	-5.08	1.18	1.24
1	A	360	SER	C-O	-5.07	1.18	1.24
1	B	396	PRO	C-O	-5.07	1.17	1.23
1	A	502	GLN	C-O	-5.07	1.18	1.24
1	B	508	LYS	C-O	-5.07	1.18	1.24
1	A	387	ALA	C-O	-5.05	1.18	1.24
1	A	403	ILE	C-O	-5.04	1.18	1.23
1	A	346	PHE	C-O	-5.02	1.17	1.23
1	B	549	LEU	C-O	-5.02	1.18	1.24
1	B	475	ALA	C-O	-5.02	1.17	1.24
1	A	363	MET	C-O	-5.02	1.18	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	477	ARG	N-CA-C	10.82	124.38	111.82
1	A	355	VAL	N-CA-C	9.57	119.52	110.53
1	B	430	VAL	N-CA-C	7.83	118.54	111.81
1	B	528	PRO	N-CA-C	-7.02	100.18	111.14
1	B	355	VAL	N-CA-C	6.99	117.10	110.53
1	B	389[A]	GLU	CA-C-O	-6.52	113.97	120.82
1	B	389[B]	GLU	CA-C-O	-6.52	113.97	120.82
1	B	427	PRO	N-CA-C	6.32	118.40	110.70
1	A	378	SER	N-CA-C	6.14	118.41	109.07
1	B	389[A]	GLU	N-CA-C	-6.12	104.52	111.07
1	B	389[B]	GLU	N-CA-C	-6.12	104.52	111.07
1	B	402	ILE	N-CA-C	5.89	116.36	108.11
1	B	414	ARG	N-CA-C	5.88	117.77	111.36
1	A	426	ILE	CA-C-N	5.69	123.81	119.66
1	A	426	ILE	C-N-CA	5.69	123.81	119.66
1	B	381	VAL	N-CA-C	5.58	115.78	110.42
1	B	499	VAL	N-CA-C	-5.56	104.95	110.62
1	A	529	LYS	N-CA-C	-5.53	107.17	114.31
1	A	460	LEU	N-CA-C	5.51	119.64	111.87
1	A	466	VAL	N-CA-C	5.51	115.80	107.75
1	A	542	SER	N-CA-C	5.34	119.06	112.54
1	A	402	ILE	CB-CA-C	-5.30	102.79	110.63
1	B	390	VAL	N-CA-C	5.27	115.49	110.53
1	B	378	SER	N-CA-C	5.26	117.06	108.76
1	B	544	GLU	N-CA-C	5.25	117.00	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ARG	N-CA-C	5.18	117.01	111.36
1	A	390	VAL	N-CA-C	5.17	115.39	110.53
1	B	459	SER	N-CA-C	5.14	117.48	110.55
1	B	426	ILE	CA-C-N	5.10	125.63	120.38
1	B	426	ILE	C-N-CA	5.10	125.63	120.38
1	B	557	LEU	N-CA-C	-5.10	106.89	114.64
1	A	511	TRP	N-CA-C	5.02	116.75	111.28

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	1540	0	1574	38	1
1	B	1544	0	1542	36	0
2	A	105	0	0	8	5
2	B	119	0	0	9	6
All	All	3308	0	3116	74	6

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 (74) 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:523:LYS:O	1:A:524:VAL:HG23	1.41	1.18
1:A:512:MET:HG3	2:A:195:HOH:O	1.68	0.93
1:A:377:LYS:CE	1:A:422:PRO:O	2.16	0.92
1:A:350:ARG:HH22	1:A:495:LEU:HB2	1.32	0.91
1:A:377:LYS:HE2	1:A:422:PRO:O	1.69	0.90
1:A:477:ARG:N	1:A:477:ARG:HD2	1.86	0.89
1:B:428:PRO:HA	2:B:265:HOH:O	1.72	0.88
1:A:523:LYS:O	1:A:524:VAL:CG2	2.29	0.75
