



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:21 AM UTC

PDB ID : 9DHC / pdb_00009dhc
Title : The Retinoblastoma Protein with Mutation S751Y
Authors : Ruiz-Rivera, A.; Castro, A.; Burke, J.R.
Deposited on : 2024-09-03
Resolution : 2.32 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

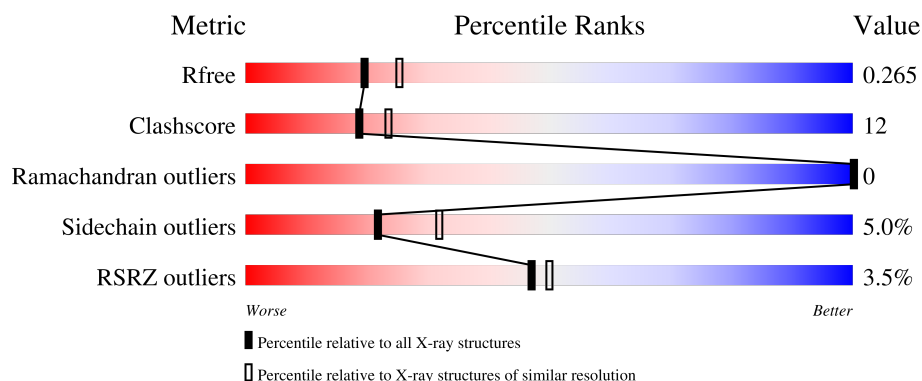
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

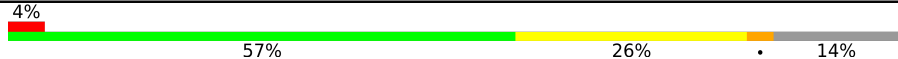
The reported resolution of this entry is 2.32 Å.

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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	390	
1	B	390	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11602 atoms, of which 5809 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 Retinoblastoma-associated protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	335	Total	C	H	N	O	S	0	0	0
			5601	1795	2826	464	496	20			
1	B	357	Total	C	H	N	O	S	0	0	0
			5923	1894	2983	493	532	21			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	GLY	-	expression tag	UNP P06400
A	378	GLU	-	expression tag	UNP P06400
A	379	PHE	-	expression tag	UNP P06400
A	608	GLU	SER	engineered mutation	UNP P06400
A	639	ALA	SER	engineered mutation	UNP P06400
A	?	-	LYS	deletion	UNP P06400
A	?	-	GLY	deletion	UNP P06400
A	?	-	SER	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	ARG	deletion	UNP P06400
A	?	-	VAL	deletion	UNP P06400
A	?	-	ASN	deletion	UNP P06400
A	?	-	SER	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	ALA	deletion	UNP P06400
A	?	-	ASN	deletion	UNP P06400
A	?	-	ALA	deletion	UNP P06400
A	?	-	GLU	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	GLN	deletion	UNP P06400
A	?	-	ALA	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	SER	deletion	UNP P06400
A	?	-	ALA	deletion	UNP P06400

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P06400
A	?	-	GLN	deletion	UNP P06400
A	?	-	THR	deletion	UNP P06400
A	?	-	GLN	deletion	UNP P06400
A	?	-	LYS	deletion	UNP P06400
A	?	-	PRO	deletion	UNP P06400
A	?	-	LEU	deletion	UNP P06400
A	751	TYR	SER	engineered mutation	UNP P06400
A	780	ALA	SER	engineered mutation	UNP P06400
B	377	GLY	-	expression tag	UNP P06400
B	378	GLU	-	expression tag	UNP P06400
B	379	PHE	-	expression tag	UNP P06400
B	608	GLU	SER	engineered mutation	UNP P06400
B	612	ALA	SER	engineered mutation	UNP P06400
B	?	-	LYS	deletion	UNP P06400
B	?	-	GLY	deletion	UNP P06400
B	?	-	SER	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	ARG	deletion	UNP P06400
B	?	-	VAL	deletion	UNP P06400
B	?	-	ASN	deletion	UNP P06400
B	?	-	SER	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	ALA	deletion	UNP P06400
B	?	-	ASN	deletion	UNP P06400
B	?	-	ALA	deletion	UNP P06400
B	?	-	GLU	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	GLN	deletion	UNP P06400
B	?	-	ALA	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	SER	deletion	UNP P06400
B	?	-	ALA	deletion	UNP P06400
B	?	-	PHE	deletion	UNP P06400
B	?	-	GLN	deletion	UNP P06400
B	?	-	THR	deletion	UNP P06400
B	?	-	GLN	deletion	UNP P06400
B	?	-	LYS	deletion	UNP P06400
B	?	-	PRO	deletion	UNP P06400
B	?	-	LEU	deletion	UNP P06400
B	751	TYR	SER	engineered mutation	UNP P06400

