Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 12:07 AM EDT

PDB ID	:	3POM
Title	:	Crystal Structure of the Unliganded Retinoblastoma Protein Pocket Domain
Authors	:	Balog, E.R.M.; Burke, J.R.; Rubin, S.M.
Deposited on	:	2010-11-23
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:

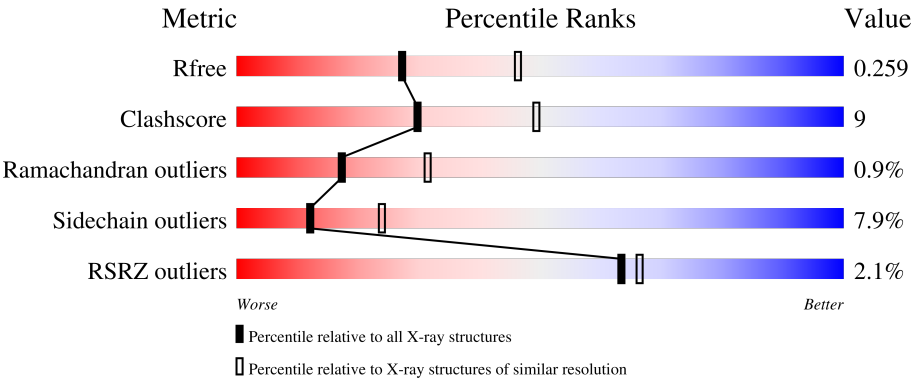
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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))
R_{free}	130704	4661 (2.50-2.50)
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 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 <=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	352	% 72% 22%
1	B	352	3% 67% 24% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5731 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 Retinoblastoma-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2811	1811	471	509	20			
1	B	332	Total	C	N	O	S	0	0	0
			2740	1770	458	492	20			

There are 18 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	578	LEU	-	LINKER	UNP P06400
A	579	VAL	-	LINKER	UNP P06400
A	580	PRO	-	LINKER	UNP P06400
A	640	ARG	-	LINKER	UNP P06400
A	641	GLY	-	LINKER	UNP P06400
A	642	SER	-	LINKER	UNP P06400
B	377	GLY	-	EXPRESSION TAG	UNP P06400
B	378	GLU	-	EXPRESSION TAG	UNP P06400
B	379	PHE	-	EXPRESSION TAG	UNP P06400
B	578	LEU	-	LINKER	UNP P06400
B	579	VAL	-	LINKER	UNP P06400
B	639	PRO	-	LINKER	UNP P06400
B	640	ARG	-	LINKER	UNP P06400
B	641	GLY	-	LINKER	UNP P06400
B	642	SER	-	LINKER	UNP P06400

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		

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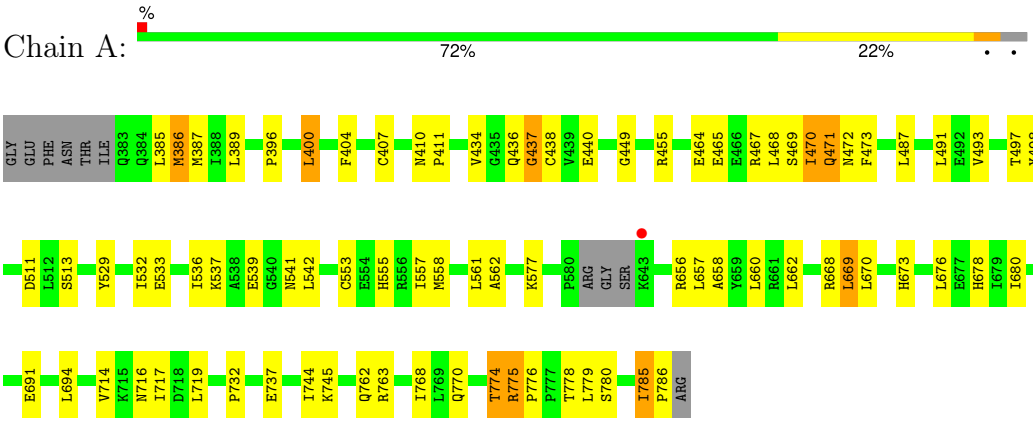
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	72	Total	O	0	0
			72	72		

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.