1:A:502:GLN:CG	2:A:191:HOH:O	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:THR:HA	1:B:558:SER:HB2	1.72	0.70
1:B:431:LEU:HD12	2:B:265:HOH:O	1.90	0.69
1:A:477:ARG:N	1:A:477:ARG:CD	2.54	0.69
1:B:443:ALA:C	2:B:239:HOH:O	2.36	0.68
1:B:377:LYS:CE	1:B:422:PRO:O	2.43	0.67
1:A:377:LYS:HE3	1:A:422:PRO:O	1.96	0.66
1:A:502:GLN:HG3	2:A:191:HOH:O	1.93	0.65
1:B:557:LEU:C	1:B:557:LEU:HD12	2.21	0.65
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.81	0.61
1:A:532:THR:HG23	2:A:104:HOH:O	2.00	0.61
1:A:502:GLN:HG2	2:A:191:HOH:O	1.98	0.61
1:B:514:LYS:HE2	1:B:539:LEU:O	2.00	0.61
1:B:350:ARG:HH22	1:B:495:LEU:HB2	1.67	0.59
1:B:377:LYS:HE2	1:B:422:PRO:O	2.03	0.58
1:B:505:VAL:O	1:B:509:GLU:HG3	2.04	0.57
1:B:496:SER:HB3	2:B:223:HOH:O	2.04	0.57
1:A:370:MET:HE2	1:A:480:PRO:HD3	1.88	0.56
1:B:557:LEU:C	1:B:557:LEU:CD1	2.80	0.54
1:B:521:PHE:CZ	1:B:527:ARG:HG2	2.43	0.54
1:A:421:SER:HB2	1:A:424:VAL:HG23	1.91	0.52
1:B:498:ASP:OD1	1:B:498:ASP:C	2.53	0.51
1:B:403:ILE:HG13	1:B:415:CYS:HB3	1.92	0.51
1:A:459:SER:C	1:A:460:LEU:HD12	2.36	0.50
1:A:343:LEU:N	1:A:344:PRO:CD	2.75	0.50
1:A:459:SER:HB2	1:A:460:LEU:HD13	1.95	0.49
1:B:377:LYS:HE3	1:B:422:PRO:O	2.13	0.48
1:A:343:LEU:CB	2:A:135:HOH:O	2.62	0.48
1:B:424:VAL:HG12	1:B:425:GLN:N	2.28	0.48
1:A:471:SER:O	1:A:472:PRO:C	2.56	0.48
1:A:493:GLN:O	1:A:493:GLN:OE1	2.32	0.47
1:A:492:ASN:HD22	1:A:495:LEU:HD23	1.79	0.47
1:B:521:PHE:CE2	1:B:527:ARG:HG2	2.50	0.47
1:B:381:VAL:HG22	1:B:405:TYR:CE2	2.50	0.47
1:B:557:LEU:HD12	1:B:558:SER:N	2.30	0.47
1:A:548:LYS:HD2	2:A:284:HOH:O	2.15	0.47
1:B:428:PRO:CA	2:B:265:HOH:O	2.47	0.46
1:A:471:SER:HA	1:A:472:PRO:HD2	1.41	0.46
1:B:372:ASN:HB3	1:B:435:PHE:O	2.17	0.45
1:A:409:TYR:CZ	1:A:430:VAL:HG21	2.51	0.44
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.83	0.43
1:B:493:GLN:CB	2:B:123:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.99	0.43
1:A:350:ARG:HD3	1:A:493:GLN:HE22	1.84	0.42
1:B:515:VAL:CG1	1:B:554:MET:HG3	2.49	0.42
1:B:477:ARG:CZ	2:B:218:HOH:O	2.67	0.42
1:B:424:VAL:CG1	1:B:425:GLN:N	2.81	0.42
1:B:473:VAL:O	1:B:474:ALA:HB3	2.20	0.42
1:B:527:ARG:HH11	1:B:527:ARG:HD2	1.59	0.42
1:A:462:LYS:HD3	1:A:463:TYR:CD2	2.55	0.42
1:A:466:VAL:HG12	2:A:183:HOH:O	2.20	0.41
1:B:381:VAL:HG22	1:B:405:TYR:CZ	2.55	0.41
1:A:462:LYS:HD3	1:A:463:TYR:CE2	2.55	0.41
1:A:372:ASN:HB3	1:A:435:PHE:O	2.19	0.41
