Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 04:47 PM EST

PDB ID	:	1GUX
Title	:	RB POCKET BOUND TO E7 LXCXE MOTIF
Authors	:	Lee, J.O.; Russo, A.A.; Pavletich, N.P.
Deposited on	:	1997-11-15
Resolution	:	1.85 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 (i) 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 (i)) were used in the production of this report:

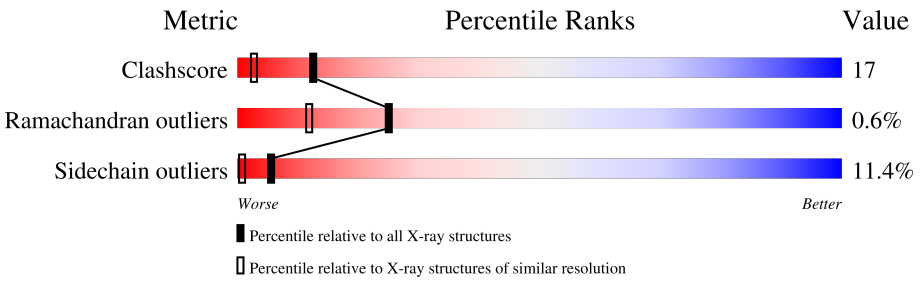
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.85 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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	52% 25% • 19%
2	B	152	55% 32% 6% 7%
3	E	9	78% 11% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3097 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 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1438	927	239	260	12	0	0	0

- Molecule 2 is a protein called RETINOBLASTOMA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1190	775	199	208	8	0	0	0

- Molecule 3 is a protein called ONCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	9	81	51	11	18	1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	228	228	228	0	0
4	B	151	151	151	0	0
4	E	9	9	9	0	0

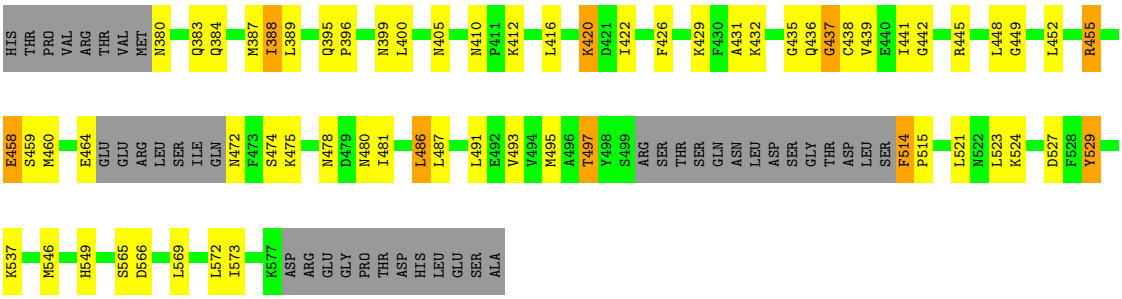
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

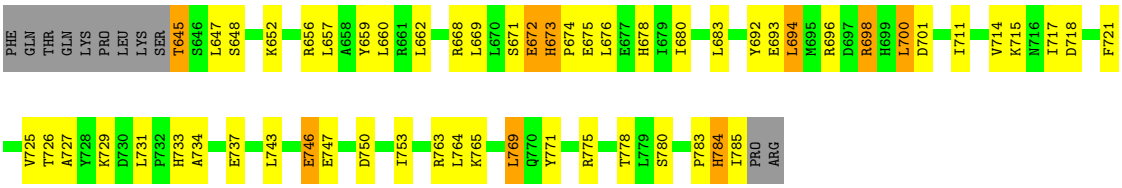
• Molecule 1: RETINOBLASTOMA PROTEIN

Chain A: 52% 25% • 19%



• Molecule 2: RETINOBLASTOMA PROTEIN

Chain B: 55% 32% 6% 7%



• Molecule 3: ONCOPROTEIN

Chain E: 78% 11% 11%

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.50Å 76.80Å 64.00Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	7.00 – 1.85	Depositor
% Data completeness (in resolution range)	93.0 (7.00-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.218 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3097	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

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	0.63	0/1463	0.72	2/1963 (0.1%)
2	B	0.62	0/1218	0.81	3/1647 (0.2%)
3	E	0.62	0/82	1.09	0/109
All	All	0.62	0/2763	0.78	5/3719 (0.1%)

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
2	B	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	698	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	514	PHE	C-N-CD	6.28	141.59	128.40
2	B	700	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	698	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	455	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	529	TYR	Sidechain
2	B	659	TYR	Sidechain
2	B	771	TYR	Sidechain

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	1438	0	1465	53	0
2	B	1190	0	1221	40	0
3	E	81	0	71	2	0
4	A	228	0	0	6	0
4	B	151	0	0	7	0
4	E	9	0	0	1	0
All	All	3097	0	2757	92	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 17.

