



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:24 PM UTC

PDB ID : 9DGK / pdb_00009dgc
Title : The Retinoblastoma Protein with Mutation M704V
Authors : Ruiz-Rivera, A.; Castro, A.; Burke, J.R.
Deposited on : 2024-09-02
Resolution : 2.38 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

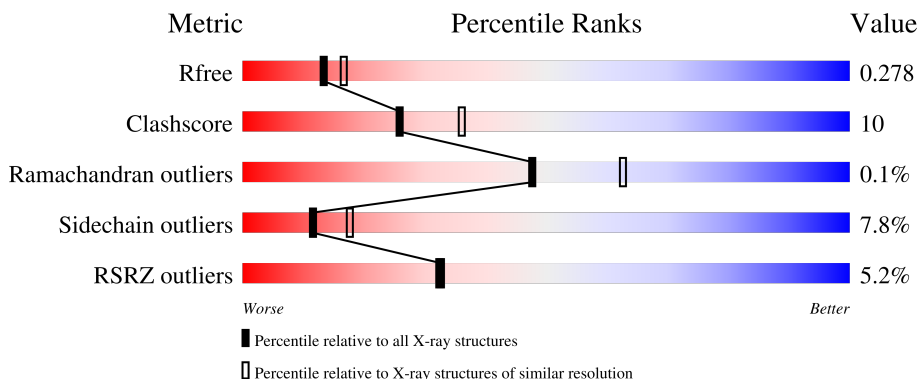
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	6% 58% 26% • 14%
1	B	390	3% 70% 19% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11477 atoms, of which 5783 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
			5590	1789	2822	464	496	19			
1	B	355	Total	C	H	N	O	S	0	0	0
			5878	1879	2961	488	530	20			

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	conflict	UNP P06400
A	639	ALA	SER	conflict	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	704	VAL	MET	engineered mutation	UNP P06400
A	780	ALA	SER	conflict	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	conflict	UNP P06400
B	639	ALA	SER	conflict	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	704	VAL	MET	engineered mutation	UNP P06400

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

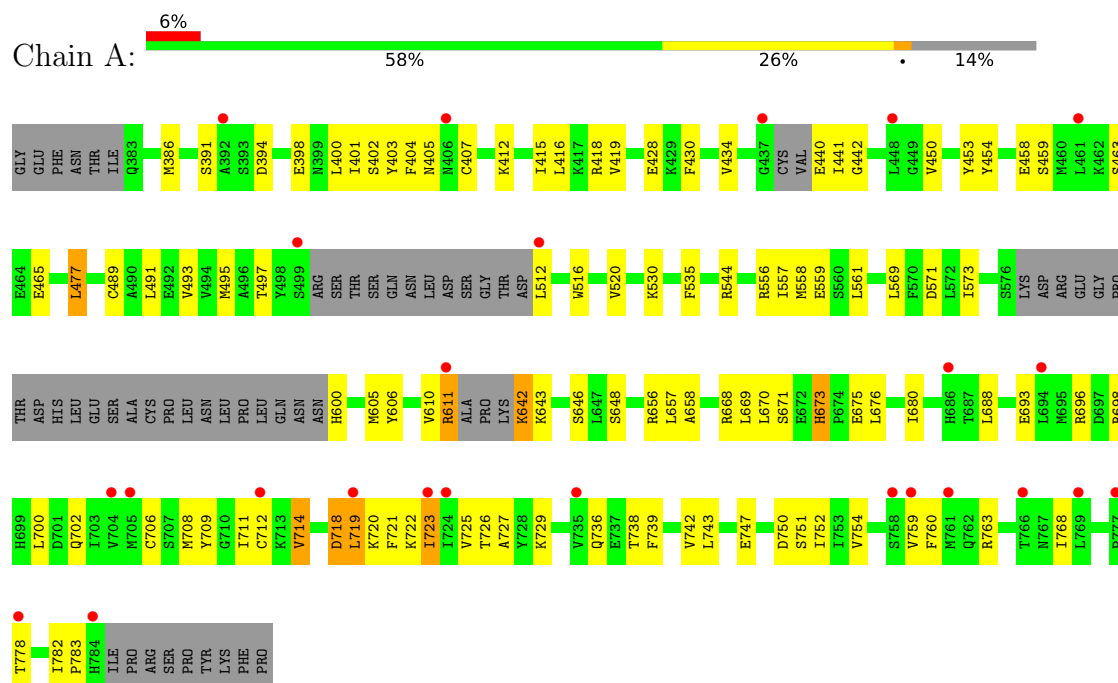
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	5	Total O 5 5	0	0

