Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BNI
Title	:	BARNASE WILDTYPE STRUCTURE AT PH 6.0
Authors	:	Cameron, A.; Henrick, K.; Fersht, A.R.; Dodson, G.; Buckle, A.M.
Deposited on	:	1995-05-17
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

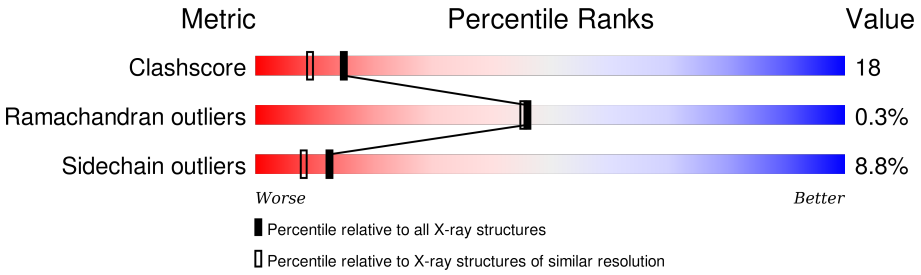
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	110	47% 34% 16%
1	B	110	45% 34% 17%
1	C	110	55% 35% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2763 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 BARNASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	6	0	0
			851	541	147	163			
1	B	108	Total	C	N	O	1	0	0
			844	537	144	163			
1	C	108	Total	C	N	O	0	0	0
			852	541	145	166			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	63	Total	O	0	0
			63	63		
2	B	72	Total	O	0	0
			72	72		
2	C	81	Total	O	0	0
			81	81		

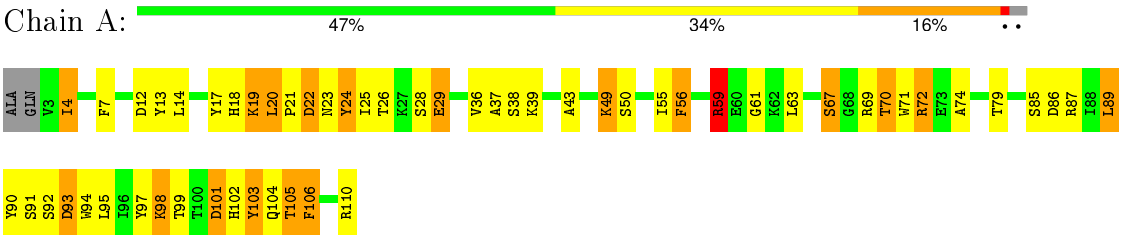
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

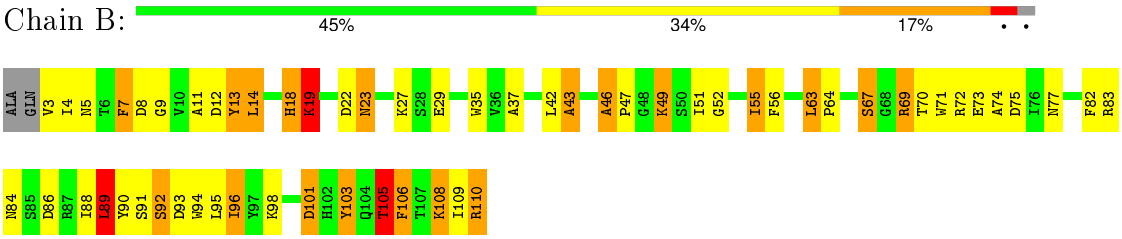
- Molecule 1: BARNASE

Chain A:



