



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:46 PM UTC

PDB ID : 1PBW / pdb_00001pbw
Title : STRUCTURE OF BCR-HOMOLOGY (BH) DOMAIN
Authors : Musacchio, A.; Cantley, L.C.; Harrison, S.C.
Deposited on : 1996-10-17
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

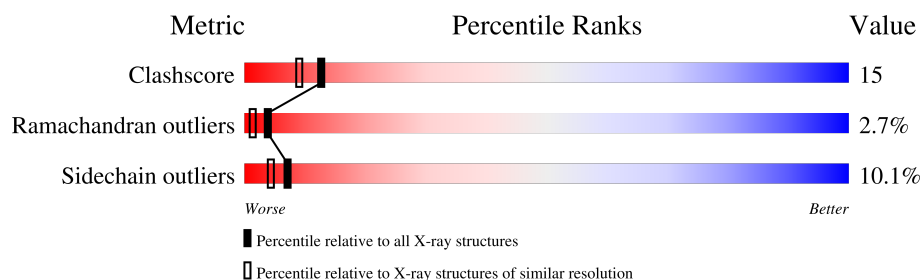
1 Overall quality at a glance

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	216	
1	B	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3284 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 PHOSPHATIDYLINOSITOL 3-KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1469	953	234	277	5			
1	B	195	Total	C	N	O	S	0	0	0
			1548	1003	250	290	5			

- Molecule 2 is water.

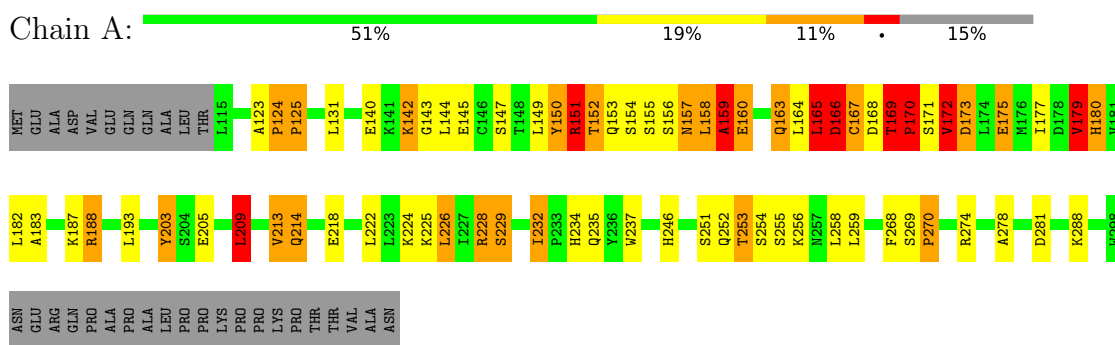
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		
2	B	143	Total	O	0	0
			143	143		

3 Residue-property plots

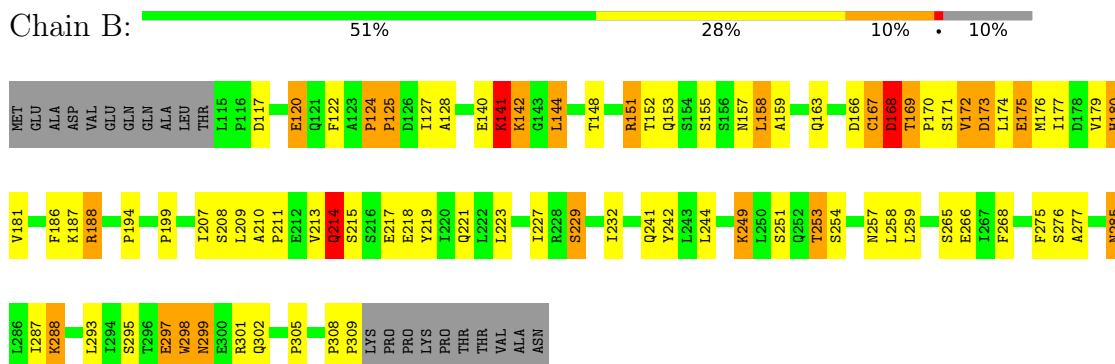
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PHOSPHATIDYLINOSITOL 3-KINASE



• Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.05Å 90.51Å 69.28Å 90.00° 97.19° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3284	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	0.99	4/1501 (0.3%)	3.03	81/2044 (4.0%)
1	B	0.89	6/1584 (0.4%)	2.39	70/2161 (3.2%)
All	All	0.94	10/3085 (0.3%)	2.72	151/4205 (3.6%)

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	2
1	B	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	PRO	N-CD	11.56	1.64	1.47
1	A	170	PRO	N-CD	9.67	1.61	1.47
1	B	308	PRO	C-O	-6.25	1.19	1.25
1	B	124	PRO	CA-C	5.77	1.57	1.52
1	A	125	PRO	N-CA	-5.76	1.40	1.47
1	B	125	PRO	N-CD	5.74	1.55	1.47
1	B	125	PRO	N-CA	-5.56	1.40	1.47
1	B	309	PRO	N-CD	5.44	1.55	1.47
1	B	151	ARG	NE-CZ	-5.10	1.27	1.33
1	A	124	PRO	CA-C	5.03	1.56	1.52

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	THR	CA-C-N	40.99	171.08	119.84
1	A	169	THR	C-N-CA	40.99	171.08	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	PRO	CA-C-N	34.09	162.45	119.84
1	A	124	PRO	C-N-CA	34.09	162.45	119.84
1	B	124	PRO	CA-C-N	27.01	153.60	119.84
1	B	124	PRO	C-N-CA	27.01	153.60	119.84
1	A	124	PRO	O-C-N	24.38	150.23	121.46
1	A	170	PRO	N-CA-CB	23.31	127.72	103.25
1	A	125	PRO	N-CA-CB	23.23	127.65	103.25
1	A	169	THR	O-C-N	22.19	146.84	121.32
1	A	125	PRO	CA-N-CD	-20.89	82.75	112.00
1	A	170	PRO	CA-N-CD	-20.28	83.61	112.00
1	B	151	ARG	CD-NE-CZ	18.98	150.97	124.40
1	B	125	PRO	CA-N-CD	-17.00	88.19	112.00
1	A	274	ARG	CD-NE-CZ	16.66	147.72	124.40
1	A	188	ARG	CD-NE-CZ	16.65	147.71	124.40
1	B	125	PRO	N-CA-CB	15.25	119.27	103.25
1	B	124	PRO	O-C-N	12.89	136.67	121.46
1	A	165	LEU	CA-C-N	12.65	145.71	121.54
1	A	165	LEU	C-N-CA	12.65	145.71	121.54
1	B	163	GLN	CB-CG-CD	11.64	132.38	112.60
1	B	241	GLN	OE1-CD-NE2	11.21	133.81	122.60
1	B	125	PRO	N-CD-CG	11.16	119.94	103.20
1	A	179	VAL	N-CA-CB	10.68	122.36	110.51
1	A	179	VAL	CB-CA-C	-10.49	98.45	111.88
1	A	153	GLN	CB-CG-CD	10.31	130.12	112.60
1	A	166	ASP	CA-CB-CG	10.26	122.86	112.60
1	B	180	HIS	CA-CB-CG	-9.83	103.97	113.80
1	A	124	PRO	CA-C-O	-9.35	107.00	120.56
1	A	158	LEU	CA-C-O	-9.29	111.70	121.55
1	A	125	PRO	N-CD-CG	9.22	117.04	103.20
1	A	124	PRO	C-N-CD	-9.04	87.94	125.00
1	B	124	PRO	CB-CA-C	9.03	121.93	110.92
1	B	308	PRO	CA-C-O	8.95	127.34	120.90
1	B	120	GLU	CB-CG-CD	-8.70	97.82	112.60
1	B	168	ASP	CA-CB-CG	8.68	121.28	112.60
1	B	299	ASN	CA-CB-CG	8.44	121.04	112.60
1	B	268	PHE	N-CA-C	8.44	123.96	112.90
1	B	285	ASN	OD1-CG-ND2	8.21	130.81	122.60
1	A	213	VAL	CA-C-O	8.10	129.86	120.71
1	A	203	TYR	CA-C-O	8.09	129.13	120.55
1	B	275	PHE	CA-CB-CG	8.05	121.85	113.80
1	B	213	VAL	CA-C-O	8.05	130.03	120.85
1	A	169	THR	CA-C-O	-7.90	109.34	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	CD-NE-CZ	7.67	135.14	124.40
1	B	151	ARG	CG-CD-NE	-7.63	95.20	112.00
1	A	123	ALA	O-C-N	7.60	127.17	121.85
1	B	241	GLN	CB-CG-CD	-7.52	99.82	112.60
1	A	169	THR	C-N-CD	-7.51	94.23	125.00
1	B	124	PRO	C-N-CD	-7.44	94.50	125.00
1	A	228	ARG	CG-CD-NE	7.39	128.25	112.00
1	B	141	LYS	CA-CB-CG	7.34	128.79	114.10
1	B	308	PRO	O-C-N	7.34	124.69	121.31
1	A	170	PRO	N-CD-CG	7.22	114.03	103.20
1	B	298	TRP	CA-CB-CG	6.95	126.80	113.60
1	B	142	LYS	N-CA-C	6.86	122.75	113.97
1	B	301	ARG	CA-C-O	6.72	129.53	121.66
1	A	225	LYS	CA-C-O	6.72	127.62	120.70
1	B	173	ASP	N-CA-CB	6.71	121.84	110.49
1	B	297	GLU	N-CA-C	-6.69	104.59	112.89
1	B	188	ARG	NE-CZ-NH1	6.54	128.04	121.50
1	B	122	PHE	O-C-N	6.51	130.10	123.26
1	B	153	GLN	OE1-CD-NE2	6.50	129.10	122.60
1	B	266	GLU	CA-C-O	6.48	127.43	120.10
1	B	186	PHE	CA-CB-CG	6.38	120.19	113.80
1	B	265	SER	O-C-N	-6.36	115.38	122.12
1	B	285	ASN	CA-CB-CG	-6.33	106.27	112.60