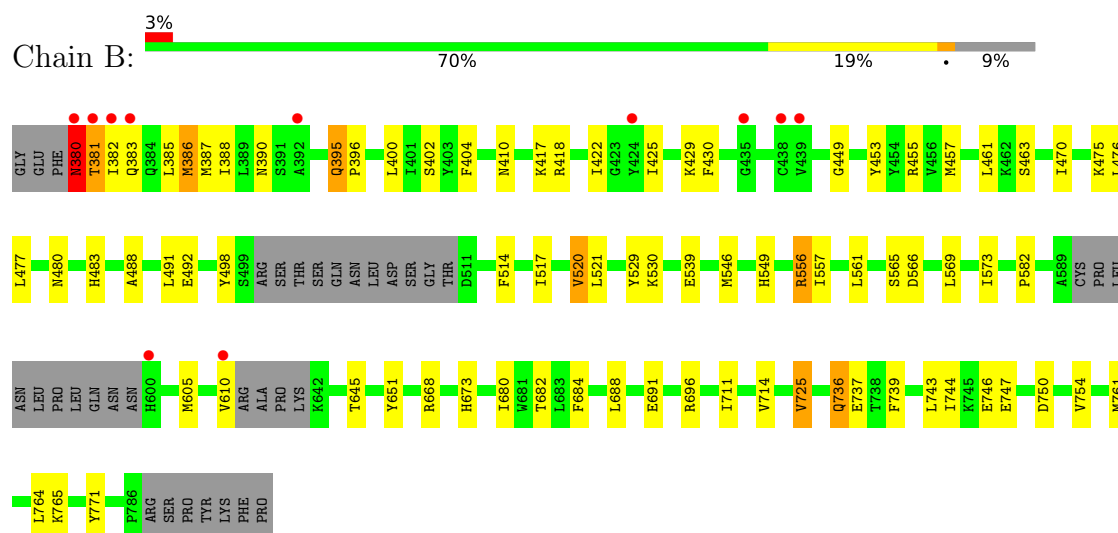
3 Residue-property plots [i](#)

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	250.84Å 250.84Å 35.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.40 – 2.38 47.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.40-2.38) 99.9 (47.40-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.220 , 0.277 0.222 , 0.278	Depositor DCC
R_{free} test set	1996 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11477	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/2823	0.78	0/3800
1	B	0.87	2/2976 (0.1%)	0.99	3/4012 (0.1%)
All	All	0.73	2/5799 (0.0%)	0.89	3/7812 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	582	PRO	C-O	-6.17	1.16	1.24
1	B	673	HIS	C-N	-5.10	1.27	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	696	ARG	CA-C-O	-5.76	114.08	120.70
1	B	380	ASN	CA-C-N	5.52	132.08	121.54
1	B	380	ASN	C-N-CA	5.52	132.08	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2768	2822	2822	64	2
1	B	2917	2961	2961	46	0
2	A	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
All	All	5694	5783	5783	109	2

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 10.