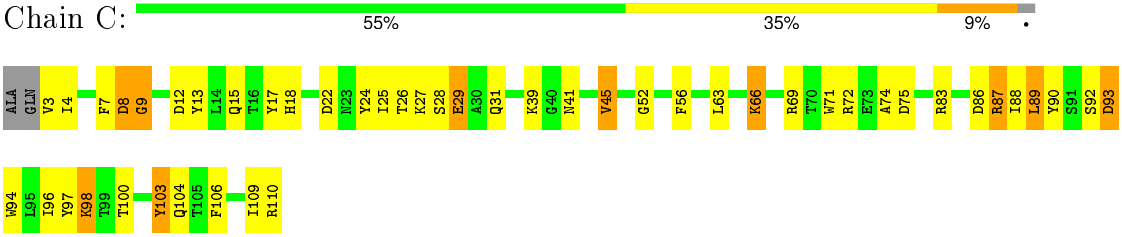
- Molecule 1: BARNASE

Chain B:



- Molecule 1: BARNASE

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	59.39Å 59.39Å 82.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	80.0 (10.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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	1.32	1/872 (0.1%)	2.51	48/1183 (4.1%)
1	B	1.53	4/865 (0.5%)	2.47	47/1175 (4.0%)
1	C	1.15	0/873	2.55	51/1183 (4.3%)
All	All	1.35	5/2610 (0.2%)	2.51	146/3541 (4.1%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	SER	CB-OG	-29.37	1.04	1.42
1	A	59	ARG	CB-CG	-23.32	0.89	1.52
1	B	82	PHE	CG-CD2	5.41	1.46	1.38
1	B	110	ARG	CZ-NH2	-5.28	1.26	1.33
1	B	84	ASN	C-O	5.26	1.33	1.23