All (92) 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:420:LYS:HE2	1:A:420:LYS:HA	1.48	0.96
2:B:673:HIS:N	2:B:674:PRO:HD3	1.97	0.79
1:A:493:VAL:HG22	1:A:546:MET:HE2	1.66	0.78
1:A:437:GLY:HA2	4:A:634:HOH:O	1.83	0.78
2:B:785:ILE:HG21	4:B:321:HOH:O	1.84	0.75
1:A:439:VAL:HG12	1:A:442:GLY:H	1.53	0.74
1:A:420:LYS:HA	1:A:420:LYS:CE	2.19	0.73
2:B:678:HIS:HE1	2:B:780:SER:O	1.71	0.72
1:A:395:GLN:HB3	1:A:396:PRO:HD2	1.72	0.71
1:A:436:GLN:HE22	1:A:439:VAL:HA	1.55	0.71
1:A:493:VAL:O	1:A:497:THR:HG23	1.92	0.70
1:A:436:GLN:NE2	1:A:439:VAL:HA	2.08	0.68
1:A:537:LYS:HG3	4:A:708:HOH:O	1.92	0.68
1:A:380:ASN:HB3	1:A:383:GLN:OE1	1.93	0.68
2:B:673:HIS:H	2:B:674:PRO:HD3	1.61	0.65
2:B:784:HIS:O	2:B:785:ILE:HG22	1.96	0.64
1:A:472:ASN:HD22	1:A:475:LYS:HB3	1.63	0.64
2:B:648:SER:O	2:B:652:LYS:HG3	2.01	0.60
2:B:694:LEU:HD13	2:B:763:ARG:NH1	2.16	0.60
2:B:765:LYS:HG2	2:B:769:LEU:HD22	1.85	0.59
1:A:431:ALA:HB2	1:A:438:CYS:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:746:GLU:O	2:B:747:GLU:HG3	2.05	0.57
1:A:514:PHE:O	1:A:514:PHE:CD2	2.58	0.57
1:A:474:SER:O	1:A:478:ASN:HB2	2.07	0.55
1:A:436:GLN:HB2	4:A:683:HOH:O	2.06	0.55
1:A:439:VAL:HG13	1:A:441:ILE:H	1.73	0.54
1:A:514:PHE:N	1:A:515:PRO:CD	2.71	0.54
1:A:426:PHE:HZ	1:A:495:MET:CE	2.21	0.53
2:B:672:GLU:H	2:B:672:GLU:CD	2.11	0.52
1:A:572:LEU:HG	2:B:647:LEU:HD22	1.92	0.52
1:A:395:GLN:NE2	1:A:416:LEU:HD22	2.25	0.52
1:A:405:ASN:HA	1:A:410:ASN:ND2	2.26	0.51
2:B:726:THR:HA	2:B:729:LYS:HE2	1.92	0.51
1:A:431:ALA:O	1:A:435:GLY:N	2.44	0.51
1:A:436:GLN:CD	1:A:439:VAL:HG22	2.31	0.51
2:B:737:GLU:HB2	4:B:131:HOH:O	2.10	0.51
1:A:400:LEU:HG	1:A:458:GLU:HG2	1.92	0.51
1:A:429:LYS:CE	1:A:432:LYS:HZ2	2.24	0.50
1:A:426:PHE:HZ	1:A:495:MET:HE1	1.77	0.50
2:B:763:ARG:HD2	4:B:78:HOH:O	2.10	0.50
1:A:565:SER:O	1:A:566:ASP:HB2	2.13	0.48
1:A:439:VAL:CG1	1:A:441:ILE:HB	2.43	0.48
1:A:399:ASN:HB3	4:A:664:HOH:O	2.13	0.48
3:E:9:ASN:ND2	4:E:146:HOH:O	2.46	0.48
1:A:405:ASN:HA	1:A:410:ASN:HD22	1.79	0.47
1:A:439:VAL:CG1	1:A:441:ILE:H	2.27	0.47
1:A:573:ILE:HG21	2:B:692:TYR:CE2	2.49	0.47
2:B:673:HIS:N	2:B:674:PRO:CD	2.70	0.47
2:B:668:ARG:NH1	2:B:727:ALA:O	2.48	0.47
2:B:701:ASP:OD2	2:B:733:HIS:HE1	1.98	0.47
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.82	0.47
1:A:395:GLN:HE22	1:A:416:LEU:HD22	1.79	0.47
1:A:524:LYS:HB2	1:A:527:ASP:OD2	2.14	0.47
1:A:384:GLN:O	1:A:388:ILE:HG23	2.16	0.46
1:A:514:PHE:HA	4:A:750:HOH:O	2.14	0.46
1:A:445:ARG:HD2	1:A:495:MET:CE	2.46	0.46
1:A:481:ILE:HD12	1:A:527:ASP:HB3	1.98	0.46
2:B:675:GLU:HB3	4:B:325:HOH:O	2.15	0.46
1:A:431:ALA:CB	1:A:438:CYS:HA	2.46	0.46
2:B:656:ARG:HD3	2:B:784:HIS:O	2.16	0.46
2:B:784:HIS:O	2:B:784:HIS:ND1	2.50	0.45
2:B:645:THR:N	4:B:166:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:LEU:HD11	2:B:717:ILE:HG13	1.99	0.45
1:A:460:MET:O	1:A:464:GLU:HG2	2.16	0.44
2:B:678:HIS:CE1	2:B:780:SER:O	2.61	0.44
1:A:388:ILE:HG13	1:A:389:LEU:N	2.32	0.44
2:B:783:PRO:HA	4:B:185:HOH:O	2.17	0.44
2:B:645:THR:HA	2:B:648:SER:OG	2.16	0.44
1:A:448:LEU:HD12	4:A:786:HOH:O	2.17	0.44
2:B:680:ILE:HA	2:B:711:ILE:HG13	2.00	0.43
2:B:656:ARG:HD3	2:B:785:ILE:HG22	1.99	0.43
2:B:676:LEU:CD2	2:B:715:LYS:HG3	2.49	0.43
2:B:731:LEU:HB2	2:B:734:ALA:HB2	2.01	0.43
2:B:693:GLU:CD	2:B:696:ARG:HH12	2.22	0.43
1:A:439:VAL:HG11	1:A:441:ILE:HB	2.01	0.43
2:B:733:HIS:H	2:B:733:HIS:CD2	2.35	0.43
1:A:422:ILE:HG23	1:A:521:LEU:HD22	2.01	0.42
1:A:546:MET:HE3	1:A:549:HIS:HD2	1.84	0.42
2:B:753:ILE:HD12	3:E:8:LEU:HG	2.00	0.42
2:B:729:LYS:HB2	2:B:729:LYS:HE3	1.77	0.42
1:A:436:GLN:NE2	1:A:439:VAL:HG22	2.34	0.41
2:B:660:LEU:HD23	2:B:660:LEU:HA	1.87	0.41
2:B:775:ARG:HE	2:B:775:ARG:HB3	1.62	0.41
2:B:769:LEU:HD12	2:B:769:LEU:HA	1.79	0.41
1:A:431:ALA:HB1	1:A:438:CYS:H	1.84	0.41
1:A:546:MET:CE	1:A:549:HIS:HD2	2.33	0.41
2:B:672:GLU:O	2:B:673:HIS:CB	2.68	0.41
2:B:698:ARG:NH2	4:B:49:HOH:O	2.46	0.41
1:A:449:GLY:HA3	1:A:491:LEU:HD23	2.03	0.40
1:A:412:LYS:O	1:A:416:LEU:HG	2.21	0.40
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.95	0.40
2:B:672:GLU:HG2	2:B:673:HIS:CE1	2.57	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	171/218 (78%)	161 (94%)	9 (5%)	1 (1%)	25	12
2	B	139/152 (91%)	132 (95%)	6 (4%)	1 (1%)	22	9
3	E	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	317/379 (84%)	298 (94%)	17 (5%)	2 (1%)	25	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	GLY
2	B	673	HIS