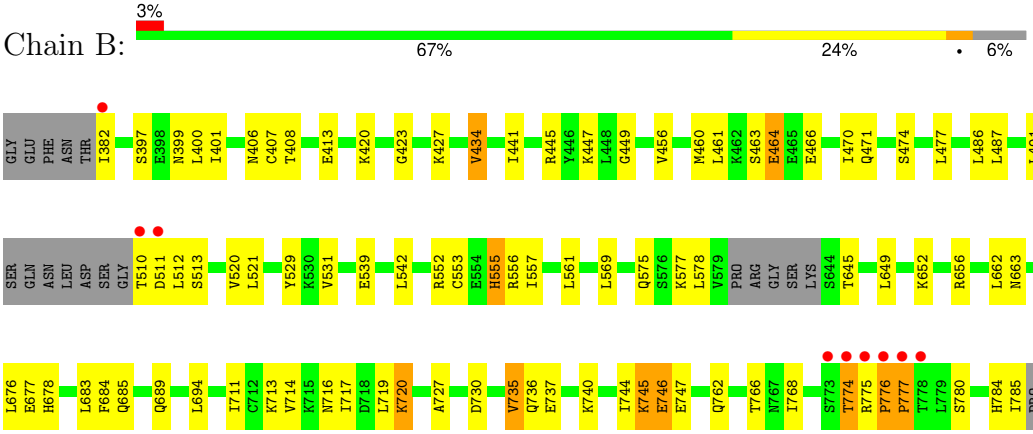
• Molecule 1: Retinoblastoma-associated protein

Chain A:



• Molecule 1: Retinoblastoma-associated protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.28Å 111.16Å 138.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 2.50 45.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.50-2.50) 99.9 (45.53-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.262 0.214 , 0.259	Depositor DCC
R_{free} test set	3324 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5731	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/2868	0.46	0/3866
1	B	0.27	0/2794	0.45	0/3763
All	All	0.27	0/5662	0.45	0/7629

There are no bond length outliers.

There are no bond angle outliers.

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	2811	0	2870	56	0
1	B	2740	0	2804	52	0
2	A	108	0	0	8	0
2	B	72	0	0	7	0
All	All	5731	0	5674	105	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 9.