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Chain	Residue	Modelled	Actual	Comment	Reference
B	780	ALA	SER	engineered mutation	UNP P06400

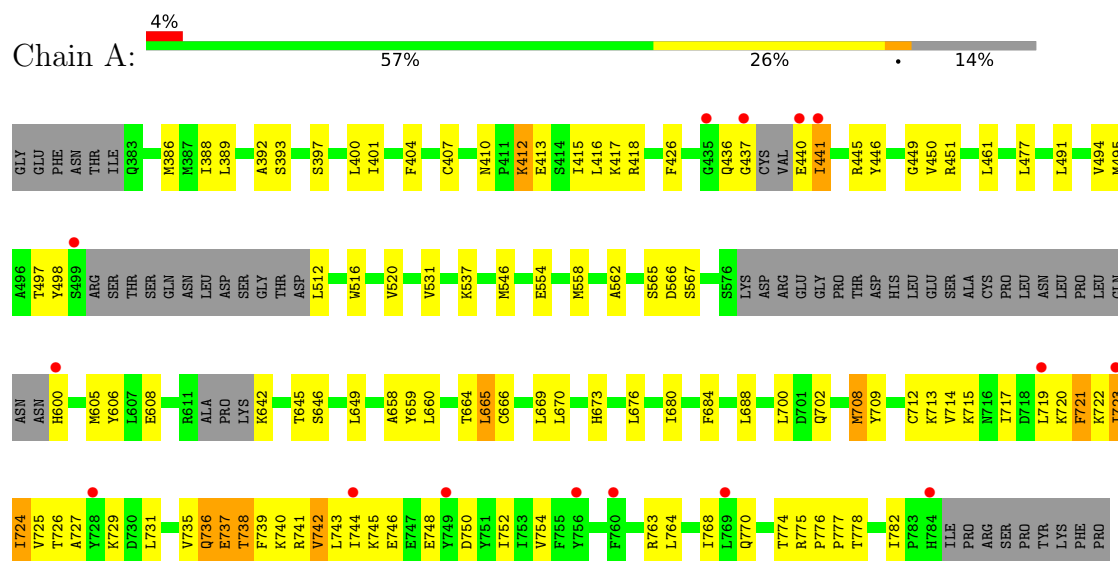
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	71	Total	O	0	0
			71	71		

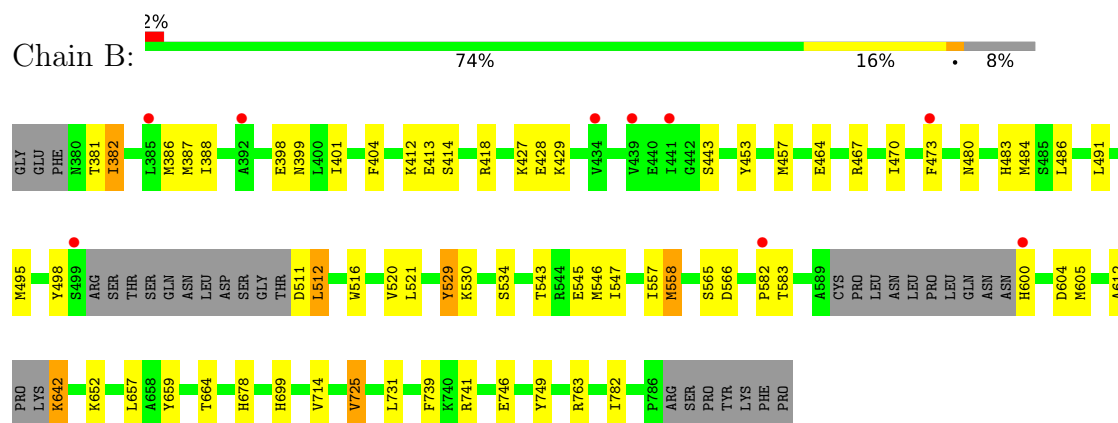
3 Residue-property plots [i](#)