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	162/200 (81%)	148 (91%)	14 (9%)	10	2
2	B	136/147 (92%)	116 (85%)	20 (15%)	3	0
3	E	9/9 (100%)	8 (89%)	1 (11%)	6	1
All	All	307/356 (86%)	272 (89%)	35 (11%)	5	1

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	MET
1	A	388	ILE
1	A	420	LYS
1	A	452	LEU
1	A	455	ARG
1	A	458	GLU
1	A	459	SER
1	A	480	ASN

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Mol	Chain	Res	Type
1	A	486	LEU
1	A	487	LEU
1	A	497	THR
1	A	523	LEU
1	A	529	TYR
1	A	569	LEU
2	B	645	THR
2	B	657	LEU
2	B	662	LEU
2	B	669	LEU
2	B	671	SER
2	B	672	GLU
2	B	683	LEU
2	B	694	LEU
2	B	700	LEU
2	B	714	VAL
2	B	718	ASP
2	B	721	PHE
2	B	725	VAL
2	B	743	LEU
2	B	746	GLU
2	B	750	ASP
2	B	764	LEU
2	B	769	LEU
2	B	778	THR
2	B	784	HIS
3	E	9	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	405	ASN
1	A	436	GLN
1	A	472	ASN
2	B	678	HIS
2	B	685	GLN
2	B	689	GLN
2	B	733	HIS

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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.