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH2	-19.30	110.65	120.30
1	C	72	ARG	NE-CZ-NH2	-18.57	111.01	120.30
1	C	17	TYR	CB-CG-CD2	-17.49	110.51	121.00
1	A	93	ASP	CB-CG-OD2	-17.39	102.65	118.30
1	A	110	ARG	NE-CZ-NH1	14.69	127.64	120.30
1	B	110	ARG	NE-CZ-NH2	14.36	127.48	120.30
1	C	17	TYR	CB-CG-CD1	14.23	129.54	121.00
1	A	59	ARG	CA-CB-CG	13.99	144.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	TYR	CB-CG-CD2	-13.93	112.64	121.00
1	B	8	ASP	CB-CG-OD1	13.29	130.26	118.30
1	B	13	TYR	CB-CG-CD2	-13.22	113.07	121.00
1	A	86	ASP	CB-CG-OD1	13.17	130.16	118.30
1	A	93	ASP	CB-CG-OD1	12.98	129.99	118.30
1	C	90	TYR	CB-CG-CD1	12.71	128.63	121.00
1	B	13	TYR	CB-CG-CD1	12.37	128.42	121.00
1	C	86	ASP	CB-CG-OD2	-11.09	108.32	118.30
1	A	59	ARG	CD-NE-CZ	10.89	138.85	123.60
1	B	67	SER	CA-CB-OG	10.74	140.19	111.20
1	C	83	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	B	105	THR	CA-CB-CG2	10.56	127.18	112.40
1	A	97	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	B	110	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	C	12	ASP	CB-CG-OD1	10.05	127.34	118.30
1	C	12	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	A	110	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	C	103	TYR	CB-CG-CD2	-9.39	115.37	121.00
1	C	103	TYR	CB-CG-CD1	9.36	126.61	121.00
1	B	8	ASP	O-C-N	9.18	138.81	123.20
1	B	93	ASP	CB-CG-OD1	9.14	126.53	118.30
1	B	22	ASP	CB-CG-OD2	9.07	126.46	118.30
1	C	8	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	C	22	ASP	CB-CG-OD1	8.90	126.31	118.30
1	B	72	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	B	83	ARG	NE-CZ-NH2	8.63	124.62	120.30
1	C	29	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	A	72	ARG	NH1-CZ-NH2	8.30	128.53	119.40
1	A	12	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	24	TYR	CB-CG-CD1	-8.12	116.13	121.00
1	C	93	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	12	ASP	CB-CG-OD1	-7.95	111.14	118.30
1	C	93	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	22	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	B	8	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	C	110	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	83	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	A	4	ILE	O-C-N	7.30	134.39	122.70
1	C	97	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	A	101	ASP	CB-CG-OD2	7.24	124.81	118.30
1	A	29	GLU	CG-CD-OE2	7.19	132.69	118.30
1	C	45	VAL	CA-CB-CG1	-7.14	100.18	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	THR	N-CA-CB	-7.11	96.80	110.30
1	B	72	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	67	SER	N-CA-CB	6.97	120.95	110.50
1	C	72	ARG	NH1-CZ-NH2	6.91	127.00	119.40
1	C	75	ASP	CB-CG-OD1	6.85	124.47	118.30
1	C	66	LYS	CG-CD-CE	6.75	132.14	111.90
1	C	18	HIS	CA-CB-CG	-6.73	102.16	113.60
1	A	97	TYR	CB-CG-CD1	6.72	125.03	121.00
1	B	89	LEU	CB-CG-CD2	-6.61	99.77	111.00
1	B	29	GLU	CG-CD-OE1	6.60	131.50	118.30
1	A	69	ARG	N-CA-CB	6.57	122.43	110.60
1	C	25	ILE	CA-C-N	6.51	131.53	117.20
1	B	89	LEU	CB-CA-C	6.51	122.57	110.20
1	A	59	ARG	CG-CD-NE	6.49	125.43	111.80
1	B	108	LYS	CD-CE-NZ	6.48	126.61	111.70
1	C	87	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	86	ASP	CB-CG-OD2	-6.38	112.55	118.30
1	A	19	LYS	CA-CB-CG	6.30	127.27	113.40
1	A	49	LYS	N-CA-CB	6.26	121.88	110.60
1	A	104	GLN	C-N-CA	6.25	137.34	121.70
1	C	15	GLN	CA-CB-CG	-6.24	99.66	113.40
1	B	14	LEU	CB-CG-CD1	-6.24	100.39	111.00
1	C	24	TYR	CA-CB-CG	-6.20	101.62	113.40