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: Retinoblastoma-associated protein



• Molecule 1: Retinoblastoma-associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	255.04Å 255.04Å 35.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.20 – 2.32 48.20 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.20-2.32) 99.9 (48.20-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.263 0.214 , 0.265	Depositor DCC
R_{free} test set	1997 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11602	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.51	0/2831	0.74	1/3810 (0.0%)
1	B	0.87	3/3000 (0.1%)	0.98	4/4043 (0.1%)
All	All	0.72	3/5831 (0.1%)	0.87	5/7853 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	763	ARG	C-O	-6.25	1.16	1.24
1	B	558	MET	C-O	-5.43	1.17	1.24
1	B	699	HIS	CE1-NE2	-5.36	1.27	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	THR	CA-C-N	8.52	129.66	121.65
1	B	381	THR	C-N-CA	8.52	129.66	121.65
1	B	382	ILE	N-CA-CB	-6.89	105.39	112.28
1	B	387	MET	N-CA-C	-6.28	104.36	111.14
1	A	412	LYS	CB-CG-CD	5.23	123.32	111.30

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	2775	2826	2826	91	0
1	B	2940	2983	2983	47	0
2	A	7	0	0	0	0
2	B	71	0	0	2	0
All	All	5793	5809	5809	137	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 (137) 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:441:ILE:H	1:A:441:ILE:HD12	1.46	0.80
1:A:605:MET:HE2	1:A:646:SER:HA	1.67	0.76
1:A:404:PHE:O	1:A:410:ASN:ND2	2.21	0.74
1:A:449:GLY:HA3	1:A:491:LEU:HD23	1.72	0.72
1:A:397:SER:O	1:A:401:ILE:HG13	1.92	0.69
1:B:470:ILE:HD12	1:B:470:ILE:H	1.57	0.69
1:A:720:LYS:O	1:A:723:ILE:HG22	1.95	0.66
1:B:382:ILE:HG23	1:B:386:MET:HG3	1.79	0.65
1:A:386:MET:HE2	1:A:497:THR:HG21	1.78	0.64
1:A:722:LYS:HA	1:A:725:VAL:HG22	1.81	0.63
1:A:709:TYR:CZ	1:A:713:LYS:HE3	2.34	0.62
1:B:520:VAL:HG12	1:B:521:LEU:HD23	1.82	0.62
1:A:743:LEU:HD11	1:A:745:LYS:O	2.00	0.61
1:B:741:ARG:HG3	1:B:749:TYR:HB3	1.82	0.61
1:A:665:LEU:HD23	1:A:708:MET:SD	2.41	0.61
1:A:669:LEU:HD22	1:A:724:ILE:HG22	1.82	0.61
1:A:386:MET:CE	1:A:497:THR:HG21	2.31	0.61
1:A:410:ASN:ND2	1:A:412:LYS:HE2	2.16	0.60
1:B:512:LEU:HD12	1:B:512:LEU:H	1.65	0.60
1:B:382:ILE:HG22	1:B:386:MET:HB3	1.84	0.59
1:B:404:PHE:CD2	1:B:412:LYS:HG2	2.37	0.59
1:B:512:LEU:HD12	1:B:512:LEU:N	2.18	0.58
1:A:735:VAL:HG23	1:A:738:THR:HG23	1.84	0.58
1:A:436:GLN:HG2	1:A:437:GLY:H	1.69	0.57
1:B:565:SER:O	1:B:566:ASP:HB2	2.04	0.57
1:A:404:PHE:HB3	1:A:412:LYS:CG	2.35	0.57
1:A:673:HIS:CB	1:A:676:LEU:HD12	2.35	0.57
1:A:660:LEU:O	1:A:664:THR:HG23	2.05	0.56
1:B:382:ILE:HG22	1:B:386:MET:CB	2.35	0.56