1	B	163	GLN	O-C-N	-6.26	115.48	122.12
1	A	173	ASP	N-CA-C	-6.19	99.78	109.25
1	A	160	GLU	N-CA-C	-6.18	104.46	111.07
1	A	253	THR	CA-C-N	6.17	129.16	120.28
1	A	253	THR	C-N-CA	6.17	129.16	120.28
1	A	170	PRO	CA-CB-CG	-6.16	92.79	104.50
1	B	229	SER	N-CA-CB	-6.14	101.20	110.05
1	B	213	VAL	N-CA-CB	6.13	117.21	110.53
1	B	242	TYR	N-CA-C	-6.12	104.53	111.14
1	A	152	THR	N-CA-CB	6.09	121.48	111.62
1	B	214	GLN	CB-CG-CD	6.04	122.86	112.60
1	B	305	PRO	O-C-N	-5.95	115.34	122.89
1	A	153	GLN	N-CA-CB	5.94	120.36	110.85
1	A	151	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	142	LYS	N-CA-C	5.91	120.77	113.50
1	B	214	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	B	181	VAL	N-CA-C	-5.85	104.81	110.72
1	A	150	TYR	CA-C-O	5.85	124.85	119.00
1	A	157	ASN	CA-C-O	-5.80	114.83	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	PRO	CB-CA-C	5.77	118.56	111.12
1	A	182	LEU	CA-C-N	5.76	128.00	120.28
1	A	182	LEU	C-N-CA	5.76	128.00	120.28
1	A	209	LEU	CA-C-O	5.76	125.71	119.15
1	A	188	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	A	268	PHE	N-CA-C	5.72	120.32	113.23
1	B	213	VAL	CA-C-N	5.71	132.44	121.54
1	B	213	VAL	C-N-CA	5.71	132.44	121.54
1	B	157	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	213	VAL	CA-C-N	5.68	130.33	120.68
1	A	213	VAL	C-N-CA	5.68	130.33	120.68
1	A	152	THR	CA-C-O	-5.67	115.15	121.51
1	A	232	ILE	N-CA-CB	5.65	118.51	111.39
1	A	237	TRP	O-C-N	-5.65	116.25	122.07
1	A	228	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	A	193	LEU	N-CA-C	-5.64	102.94	109.93
1	B	287	ILE	CA-C-O	5.63	126.81	120.95
1	A	214	GLN	N-CA-C	5.62	119.31	112.23
1	A	172	VAL	N-CA-CB	5.61	120.48	111.23
1	A	153	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	166	ASP	CA-C-O	5.60	128.51	120.51
1	A	156	SER	N-CA-C	5.59	117.75	110.43
1	B	276	SER	N-CA-CB	-5.57	102.48	110.44
1	A	170	PRO	N-CA-C	-5.54	101.07	112.47
1	B	277	ALA	N-CA-C	-5.53	106.03	112.89
1	B	120	GLU	CB-CA-C	-5.50	100.31	109.55
1	A	154	SER	N-CA-C	-5.49	101.36	109.86
1	A	288	LYS	O-C-N	-5.48	116.31	122.12
1	B	167	CYS	CB-CA-C	5.47	118.76	109.84
1	A	281	ASP	N-CA-CB	5.46	118.71	110.30
1	B	244	LEU	CA-C-N	5.44	128.02	120.29
1	B	244	LEU	C-N-CA	5.44	128.02	120.29
1	A	246	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	235	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	153	GLN	N-CA-C	-5.43	101.32	109.95
1	B	221	GLN	CB-CG-CD	5.40	121.78	112.60
1	B	229	SER	CA-C-N	5.38	125.05	119.56
1	B	229	SER	C-N-CA	5.38	125.05	119.56
1	A	253	THR	CA-C-O	5.37	127.04	120.55
1	B	127	ILE	CA-C-O	-5.36	113.04	119.36
1	B	187	LYS	N-CA-CB	5.35	117.98	110.12
1	A	229	SER	CA-C-N	5.35	125.01	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	SER	C-N-CA	5.35	125.01	119.56
1	B	159	ALA	N-CA-C	5.34	117.10	111.28
1	A	159	ALA	N-CA-CB	5.33	119.50	110.49
1	A	142	LYS	N-CA-CB	-5.33	102.69	110.53
1	A	232	ILE	N-CA-C	-5.26	101.73	107.73
1	A	180	HIS	CA-CB-CG	-5.25	108.56	113.80
1	A	274	ARG	CG-CD-NE	-5.23	100.50	112.00
1	B	168	ASP	CA-C-O	5.22	127.98	120.51
1	A	140	GLU	CA-C-N	5.22	127.27	120.28
1	A	140	GLU	C-N-CA	5.22	127.27	120.28
1	A	165	LEU	CA-C-O	5.21	127.97	120.51
1	A	143	GLY	CA-C-O	-5.18	111.56	120.57
1	A	255	SER	N-CA-C	-5.16	104.92	111.11
1	A	270	PRO	O-C-N	-5.13	115.60	122.22
1	B	122	PHE	CA-C-O	-5.08	116.00	121.38
1	B	142	LYS	CB-CA-C	-5.07	100.56	109.07
1	B	309	PRO	N-CA-CB	5.07	108.58	103.00
1	B	128	ALA	CA-C-O	-5.05	115.79	120.13
1	A	252	GLN	CB-CG-CD	-5.04	104.03	112.60
1	B	227	ILE	CA-C-O	-5.04	115.03	120.47
1	A	159	ALA	N-CA-C	-5.03	100.10	110.80
1	B	127	ILE	N-CA-C	5.02	119.95	113.07
1	B	167	CYS	N-CA-C	-5.01	101.80	109.76