1	C	13	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	B	103	TYR	CB-CG-CD2	6.12	124.67	121.00
1	A	37	ALA	CB-CA-C	6.11	119.27	110.10
1	B	92	SER	O-C-N	6.09	132.45	122.70
1	B	8	ASP	CA-C-O	-6.04	107.41	120.10
1	C	90	TYR	CZ-CE2-CD2	-6.04	114.36	119.80
1	A	20	LEU	O-C-N	6.01	132.52	121.10
1	A	22	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	59	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	109	ILE	O-C-N	-6.00	113.10	122.70
1	C	17	TYR	O-C-N	5.99	132.28	122.70
1	C	22	ASP	OD1-CG-OD2	-5.97	111.95	123.30
1	A	29	GLU	CA-CB-CG	5.97	126.53	113.40
1	B	69	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	C	9	GLY	O-C-N	5.97	132.25	122.70
1	C	72	ARG	CD-NE-CZ	5.96	131.95	123.60
1	C	66	LYS	CD-CE-NZ	5.90	125.27	111.70
1	A	72	ARG	CD-NE-CZ	-5.90	115.34	123.60
1	C	17	TYR	CB-CA-C	-5.87	98.66	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	LYS	CA-C-O	5.86	132.41	120.10
1	B	4	ILE	CA-CB-CG1	-5.81	99.95	111.00
1	A	29	GLU	C-N-CA	5.77	136.12	121.70
1	A	49	LYS	C-N-CA	5.76	136.10	121.70
1	B	23	ASN	O-C-N	-5.76	113.49	122.70
1	A	49	LYS	CA-C-N	-5.75	104.54	117.20
1	C	104	GLN	O-C-N	-5.74	113.51	122.70
1	B	67	SER	CA-C-N	-5.74	104.73	116.20
1	A	22	ASP	CA-CB-CG	5.71	125.96	113.40
1	B	46	ALA	O-C-N	5.70	131.93	121.10
1	B	43	ALA	CB-CA-C	5.70	118.64	110.10
1	B	72	ARG	O-C-N	5.70	131.81	122.70
1	A	29	GLU	OE1-CD-OE2	-5.67	116.50	123.30
1	C	45	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	A	67	SER	CA-C-O	5.64	131.94	120.10
1	B	101	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	15	GLN	CB-CG-CD	5.58	126.11	111.60
1	B	110	ARG	CD-NE-CZ	-5.57	115.80	123.60
1	A	56	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	A	72	ARG	CB-CG-CD	-5.53	97.22	111.60
1	A	61	GLY	C-N-CA	5.52	135.50	121.70
1	B	11	ALA	O-C-N	5.50	131.50	122.70
1	A	106	PHE	CB-CG-CD1	-5.49	116.95	120.80
1	A	110	ARG	CD-NE-CZ	5.49	131.29	123.60
1	A	74	ALA	C-N-CA	5.49	135.41	121.70
1	B	106	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	B	63	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	C	39	LYS	CA-C-O	-5.43	108.69	120.10
1	C	7	PHE	O-C-N	-5.39	114.07	122.70
1	A	59	ARG	CB-CG-CD	5.38	125.58	111.60
1	C	41	ASN	O-C-N	5.38	131.30	122.70
1	C	17	TYR	CA-CB-CG	-5.35	103.23	113.40
1	A	79	THR	CA-C-N	5.34	128.96	117.20
1	A	103	TYR	CB-CG-CD2	5.28	124.17	121.00
1	C	83	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
1	A	24	TYR	CB-CG-CD2	5.21	124.12	121.00
1	B	72	ARG	N-CA-CB	5.20	119.96	110.60
1	C	24	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	97	TYR	CB-CG-CD1	5.19	124.11	121.00
1	C	94	TRP	CA-CB-CG	-5.18	103.85	113.70
1	C	71	TRP	O-C-N	5.14	130.92	122.70
1	B	55	ILE	O-C-N	5.11	130.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	18	HIS	C-N-CA	5.10	134.45	121.70
1	C	13	TYR	CG-CD2-CE2	-5.07	117.25	121.30
1	C	103	TYR	CA-CB-CG	5.07	123.03	113.40
1	B	103	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	B	70	THR	CA-CB-OG1	-5.06	98.37	109.00
1	A	28	SER	CB-CA-C	5.04	119.68	110.10
1	C	29	GLU	CG-CD-OE1	5.04	128.38	118.30
1	A	105	THR	N-CA-CB	5.03	119.86	110.30
1	C	100	THR	CA-CB-CG2	5.03	119.44	112.40
1	B	7	PHE	CB-CG-CD1	5.02	124.31	120.80
1	B	37	ALA	O-C-N	5.01	130.72	122.70
1	B	19	LYS	CA-C-O	5.01	130.62	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ARG	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	851	0	809	35	0
1	B	844	0	796	33	0
1	C	852	0	809	20	0
2	A	63	0	0	2	0
2	B	72	0	0	2	0
2	C	81	0	0	0	0
All	All	2763	0	2414	87	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 18.