All (109) 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:658:ALA:HB2	1:A:700:LEU:HD21	1.36	1.07
1:A:386:MET:HE3	1:A:497:THR:HG21	1.51	0.89
1:B:380:ASN:HD22	1:B:380:ASN:N	1.84	0.76
1:B:385:LEU:HA	1:B:388:ILE:HD12	1.69	0.74
1:A:702:GLN:HE21	1:A:742:VAL:HG22	1.52	0.73
1:B:682:THR:HG22	1:B:771:TYR:OH	1.88	0.72
1:B:461:LEU:HD21	1:B:477:LEU:HD21	1.71	0.71
1:A:698:ARG:NH1	1:A:743:LEU:O	2.26	0.67
1:B:383:GLN:HB2	1:B:386:MET:HB2	1.77	0.66
1:B:546:MET:HE3	1:B:549:HIS:HB3	1.77	0.66
1:A:778:THR:HG21	1:B:737:GLU:OE1	1.99	0.62
1:A:400:LEU:HD13	1:A:458:GLU:HA	1.81	0.62
1:A:680:ILE:HD13	1:A:708:MET:HG2	1.82	0.62
1:A:512:LEU:HG	1:A:512:LEU:O	2.00	0.61
1:A:709:TYR:HE1	1:A:720:LYS:HG2	1.66	0.61
1:A:714:VAL:HG11	1:A:768:ILE:HG22	1.83	0.60
1:B:449:GLY:HA3	1:B:491:LEU:HD23	1.83	0.60
1:B:529:TYR:HB2	1:B:557:ILE:HG21	1.84	0.59
1:A:611:ARG:HH11	1:A:611:ARG:HA	1.68	0.59
1:B:418:ARG:HD3	1:B:480:ASN:OD1	2.03	0.59
1:A:600:HIS:N	2:A:802:HOH:O	2.37	0.58
1:A:386:MET:HE3	1:A:497:THR:CG2	2.28	0.58
1:A:430:PHE:O	1:A:434:VAL:HG22	2.03	0.58
1:A:725:VAL:HG13	1:A:739:PHE:CD2	2.40	0.56
1:A:605:MET:HE2	1:A:646:SER:HA	1.87	0.56
1:A:670:LEU:HD11	1:A:712:CYS:SG	2.46	0.56
1:B:429:LYS:HD3	1:B:520:VAL:HG22	1.87	0.56
1:A:702:GLN:NE2	1:A:742:VAL:HG22	2.20	0.55
1:B:691:GLU:HG3	1:B:764:LEU:HD21	1.89	0.55
1:A:750:ASP:OD1	1:A:754:VAL:HG21	2.06	0.55
1:B:546:MET:HE3	1:B:546:MET:HA	1.88	0.54
1:B:492:GLU:OE2	1:B:514:PHE:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:LEU:HD21	1:A:727:ALA:CB	2.38	0.54
1:A:750:ASP:CG	1:A:754:VAL:HG21	2.32	0.54
1:A:530:LYS:HD3	1:A:605:MET:HB3	1.89	0.53
1:A:642:LYS:HE2	1:A:643:LYS:HG2	1.90	0.53
1:B:498:TYR:N	1:B:498:TYR:CD2	2.75	0.53
1:B:557:ILE:HA	1:B:561:LEU:HB2	1.91	0.53
1:A:656:ARG:NH1	1:A:783:PRO:O	2.42	0.52
1:A:401:ILE:HD12	1:A:402:SER:N	2.25	0.51
1:B:530:LYS:HD3	1:B:605:MET:HB3	1.93	0.51
1:B:418:ARG:NH1	1:B:480:ASN:HA	2.27	0.50
1:B:488:ALA:HB2	1:B:521:LEU:HD12	1.92	0.50
1:B:546:MET:HE1	1:B:549:HIS:ND1	2.27	0.50
1:A:702:GLN:NE2	1:A:738:THR:O	2.44	0.50
1:B:453:TYR:CZ	1:B:457:MET:CE	2.95	0.50
1:A:725:VAL:HG11	1:A:739:PHE:CD1	2.46	0.50
1:A:416:LEU:O	1:A:419:VAL:HG22	2.12	0.49
1:A:398:GLU:O	1:A:401:ILE:HG13	2.13	0.49
1:A:405:ASN:C	2:A:801:HOH:O	2.56	0.49
1:A:669:LEU:HD22	1:A:723:ILE:CG1	2.43	0.48
1:A:718:ASP:O	1:A:718:ASP:CG	2.56	0.48
1:B:743:LEU:HD12	1:B:744:ILE:N	2.28	0.48