1:A:520:LYS:O	1:A:523:LYS:HB2	2.20	0.41
1:B:527:ARG:HA	1:B:527:ARG:HD3	1.32	0.41
1:A:379:ARG:HG3	1:A:422:PRO:HG2	2.01	0.41
1:B:385:GLN:NE2	2:B:295:HOH:O	2.37	0.41
1:A:492:ASN:HD22	1:A:495:LEU:CD2	2.34	0.41
1:A:523:LYS:C	1:A:524:VAL:HG23	2.34	0.41
1:B:495:LEU:HD23	1:B:495:LEU:HA	1.61	0.41
1:A:400:VAL:CG1	1:A:402:ILE:HD11	2.51	0.40
1:A:462:LYS:H	1:A:462:LYS:HG3	1.53	0.40
1:B:497:VAL:HG12	1:B:498:ASP:N	2.36	0.40
1:B:527:ARG:HG3	1:B:531:ASP:HB2	2.03	0.40
1:B:428:PRO:C	2:B:265:HOH:O	2.65	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:HOH:O	2:B:218:HOH:O[6_655]	1.47	0.73
2:A:199:HOH:O	2:B:254:HOH:O[7_645]	1.78	0.42
1:A:463:TYR:O	2:B:217:HOH:O[6_655]	1.80	0.40
2:A:132:HOH:O	2:B:217:HOH:O[6_655]	1.86	0.34
2:A:161:HOH:O	2:B:219:HOH:O[6_655]	1.92	0.28
2:A:181:HOH:O	2:B:99:HOH:O[6_655]	1.97	0.23

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	188/226 (83%)	186 (99%)	2 (1%)	0	100	100
1	B	194/226 (86%)	190 (98%)	4 (2%)	0	100	100
All	All	382/452 (84%)	376 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	172/201 (86%)	160 (93%)	12 (7%)	14	10
1	B	167/201 (83%)	158 (95%)	9 (5%)	20	17
All	All	339/402 (84%)	318 (94%)	21 (6%)	16	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	379	ARG
1	A	402	ILE
1	A	434	GLU
1	A	461	SER
1	A	462	LYS
1	A	477	ARG
1	A	491	THR
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	495	LEU
1	A	496	SER
1	A	497	VAL
1	A	513	ASN
1	B	379	ARG
1	B	459	SER
1	B	496	SER
1	B	497	VAL
1	B	498	ASP
1	B	527	ARG
1	B	528	PRO
1	B	543	GLU
1	B	557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	A	373	GLN
1	A	429	HIS
1	A	492	ASN
1	A	493	GLN
1	B	429	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	196/226 (86%)	0.23	12 (6%)	27 26	14, 27, 53, 64	1 (0%)
1	B	199/226 (88%)	0.14	7 (3%)	47 46	13, 26, 48, 64	3 (1%)
All	All	395/452 (87%)	0.19	19 (4%)	35 34	13, 26, 51, 64	4 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	GLN	6.4
1	A	524	VAL	3.7
1	A	472	PRO	3.6
1	A	494	ASN	3.6
1	A	558	SER	3.6
1	B	428	PRO	3.4
1	A	477	ARG	3.2
1	B	558	SER	2.9
1	A	493	GLN	2.8
1	A	459	SER	2.8
1	B	497	VAL	2.8
1	B	557	LEU	2.7
1	A	528	PRO	2.7
1	A	343	LEU	2.7
1	B	494	ASN	2.5
1	A	495	LEU	2.4
1	A	471	SER	2.3
1	A	445	ALA	2.2
1	B	528	PRO	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 [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.