All (87) 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:B:14:LEU:O	1:B:18:HIS:HA	1.75	0.86
1:A:101:ASP:O	1:A:102:HIS:HB2	1.81	0.79
1:B:101:ASP:OD2	1:B:105:THR:OG1	2.01	0.78
1:B:18:HIS:HB3	1:B:94:TRP:CZ2	2.21	0.74
1:A:14:LEU:O	1:A:18:HIS:HA	1.87	0.74
1:B:14:LEU:O	1:B:18:HIS:CA	2.37	0.73
1:A:14:LEU:HD22	1:A:94:TRP:HZ3	1.57	0.70
1:A:36:VAL:HB	1:A:39:LYS:HG3	1.73	0.70
1:A:13:TYR:CE2	1:A:17:TYR:CE2	2.80	0.69
1:C:66:LYS:NZ	1:C:93:ASP:OD2	2.26	0.68
1:C:74:ALA:HB3	1:C:88:ILE:HG22	1.77	0.66
1:A:26:THR:OG1	1:A:29:GLU:HG3	1.96	0.66
1:C:63:LEU:HD11	1:C:89:LEU:HD22	1.78	0.65
1:B:56:PHE:CE2	1:B:63:LEU:HD12	2.31	0.65
1:B:69:ARG:HG3	1:B:91:SER:HB2	1.79	0.65
1:B:89:LEU:HD13	1:B:106:PHE:HE1	1.61	0.64
1:B:56:PHE:HE2	1:B:63:LEU:HD12	1.63	0.62
1:B:77:ASN:ND2	1:B:86:ASP:OD2	2.27	0.61
1:C:26:THR:OG1	1:C:29:GLU:HG3	2.02	0.59
1:B:64:PRO:O	1:B:69:ARG:NH1	2.36	0.59
1:B:5:ASN:HB2	2:B:123:HOH:O	2.02	0.59
1:B:7:PHE:CE1	1:B:98:LYS:HB2	2.38	0.59
1:B:14:LEU:O	1:B:18:HIS:N	2.36	0.58
1:B:96:ILE:HG13	1:B:110:ARG:HB2	1.85	0.57
1:C:28:SER:HA	1:C:31:GLN:HE21	1.68	0.57
1:A:13:TYR:CD2	1:A:17:TYR:CE2	2.93	0.57
1:C:56:PHE:CD2	1:C:89:LEU:CD2	2.88	0.57
1:B:13:TYR:HD1	1:B:19:LYS:O	1.88	0.56
1:A:90:TYR:HA	1:A:95:LEU:O	2.06	0.56
1:C:3:VAL:C	1:C:4:ILE:HD12	2.25	0.56
1:C:98:LYS:HG2	1:C:109:ILE:HG21	1.88	0.55
1:A:56:PHE:CE2	1:A:63:LEU:HD12	2.42	0.55
1:B:108:LYS:HD3	1:C:45:VAL:HA	1.87	0.54
1:A:101:ASP:O	1:A:102:HIS:CB	2.50	0.54
1:A:71:TRP:CH2	1:A:91:SER:HB3	2.42	0.54
1:B:3:VAL:HG12	1:B:23:ASN:HB3	1.89	0.53
1:A:25:ILE:HG23	1:A:49:LYS:HD2	1.89	0.53
1:B:63:LEU:HD11	1:B:89:LEU:HD22	1.90	0.53
1:C:56:PHE:CG	1:C:89:LEU:HD21	2.44	0.53
1:A:13:TYR:HD1	1:A:19:LYS:O	1.91	0.52
1:B:13:TYR:CD1	1:B:19:LYS:O	2.62	0.52
1:A:55:ILE:HD13	1:A:72:ARG:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB3	2:A:139:HOH:O	2.07	0.52
1:B:74:ALA:HB3	1:B:88:ILE:CG2	2.40	0.51
1:A:14:LEU:O	1:A:18:HIS:CA	2.57	0.51
1:A:71:TRP:CZ3	1:A:91:SER:HB3	2.44	0.51
1:C:98:LYS:HG2	1:C:109:ILE:CG2	2.40	0.51
1:B:46:ALA:HB1	1:B:49:LYS:HG3	1.93	0.50
1:A:71:TRP:O	1:A:72:ARG:HG3	2.12	0.49
1:A:13:TYR:CD1	1:A:19:LYS:O	2.65	0.49
1:B:18:HIS:HB3	1:B:94:TRP:CE2	2.47	0.49
1:C:4:ILE:HG21	1:C:9:GLY:C	2.32	0.49
1:A:23:ASN:O	1:A:49:LYS:HD3	2.12	0.49
1:B:35:TRP:CD1	1:B:42:LEU:HB2	2.47	0.49