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	PRO	Peptide
1	A	169	THR	Peptide
1	B	124	PRO	Mainchain,Peptide

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	1469	0	1506	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1548	0	1584	46	0
2	A	124	0	0	10	1
2	B	143	0	0	13	1
All	All	3284	0	3090	93	1

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 15.

All (93) 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:172:VAL:HG22	1:B:172:VAL:HG21	1.52	0.92
1:A:131:LEU:HD13	1:A:166:ASP:HB2	1.58	0.85
1:B:166:ASP:HB3	2:B:386:HOH:O	1.82	0.79
1:B:210:ALA:HB3	1:B:211:PRO:HD3	1.66	0.76
1:A:163:GLN:HG3	1:A:170:PRO:HG2	1.68	0.74
1:B:144:LEU:HD13	1:B:253:THR:HG21	1.68	0.74
2:A:354:HOH:O	1:B:179:VAL:HG23	1.89	0.72
1:A:232:ILE:O	2:A:338:HOH:O	2.11	0.68
1:B:180:HIS:HB3	2:B:451:HOH:O	1.94	0.67
1:A:155:SER:HB3	2:A:441:HOH:O	1.94	0.67
1:A:151:ARG:HG3	1:A:151:ARG:HH11	1.59	0.66
1:A:251:SER:O	1:A:254:SER:HB2	1.95	0.66
1:B:120:GLU:OE1	2:B:413:HOH:O	2.13	0.66
1:A:234:HIS:HB2	2:A:427:HOH:O	1.95	0.65
1:B:297:GLU:O	2:B:379:HOH:O	2.14	0.65
1:A:142:LYS:HD2	1:A:175:GLU:OE1	1.98	0.63
1:A:158:LEU:O	1:A:159:ALA:CB	2.46	0.63
1:A:145:GLU:HG2	1:A:256:LYS:HD2	1.80	0.62
1:B:299:ASN:ND2	2:B:419:HOH:O	2.32	0.62
1:A:158:LEU:O	1:A:159:ALA:HB3	2.01	0.61
1:A:253:THR:O	1:A:253:THR:HG22	2.02	0.59
1:B:170:PRO:O	1:B:171:SER:HB3	2.03	0.59
1:B:214:GLN:OE1	1:B:218:GLU:HB3	2.02	0.59
1:A:253:THR:HG22	1:A:256:LYS:HB2	1.85	0.58
1:A:224:LYS:O	1:A:228:ARG:HD3	2.03	0.58
1:A:214:GLN:H	1:A:214:GLN:CD	2.08	0.57
1:B:293:LEU:O	1:B:297:GLU:HG2	2.04	0.57
1:B:232:ILE:O	2:B:335:HOH:O	2.17	0.57
1:B:297:GLU:HA	2:B:424:HOH:O	2.05	0.57
1:B:167:CYS:O	1:B:168:ASP:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:H	1:B:214:GLN:CD	2.13	0.56
1:A:151:ARG:NH2	1:A:258:LEU:HB2	2.19	0.56
1:A:222:LEU:HG	1:A:226:LEU:HD22	1.88	0.55
1:B:253:THR:HG23	1:B:257:ASN:ND2	2.21	0.54
1:A:164:LEU:O	1:A:166:ASP:OD1	2.25	0.54
1:A:157:ASN:HB3	2:A:350:HOH:O	2.06	0.54
1:A:214:GLN:HB2	1:A:218:GLU:OE1	2.08	0.54
1:A:151:ARG:HG3	1:A:151:ARG:NH1	2.20	0.53
1:B:140:GLU:OE1	1:B:249:LYS:HE2	2.09	0.53
1:A:183:ALA:O	1:A:187:LYS:HG3	2.09	0.53
1:B:251:SER:HA	1:B:259:LEU:O	2.09	0.52
1:A:167:CYS:SG	1:A:168:ASP:N	2.83	0.51