1:A:706:CYS:HB3	1:A:760:PHE:CE2	2.49	0.48
1:A:658:ALA:CB	1:A:700:LEU:HD21	2.25	0.48
1:A:512:LEU:O	1:A:512:LEU:CG	2.62	0.47
1:A:718:ASP:HB2	1:A:720:LYS:NZ	2.30	0.47
1:A:673:HIS:HB3	1:A:675:GLU:CD	2.39	0.47
1:A:440:GLU:HG3	1:A:441:ILE:N	2.29	0.47
1:A:516:TRP:O	1:A:520:VAL:HG23	2.15	0.47
1:A:696:ARG:CZ	1:A:696:ARG:HB2	2.45	0.47
1:B:746:GLU:OE1	1:B:746:GLU:HA	2.15	0.47
1:A:669:LEU:HD22	1:A:723:ILE:HD11	1.97	0.47
1:A:403:TYR:HE1	1:A:465:GLU:OE2	1.98	0.46
1:B:430:PHE:C	1:B:430:PHE:CD2	2.93	0.46
1:B:761:MET:O	1:B:765:LYS:N	2.48	0.46
1:B:529:TYR:CD2	1:B:529:TYR:C	2.93	0.46
1:A:491:LEU:O	1:A:495:MET:HG2	2.14	0.46
1:A:415:ILE:HD11	1:A:477:LEU:HD12	1.98	0.45
1:B:422:ILE:HA	1:B:425:ILE:HD12	1.99	0.45
1:B:453:TYR:OH	1:B:483:HIS:ND1	2.43	0.45
1:B:569:LEU:O	1:B:573:ILE:HG13	2.17	0.45
1:B:725:VAL:HG22	1:B:739:PHE:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:O	1:A:407:CYS:HB2	2.17	0.44
1:B:455:ARG:NE	1:B:539:GLU:OE1	2.47	0.44
1:A:489:CYS:HB3	1:A:535:PHE:CE2	2.52	0.44
1:B:404:PHE:CD1	1:B:404:PHE:N	2.82	0.44
1:A:709:TYR:CD1	1:A:720:LYS:HA	2.53	0.44
1:B:491:LEU:HD12	1:B:517:ILE:HD11	2.00	0.44
1:B:684:PHE:CD2	1:B:684:PHE:C	2.95	0.43
1:A:569:LEU:O	1:A:573:ILE:HG13	2.19	0.43
1:B:386:MET:O	1:B:390:ASN:OD1	2.37	0.43
1:B:395:GLN:O	1:B:396:PRO:C	2.62	0.43
1:A:719:LEU:HD13	1:A:719:LEU:HA	1.89	0.42
1:B:556:ARG:HH11	1:B:556:ARG:HG3	1.83	0.42
1:A:530:LYS:HB2	1:A:606:TYR:CZ	2.54	0.42
1:B:404:PHE:O	1:B:410:ASN:ND2	2.52	0.42
1:A:558:MET:HE2	1:A:657:LEU:HD22	2.02	0.42
1:A:557:ILE:HA	1:A:561:LEU:HB2	2.00	0.42
1:A:404:PHE:HD2	1:A:412:LYS:HB2	1.84	0.42
1:A:721:PHE:CE2	1:A:752:ILE:HG12	2.55	0.42
1:A:430:PHE:CE2	1:A:442:GLY:N	2.88	0.41
1:A:430:PHE:CD2	1:A:442:GLY:CA	3.04	0.41
1:B:680:ILE:HG12	1:B:711:ILE:HB	2.02	0.41
1:A:673:HIS:HB3	1:A:675:GLU:OE2	2.20	0.41
1:A:721:PHE:O	1:A:725:VAL:HG23	2.20	0.41
1:B:475:LYS:O	1:B:476:LEU:C	2.62	0.41
1:A:669:LEU:HD21	1:A:727:ALA:HB2	2.03	0.41
1:A:415:ILE:HA	1:A:418:ARG:NH1	2.36	0.41
1:A:556:ARG:HA	1:A:559:GLU:HG2	2.02	0.41
1:B:400:LEU:CD2	1:B:461:LEU:HD12	2.51	0.41
1:A:402:SER:O	1:A:405:ASN:N	2.53	0.41
1:A:453:TYR:HE2	1:A:454:TYR:CE1	2.39	0.41
1:A:736:GLN:HA	1:A:739:PHE:CE2	2.56	0.41
1:B:565:SER:O	1:B:566:ASP:HB2	2.21	0.41
1:B:477:LEU:HD23	1:B:477:LEU:HA	1.92	0.41
1:B:736:GLN:HA	1:B:739:PHE:CE2	2.56	0.41
1:B:556:ARG:HG3	1:B:556:ARG:NH1	2.36	0.40
1:B:750:ASP:HB3	1:B:754:VAL:HB	2.04	0.40