1:A:658:ALA:HB1	1:A:684:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:TYR:CZ	1:A:713:LYS:CE	2.89	0.56
1:A:736:GLN:HB2	1:A:740:LYS:HD3	1.87	0.56
1:A:410:ASN:CG	1:A:412:LYS:HE2	2.30	0.55
1:A:436:GLN:HG2	1:A:437:GLY:N	2.21	0.55
1:B:453:TYR:CZ	1:B:457:MET:CE	2.89	0.55
1:B:398:GLU:O	1:B:401:ILE:HG13	2.06	0.55
1:A:404:PHE:HB3	1:A:412:LYS:HG2	1.88	0.55
1:A:714:VAL:HG21	1:A:768:ILE:HG22	1.88	0.54
1:B:382:ILE:CG2	1:B:386:MET:HB3	2.37	0.54
1:B:404:PHE:HD2	1:B:412:LYS:HG2	1.71	0.54
1:A:516:TRP:CZ2	1:A:520:VAL:HG21	2.43	0.54
1:B:725:VAL:HG13	1:B:739:PHE:CZ	2.43	0.53
1:A:441:ILE:H	1:A:441:ILE:CD1	2.13	0.53
1:A:665:LEU:O	1:A:669:LEU:HD12	2.10	0.52
1:B:725:VAL:HG22	1:B:739:PHE:CG	2.45	0.52
1:A:658:ALA:HB2	1:A:700:LEU:HD21	1.91	0.51
1:A:416:LEU:HD12	1:A:417:LYS:N	2.24	0.51
1:A:512:LEU:HD11	1:A:516:TRP:CE2	2.45	0.51
1:A:670:LEU:HD22	1:A:673:HIS:HB2	1.93	0.51
1:A:440:GLU:CD	1:A:440:GLU:O	2.53	0.51
1:A:659:TYR:CZ	1:A:782:ILE:HD12	2.45	0.51
1:B:612:ALA:O	1:B:642:LYS:N	2.44	0.51
1:A:600:HIS:HB2	1:A:649:LEU:HD22	1.93	0.51
1:B:495:MET:HE1	1:B:512:LEU:HD22	1.93	0.51
1:A:676:LEU:HD21	1:A:715:LYS:HG3	1.93	0.50
1:A:461:LEU:HD21	1:A:477:LEU:HD21	1.93	0.50
1:B:484:MET:HE1	1:B:521:LEU:HB3	1.94	0.50
1:A:721:PHE:CD1	1:A:724:ILE:HD11	2.47	0.50
1:B:382:ILE:CG2	1:B:386:MET:CB	2.90	0.50
1:A:554:GLU:HG2	1:A:558:MET:HE3	1.92	0.50
1:A:565:SER:O	1:A:566:ASP:HB2	2.11	0.49
1:A:407:CYS:SG	1:A:477:LEU:HD12	2.52	0.49
1:B:427:LYS:HE2	1:B:443:SER:HA	1.93	0.49
1:B:386:MET:CE	1:B:498:TYR:HE1	2.26	0.49
1:A:393:SER:O	1:A:451:ARG:HG2	2.13	0.49
1:A:410:ASN:OD1	1:A:412:LYS:HG3	2.13	0.48
1:B:386:MET:HE2	1:B:498:TYR:HE1	1.78	0.48
1:A:446:TYR:CE2	1:A:450:VAL:HG21	2.48	0.48
1:A:770:GLN:HB3	1:A:777:PRO:HD3	1.96	0.48
1:A:516:TRP:CE2	1:A:520:VAL:HG21	2.49	0.47
1:A:389:LEU:O	1:A:451:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:THR:O	1:A:729:LYS:HG2	2.14	0.47
1:B:664:THR:HG21	1:B:731:LEU:CD2	2.44	0.47
1:A:516:TRP:CE2	1:A:520:VAL:CG2	2.97	0.47
1:A:410:ASN:OD1	1:A:412:LYS:HE2	2.15	0.47
1:A:669:LEU:HD11	1:A:727:ALA:CB	2.44	0.47
1:A:775:ARG:HG2	1:A:775:ARG:O	2.15	0.47
1:B:491:LEU:O	1:B:495:MET:HG2	2.15	0.47
1:B:520:VAL:HG12	1:B:521:LEU:CD2	2.44	0.47
1:B:558:MET:HE3	1:B:657:LEU:HD22	1.95	0.47
1:B:453:TYR:OH	1:B:483:HIS:ND1	2.42	0.46
1:B:470:ILE:HD12	1:B:470:ILE:N	2.26	0.46
1:A:461:LEU:HD11	1:A:477:LEU:HD21	1.97	0.46
1:A:721:PHE:O	1:A:724:ILE:HG13	2.16	0.46
1:B:382:ILE:HG22	1:B:382:ILE:O	2.14	0.46
1:B:404:PHE:CB	1:B:412:LYS:HG2	2.46	0.46
1:B:470:ILE:H	1:B:470:ILE:CD1	2.26	0.46
1:A:712:CYS:SG	1:A:719:LEU:HD21	2.56	0.46
1:A:743:LEU:HD12	1:A:748:GLU:O	2.16	0.46
1:A:702:GLN:CD	1:A:742:VAL:HG13	2.41	0.45