1:A:164:LEU:O	1:A:166:ASP:N	2.43	0.51
1:B:144:LEU:CD1	1:B:253:THR:HG21	2.38	0.51
1:B:180:HIS:HD2	2:B:322:HOH:O	1.93	0.51
1:B:141:LYS:HE3	1:B:175:GLU:OE2	2.10	0.50
1:B:168:ASP:OD2	1:B:169:THR:HG22	2.12	0.49
1:A:167:CYS:HB3	2:A:420:HOH:O	2.12	0.49
1:B:171:SER:HA	2:B:440:HOH:O	2.12	0.49
1:A:160:GLU:HG3	2:A:350:HOH:O	2.12	0.49
1:A:205:GLU:O	1:A:209:LEU:HB2	2.13	0.49
1:B:254:SER:O	1:B:258:LEU:HA	2.13	0.49
1:B:298:TRP:CZ3	1:B:302:GLN:HG3	2.48	0.49
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.28	0.49
1:B:158:LEU:CD1	1:B:188:ARG:HD3	2.43	0.48
1:A:149:LEU:O	1:A:150:TYR:HB2	2.13	0.48
1:A:163:GLN:HG3	1:A:170:PRO:CG	2.42	0.48
1:A:224:LYS:HB3	1:A:228:ARG:HH11	1.77	0.48
1:A:172:VAL:CG2	1:A:177:ILE:HD11	2.44	0.47
1:A:131:LEU:HD21	1:A:165:LEU:HD12	1.96	0.47
1:A:151:ARG:HH21	1:A:258:LEU:HB2	1.80	0.47
1:A:222:LEU:O	1:A:226:LEU:HB2	2.16	0.46
1:B:158:LEU:HD13	1:B:188:ARG:HD3	1.97	0.46
1:B:180:HIS:CB	2:B:451:HOH:O	2.60	0.46
1:A:142:LYS:HB3	1:A:179:VAL:HG13	1.99	0.45
1:B:141:LYS:HE3	1:B:175:GLU:HG2	1.99	0.45
1:B:214:GLN:HG2	1:B:215:SER:H	1.80	0.45
1:A:224:LYS:HB3	1:A:228:ARG:NH1	2.31	0.45
1:B:285:ASN:HB2	2:B:448:HOH:O	2.16	0.44
1:B:117:ASP:HA	1:B:194:PRO:HG2	1.99	0.44
1:B:142:LYS:HE2	1:B:177:ILE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:N	1:A:270:PRO:CD	2.81	0.44
1:A:251:SER:HA	1:A:259:LEU:O	2.18	0.43
1:A:180:HIS:HD2	2:A:320:HOH:O	2.01	0.43
1:B:208:SER:O	1:B:211:PRO:HD2	2.18	0.43
1:A:203:TYR:OH	1:A:278:ALA:HB2	2.18	0.42
1:A:213:VAL:O	2:A:443:HOH:O	2.22	0.42
1:B:288:LYS:HA	1:B:288:LYS:HD3	1.84	0.42
1:A:160:GLU:HB3	1:B:176:MET:HE3	2.01	0.42
1:B:148:THR:HB	1:B:152:THR:HG23	2.00	0.42
1:A:147:SER:HB2	1:A:258:LEU:HG	2.01	0.42
1:A:169:THR:HG22	1:A:170:PRO:O	2.20	0.42
1:B:144:LEU:HB2	2:B:360:HOH:O	2.19	0.41
1:B:167:CYS:O	1:B:168:ASP:CB	2.67	0.41
1:B:214:GLN:HG2	1:B:218:GLU:HB2	2.01	0.41
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.91	0.41
1:A:144:LEU:HD13	2:A:414:HOH:O	2.19	0.41
1:B:254:SER:HA	1:B:257:ASN:OD1	2.21	0.41
1:B:167:CYS:HA	2:B:458:HOH:O	2.21	0.41
1:A:145:GLU:HG2	1:A:256:LYS:CD	2.48	0.40
1:B:298:TRP:HZ3	1:B:302:GLN:HG3	1.86	0.40
1:A:173:ASP:OD1	1:A:175:GLU:HB2	2.21	0.40
1:A:172:VAL:HB	1:A:173:ASP:H	1.58	0.40