All (105) 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:785:ILE:HB	1:A:786:PRO:HD3	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ARG:HH12	1:B:730:ASP:HB2	1.48	0.77
1:B:423:GLY:O	1:B:427:LYS:HG2	1.83	0.77
1:B:670:LEU:HD21	1:B:719:LEU:HD22	1.66	0.76
1:A:504:GLN:HA	2:A:130:HOH:O	1.86	0.74
1:A:533:GLU:HG2	1:A:537:LYS:HE3	1.69	0.74
1:B:774:THR:O	1:B:776:PRO:HD3	1.89	0.72
1:B:668:ARG:HH22	1:B:730:ASP:HB3	1.55	0.71
1:A:470:ILE:HD13	1:B:470:ILE:HD12	1.72	0.71
1:A:714:VAL:HG11	1:A:768:ILE:HG22	1.73	0.71
1:A:678:HIS:HE1	1:A:780:SER:O	1.74	0.70
1:B:557:ILE:HA	1:B:561:LEU:HB2	1.77	0.65
1:A:676:LEU:HD11	1:A:717:ILE:HD12	1.79	0.64
1:B:678:HIS:HE1	1:B:780:SER:O	1.80	0.64
1:B:784:HIS:CD2	1:B:785:ILE:HG12	2.34	0.63
1:A:493:VAL:O	1:A:497:THR:HG23	1.99	0.62
1:B:685:GLN:HE22	1:B:689:GLN:NE2	1.97	0.62
1:A:785:ILE:CB	1:A:786:PRO:HD3	2.25	0.61
1:A:557:ILE:HA	1:A:561:LEU:HB2	1.81	0.61
1:A:467:ARG:HH22	1:B:464:GLU:CD	2.04	0.61
1:A:785:ILE:HB	1:A:786:PRO:CD	2.26	0.60
1:A:774:THR:HG23	1:A:775:ARG:HD3	1.84	0.60
1:B:408:THR:H	1:B:474:SER:HB2	1.65	0.60
1:B:652:LYS:CE	1:B:656:ARG:HH22	2.16	0.59
1:A:386:MET:HE3	1:A:389:LEU:HD12	1.86	0.58
1:A:691:GLU:OE1	1:A:763:ARG:NE	2.37	0.58
1:A:438:CYS:HB3	1:A:440:GLU:OE1	2.03	0.58
1:A:449:GLY:HA3	1:A:491:LEU:HD23	1.86	0.57
1:B:512:LEU:HA	2:B:157:HOH:O	2.03	0.57
1:B:775:ARG:O	1:B:777:PRO:HD3	2.05	0.56
1:A:471:GLN:HA	1:A:473:PHE:CE1	2.40	0.56
1:B:539:GLU:HG3	1:B:542:LEU:HG	1.87	0.56
1:A:668:ARG:HG2	1:A:669:LEU:HD13	1.86	0.56
1:B:449:GLY:HA3	1:B:491:LEU:HD23	1.87	0.56
1:B:735:VAL:HG22	1:B:737:GLU:H	1.70	0.56
1:B:397:SER:O	1:B:401:ILE:HG13	2.04	0.56
1:B:407:CYS:SG	1:B:477:LEU:HD12	2.47	0.54
1:B:676:LEU:HD11	1:B:717:ILE:HD12	1.89	0.53
1:A:539:GLU:HG3	1:A:542:LEU:HG	1.89	0.53
1:A:396:PRO:HB3	1:A:400:LEU:HD12	1.90	0.53
1:B:441:ILE:O	1:B:445:ARG:HG2	2.10	0.52
1:A:400:LEU:HD13	1:A:404:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ARG:NH1	1:B:727:ALA:O	2.42	0.52
1:A:471:GLN:HG2	2:A:174:HOH:O	2.09	0.52
1:B:652:LYS:HE3	1:B:656:ARG:HH22	1.74	0.52
1:B:500:ARG:O	1:B:500:ARG:HG2	2.10	0.52
1:A:557:ILE:HG22	1:A:562:ALA:HB2	1.90	0.52
1:B:744:ILE:HG22	1:B:745:LYS:HD3	1.92	0.52
1:A:686:HIS:HE1	2:A:40:HOH:O	1.92	0.51
1:A:670:LEU:HD21	1:A:719:LEU:HD22	1.93	0.51
1:B:555:HIS:HD2	2:B:97:HOH:O	1.92	0.50
1:B:382:ILE:HD11	1:B:500:ARG:NE	2.27	0.50
1:A:511:ASP:HA	2:A:66:HOH:O	2.12	0.49
1:A:468:LEU:O	1:A:470:ILE:HG22	2.11	0.49
1:B:645:THR:O	1:B:649:LEU:HG	2.11	0.49
1:B:447:LYS:HB3	2:B:35:HOH:O	2.12	0.49
1:A:465:GLU:O	1:A:469:SER:HA	2.13	0.49
1:B:737:GLU:HB2	2:B:64:HOH:O	2.13	0.49
1:A:676:LEU:O	1:A:680:ILE:HG13	2.13	0.48
1:A:774:THR:HG21	1:A:775:ARG:NH1	2.28	0.48
1:B:463:SER:O	1:B:466:GLU:HB3	2.13	0.48
1:B:552:ARG:O	1:B:556:ARG:HG3	2.12	0.48
1:B:676:LEU:HD11	1:B:717:ILE:CD1	2.44	0.48
1:A:455:ARG:NH2	1:A:541:ASN:HD22	2.11	0.48
1:B:668:ARG:HH22	1:B:730:ASP:CB	2.25	0.48
1:A:658:ALA:HB1	1:A:684:PHE:CE2	2.49	0.47
1:A:455:ARG:HH22	1:A:541:ASN:HD22	1.62	0.47
1:B:434:VAL:HA	2:B:113:HOH:O	2.15	0.47
1:B:511:ASP:HB3	1:B:513:SER:OG	2.14	0.47
1:B:736:GLN:O	1:B:740:LYS:HB2	2.14	0.47
1:B:663:ASN:HA	1:B:677:GLU:OE1	2.15	0.47
1:B:456:VAL:O	1:B:460:MET:HG3	2.15	0.46
1:A:404:PHE:HB3	1:A:411:PRO:HD2	1.97	0.46
1:B:461:LEU:HD11	1:B:477:LEU:HD21	1.98	0.46
1:B:714:VAL:HG11	1:B:768:ILE:HG22	1.97	0.46
1:A:436:GLN:O	1:A:437:GLY:O	2.34	0.45
1:A:553:CYS:O	1:A:557:ILE:HG12	2.15	0.45
1:A:471:GLN:HA	1:A:473:PHE:HE1	1.82	0.45
1:A:673:HIS:CD2	1:A:717:ILE:HD13	2.52	0.45
1:A:410:ASN:HA	1:A:411:PRO:HD3	1.75	0.45
1:B:745:LYS:HB3	1:B:746:GLU:H	1.46	0.45
1:A:470:ILE:CG1	1:A:471:GLN:N	2.79	0.44
1:A:555:HIS:HD2	2:A:84:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:LYS:HA	1:A:577:LYS:HD2	1.78	0.44
1:A:407:CYS:HA	1:A:472:ASN:OD1	2.18	0.44
1:A:555:HIS:HA	1:A:558:MET:HE2	1.99	0.44
1:B:577:LYS:O	1:B:578:LEU:HD23	2.18	0.44
1:B:678:HIS:CE1	1:B:780:SER:O	2.67	0.43
1:B:520:VAL:HG12	1:B:521:LEU:HD12	2.00	0.43
1:A:770:GLN:O	1:A:776:PRO:HA	2.19	0.43
1:B:510:THR:HB	2:B:94:HOH:O	2.18	0.43
1:A:470:ILE:CD1	1:B:470:ILE:HD12	2.43	0.43
1:A:737:GLU:HB2	2:A:45:HOH:O	2.18	0.43
1:B:711:ILE:HD13	1:B:711:ILE:HA	1.88	0.42
1:A:498:TYR:C	1:A:500:ARG:H	2.22	0.42
1:A:449:GLY:HA3	1:A:491:LEU:CD2	2.49	0.42
1:B:720:LYS:HG3	2:B:102:HOH:O	2.19	0.42
1:B:553:CYS:O	1:B:557:ILE:HG13	2.19	0.42
1:A:500:ARG:HB3	2:A:177:HOH:O	2.19	0.41
1:A:744:ILE:HG22	1:A:745:LYS:HD3	2.02	0.41
1:B:735:VAL:HG22	1:B:737:GLU:N	2.36	0.41
1:A:656:ARG:O	1:A:660:LEU:HB2	2.20	0.41
1:A:558:MET:HE3	1:A:657:LEU:HD22	2.03	0.41
1:A:555:HIS:CD2	2:A:84:HOH:O	2.74	0.41
1:A:532:ILE:O	1:A:536:ILE:HG12	2.21	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	338/352 (96%)	319 (94%)	16 (5%)	3 (1%)	17	31
1	B	326/352 (93%)	303 (93%)	20 (6%)	3 (1%)	17	31
All	All	664/704 (94%)	622 (94%)	36 (5%)	6 (1%)	17	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	GLY
1	A	785	ILE
1	B	777	PRO
1	B	746	GLU
1	A	732	PRO
1	B	776	PRO