1:A:774:THR:OG1	1:B:511:ASP:O	2.28	0.45
1:B:545:GLU:HG3	2:B:834:HOH:O	2.17	0.45
1:A:426:PHE:CD2	1:A:446:TYR:HB2	2.52	0.45
1:A:743:LEU:CD1	1:A:745:LYS:O	2.65	0.45
1:B:600:HIS:N	1:B:604:ASP:OD2	2.49	0.45
1:B:464:GLU:OE1	1:B:467:ARG:HD3	2.18	0.44
1:A:673:HIS:CE1	1:A:717:ILE:HG13	2.52	0.44
1:B:543:THR:O	1:B:547:ILE:HG13	2.17	0.44
1:A:400:LEU:O	1:A:400:LEU:HD12	2.17	0.44
1:B:516:TRP:CZ2	1:B:520:VAL:HG21	2.53	0.44
1:B:582:PRO:O	1:B:583:THR:C	2.60	0.43
1:A:739:PHE:O	1:A:752:ILE:HB	2.18	0.43
1:A:673:HIS:HB3	1:A:676:LEU:HG	1.99	0.43
1:A:495:MET:HA	1:A:495:MET:HE2	2.00	0.43
1:A:416:LEU:HD12	1:A:417:LYS:HG3	2.01	0.43
1:A:562:ALA:O	1:A:567:SER:OG	2.34	0.43
1:A:608:GLU:OE2	1:A:645:THR:N	2.52	0.43
1:A:726:THR:HA	1:A:729:LYS:HE2	2.01	0.43
1:A:388:ILE:O	1:A:392:ALA:HB2	2.19	0.43
1:A:702:GLN:NE2	1:A:742:VAL:HG13	2.34	0.42
1:B:659:TYR:CE1	1:B:782:ILE:HD12	2.53	0.42
1:A:491:LEU:O	1:A:495:MET:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LYS:HD3	1:B:605:MET:HB3	2.01	0.42
1:A:676:LEU:O	1:A:680:ILE:HG13	2.19	0.42
1:B:741:ARG:HG3	1:B:749:TYR:CB	2.50	0.42
1:A:410:ASN:HD21	1:A:412:LYS:HE2	1.82	0.42
1:B:484:MET:HB3	1:B:484:MET:HE3	1.88	0.42
1:A:744:ILE:HD11	1:A:754:VAL:HB	2.02	0.42
1:B:453:TYR:CE1	1:B:486:LEU:HD23	2.55	0.42
1:A:659:TYR:CE1	1:A:782:ILE:HD12	2.56	0.41
1:A:666:CYS:SG	1:A:708:MET:HE3	2.60	0.41
1:B:678:HIS:HB2	2:B:828:HOH:O	2.20	0.41
1:A:673:HIS:HB3	1:A:676:LEU:CG	2.50	0.41
1:A:764:LEU:O	1:A:768:ILE:HG13	2.20	0.41
1:A:445:ARG:NH2	1:A:498:TYR:HB3	2.35	0.41
1:A:491:LEU:O	1:A:494:VAL:HG22	2.20	0.41
1:B:418:ARG:NH1	1:B:480:ASN:HA	2.35	0.41
1:A:413:GLU:HB3	1:A:417:LYS:NZ	2.36	0.41
1:A:737:GLU:HA	1:A:740:LYS:HB2	2.02	0.41
1:A:684:PHE:O	1:A:688:LEU:HG	2.21	0.41
1:A:531:VAL:HB	1:A:606:TYR:OH	2.21	0.41
1:A:741:ARG:HA	1:A:750:ASP:O	2.21	0.41
1:A:745:LYS:O	1:A:746:GLU:C	2.64	0.40
1:A:770:GLN:O	1:A:776:PRO:HA	2.21	0.40
1:B:529:TYR:HB2	1:B:557:ILE:HG21	2.02	0.40
1:A:415:ILE:HA	1:A:418:ARG:NH1	2.36	0.40
1:A:714:VAL:HG21	1:A:768:ILE:CG2	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/390 (83%)	318 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	349/390 (90%)	338 (97%)	11 (3%)	0	100	100
All	All	674/780 (86%)	656 (97%)	18 (3%)	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	312/362 (86%)	296 (95%)	16 (5%)	21	31
1	B	331/362 (91%)	315 (95%)	16 (5%)	23	33
All	All	643/724 (89%)	611 (95%)	32 (5%)	22	32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	ILE
1	A	537	LYS
1	A	546	MET
1	A	642	LYS
1	A	665	LEU
1	A	708	MET
1	A	721	PHE
1	A	723	ILE
1	A	724	ILE
1	A	731	LEU
1	A	736	GLN
1	A	737	GLU
1	A	738	THR
1	A	742	VAL
1	A	763	ARG
1	A	778	THR
1	B	388	ILE
1	B	399	ASN