All (1) 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:403:HOH:O	2:B:418:HOH:O[2_555]	2.00	0.20

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	182/216 (84%)	169 (93%)	7 (4%)	6 (3%)	3	1
1	B	193/216 (89%)	182 (94%)	7 (4%)	4 (2%)	5	2
All	All	375/432 (87%)	351 (94%)	14 (4%)	10 (3%)	4	1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	159	ALA
1	A	170	PRO
1	A	171	SER
1	B	125	PRO
1	B	168	ASP
1	B	173	ASP
1	A	166	ASP
1	A	169	THR
1	B	214	GLN

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	158/197 (80%)	145 (92%)	13 (8%)	10	7
1	B	178/197 (90%)	157 (88%)	21 (12%)	5	3
All	All	336/394 (85%)	302 (90%)	34 (10%)	7	4

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ARG
1	A	152	THR
1	A	163	GLN
1	A	165	LEU
1	A	167	CYS
1	A	169	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	VAL
1	A	175	GLU
1	A	179	VAL
1	A	188	ARG
1	A	209	LEU
1	A	226	LEU
1	A	229	SER
1	B	141	LYS
1	B	144	LEU
1	B	151	ARG
1	B	155	SER
1	B	158	LEU
1	B	168	ASP
1	B	169	THR
1	B	172	VAL
1	B	174	LEU
1	B	175	GLU
1	B	207	ILE
1	B	209	LEU
1	B	214	GLN
1	B	217	GLU
1	B	219	TYR
1	B	223	LEU
1	B	229	SER
1	B	249	LYS
1	B	253	THR
1	B	288	LYS
1	B	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	180	HIS
1	B	180	HIS

5.3.3 RNA ⓘ

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.