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	321/329 (98%)	300 (94%)	21 (6%)	17 33
1	B	312/329 (95%)	283 (91%)	29 (9%)	9 17
All	All	633/658 (96%)	583 (92%)	50 (8%)	12 24

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

Mol	Chain	Res	Type
1	A	385	LEU
1	A	386	MET
1	A	387	MET
1	A	400	LEU
1	A	434	VAL
1	A	464	GLU
1	A	470	ILE
1	A	471	GLN
1	A	487	LEU
1	A	513	SER
1	A	529	TYR
1	A	662	LEU
1	A	669	LEU
1	A	683	LEU
1	A	694	LEU
1	A	716	ASN
1	A	762	GLN

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Mol	Chain	Res	Type
1	A	774	THR
1	A	775	ARG
1	A	778	THR
1	A	779	LEU
1	B	399	ASN
1	B	400	LEU
1	B	406	ASN
1	B	413	GLU
1	B	420	LYS
1	B	434	VAL
1	B	464	GLU
1	B	471	GLN
1	B	486	LEU
1	B	487	LEU
1	B	529	TYR
1	B	531	VAL
1	B	555	HIS
1	B	569	LEU
1	B	575	GLN
1	B	662	LEU
1	B	669	LEU
1	B	683	LEU
1	B	684	PHE
1	B	694	LEU
1	B	713	LYS
1	B	716	ASN
1	B	720	LYS
1	B	735	VAL
1	B	745	LYS
1	B	747	GLU
1	B	762	GLN
1	B	766	THR
1	B	774	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	406	ASN
1	A	471	GLN
1	A	541	ASN
1	A	678	HIS

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Mol	Chain	Res	Type
1	A	686	HIS
1	A	689	GLN
1	A	690	ASN
1	A	716	ASN
1	A	736	GLN
1	A	767	ASN
1	A	770	GLN
1	B	383	GLN
1	B	406	ASN
1	B	471	GLN
1	B	541	ASN
1	B	555	HIS
1	B	678	HIS
1	B	689	GLN
1	B	690	ASN
1	B	716	ASN
1	B	736	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	342/352 (97%)	0.02	3 (0%) 84 86	0, 10, 35, 61	0
1	B	332/352 (94%)	-0.02	11 (3%) 46 50	3, 15, 44, 88	0
All	All	674/704 (95%)	-0.00	14 (2%) 63 66	0, 13, 41, 88	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	778	THR	6.0
1	B	501	SER	5.2
1	B	777	PRO	5.1
1	B	774	THR	4.7
1	B	382	ILE	4.2
1	B	776	PRO	3.5
1	B	510	THR	3.3
1	B	511	ASP	3.0
1	B	775	ARG	3.0
1	B	500	ARG	2.5
1	A	500	ARG	2.4
1	A	643	LYS	2.3
1	A	499	SER	2.2
1	B	773	SER	2.1

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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.