All (2) 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)
1:A:544:ARG:NH1	1:A:571:ASP:OD1[1_554]	2.12	0.08
1:A:668:ARG:HH22	1:A:693:GLU:OE1[1_554]	1.53	0.07

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	325/390 (83%)	314 (97%)	11 (3%)	0	100	100
1	B	347/390 (89%)	336 (97%)	10 (3%)	1 (0%)	36	48
All	All	672/780 (86%)	650 (97%)	21 (3%)	1 (0%)	48	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	381	THR

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	312/362 (86%)	283 (91%)	29 (9%)	8	12
1	B	330/362 (91%)	309 (94%)	21 (6%)	16	25
All	All	642/724 (89%)	592 (92%)	50 (8%)	11	18

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	391	SER
1	A	394	ASP
1	A	428	GLU
1	A	450	VAL
1	A	459	SER
1	A	463	SER
1	A	477	LEU
1	A	493	VAL
1	A	610	VAL
1	A	611	ARG
1	A	642	LYS
1	A	648	SER
1	A	671	SER
1	A	673	HIS
1	A	676	LEU
1	A	688	LEU
1	A	711	ILE
1	A	714	VAL
1	A	718	ASP
1	A	719	LEU
1	A	722	LYS
1	A	723	ILE
1	A	726	THR
1	A	729	LYS
1	A	747	GLU
1	A	751	SER
1	A	759	VAL
1	A	763	ARG
1	A	782	ILE
1	B	380	ASN
1	B	381	THR
1	B	382	ILE
1	B	386	MET
1	B	387	MET
1	B	395	GLN
1	B	402	SER
1	B	417	LYS
1	B	463	SER
1	B	470	ILE
1	B	520	VAL
1	B	556	ARG
1	B	610	VAL
1	B	645	THR

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Mol	Chain	Res	Type
1	B	651	TYR
1	B	668	ARG
1	B	688	LEU
1	B	714	VAL
1	B	725	VAL
1	B	736	GLN
1	B	747	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	HIS
1	A	686	HIS
1	A	690	ASN
1	A	733	HIS
1	B	384	GLN
1	B	390	ASN
1	B	472	ASN
1	B	673	HIS
1	B	686	HIS
1	B	689	GLN
1	B	762	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

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%)	0.81	25 (7%) 20 19	65, 101, 139, 162	0
1	B	355/390 (91%)	0.10	11 (3%) 51 51	29, 55, 97, 142	0
All	All	690/780 (88%)	0.44	36 (5%) 33 32	29, 80, 133, 162	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	VAL	4.4
1	B	380	ASN	3.9
1	A	719	LEU	3.8
1	B	438	CYS	3.6
1	B	382	ILE	3.5
1	B	424	TYR	3.3
1	A	437	GLY	3.2
1	B	381	THR	3.2
1	B	610	VAL	3.1
1	A	499	SER	2.9
1	B	439	VAL	2.8
1	A	723	ILE	2.7
1	A	512	LEU	2.6
1	A	758	SER	2.6
1	A	461	LEU	2.6
1	A	705	MET	2.6
1	B	383	GLN	2.5
1	A	392	ALA	2.5
1	A	704	VAL	2.4
1	A	694	LEU	2.4
1	A	777	PRO	2.3
1	B	392	ALA	2.3
1	A	448	LEU	2.3
1	A	406	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	712	CYS	2.2
1	A	784	HIS	2.2
1	B	435	GLY	2.2
1	A	778	THR	2.2
1	A	761	MET	2.1
1	A	769	LEU	2.1
1	A	686	HIS	2.1
1	A	766	THR	2.0
1	A	611	ARG	2.0
1	A	735	VAL	2.0
1	B	600	HIS	2.0
1	A	724	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.