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Mol	Chain	Res	Type
1	B	413	GLU
1	B	414	SER
1	B	428	GLU
1	B	429	LYS
1	B	473	PHE
1	B	512	LEU
1	B	529	TYR
1	B	534	SER
1	B	546	MET
1	B	642	LYS
1	B	652	LYS
1	B	714	VAL
1	B	725	VAL
1	B	746	GLU

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	541	ASN
1	A	575	GLN
1	A	767	ASN
1	B	686	HIS
1	B	690	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	335/390 (85%)	0.59	15 (4%) 38 40	66, 107, 142, 190	0
1	B	357/390 (91%)	0.00	9 (2%) 58 61	37, 61, 106, 153	0
All	All	692/780 (88%)	0.29	24 (3%) 47 50	37, 86, 136, 190	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	SER	3.6
1	A	437	GLY	3.6
1	A	441	ILE	2.7
1	A	749	TYR	2.6
1	B	600	HIS	2.6
1	B	392	ALA	2.6
1	B	434	VAL	2.5
1	A	760	PHE	2.5
1	B	385	LEU	2.5
1	B	473	PHE	2.4
1	A	744	ILE	2.4
1	A	769	LEU	2.3
1	B	582	PRO	2.2
1	A	440	GLU	2.2
1	A	756	TYR	2.1
1	A	600	HIS	2.1
1	B	499	SER	2.1
1	B	439	VAL	2.1
1	A	723	ILE	2.1
1	B	441	ILE	2.1
1	A	728	TYR	2.0
1	A	435	GLY	2.0
1	A	784	HIS	2.0
1	A	719	LEU	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.