1:A:4:ILE:HD12	1:A:21:PRO:HB3	1.95	0.48
1:A:87:ARG:HB2	1:A:99:THR:HG22	1.96	0.48
1:B:56:PHE:HB2	1:B:73:GLU:HG2	1.95	0.48
1:C:87:ARG:HG3	1:C:103:TYR:CE1	2.49	0.48
1:C:106:PHE:CD1	1:C:106:PHE:N	2.82	0.48
1:B:52:GLY:HA2	1:B:74:ALA:HA	1.95	0.47
1:A:13:TYR:CD2	1:A:17:TYR:HE2	2.32	0.47
1:B:74:ALA:HB3	1:B:88:ILE:HG22	1.97	0.47
1:A:89:LEU:HD13	1:A:106:PHE:HE2	1.81	0.46
1:A:24:TYR:HA	1:A:50:SER:O	2.16	0.46
1:B:89:LEU:HD13	1:B:106:PHE:CE1	2.48	0.46
1:B:64:PRO:HG2	1:B:71:TRP:HZ2	1.81	0.46
1:A:89:LEU:HD13	1:A:106:PHE:CE2	2.51	0.45
1:B:43:ALA:O	1:B:47:PRO:HG3	2.16	0.45
1:C:98:LYS:HG3	1:C:98:LYS:H	1.64	0.45
1:A:56:PHE:HE2	1:A:63:LEU:HD12	1.81	0.45
1:C:74:ALA:HB3	1:C:88:ILE:CG2	2.44	0.44
1:C:27:LYS:O	1:C:31:GLN:HG3	2.18	0.44
1:A:56:PHE:CG	1:A:89:LEU:HD21	2.53	0.44
1:B:101:ASP:CG	1:B:105:THR:OG1	2.57	0.43
1:A:20:LEU:HA	1:A:21:PRO:HD3	1.86	0.43
1:A:14:LEU:O	1:A:18:HIS:N	2.52	0.43
1:A:98:LYS:HG3	1:A:98:LYS:O	2.16	0.42
1:B:9:GLY:HA3	2:B:146:HOH:O	2.20	0.42
1:B:90:TYR:HA	1:B:95:LEU:O	2.20	0.42
1:B:51:ILE:O	1:B:75:ASP:HB2	2.19	0.41
1:A:13:TYR:CZ	1:A:17:TYR:CD2	3.08	0.41
1:C:63:LEU:CD1	1:C:89:LEU:HD22	2.47	0.41
1:C:52:GLY:HA2	1:C:74:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:HA	2:A:158:HOH:O	2.20	0.41
1:A:7:PHE:CE1	1:A:98:LYS:HB2	2.55	0.41
1:A:85:SER:HB3	1:A:102:HIS:CE1	2.56	0.41
1:C:69:ARG:HA	1:C:92:SER:OG	2.22	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	106/110 (96%)	101 (95%)	5 (5%)	0	100 100
1	B	106/110 (96%)	100 (94%)	5 (5%)	1 (1%)	21 15
1	C	106/110 (96%)	106 (100%)	0	0	100 100
All	All	318/330 (96%)	307 (96%)	10 (3%)	1 (0%)	46 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	LYS

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	87/92 (95%)	76 (87%)	11 (13%)	5 3
1	B	86/92 (94%)	78 (91%)	8 (9%)	11 7
1	C	88/92 (96%)	84 (96%)	4 (4%)	34 32
All	All	261/276 (95%)	238 (91%)	23 (9%)	12 8

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	38	SER
1	A	59	ARG
1	A	67	SER
1	A	70	THR
1	A	89	LEU
1	A	92	SER
1	A	93	ASP
1	A	98	LYS
1	A	103	TYR
1	A	105	THR
1	B	49	LYS
1	B	55	ILE
1	B	67	SER
1	B	89	LEU
1	B	92	SER
1	B	96	ILE
1	B	103	TYR
1	B	105	THR
1	C	8	ASP
1	C	89	LEU
1	C	96	ILE
1	C	98	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	HIS
1	B	31	GLN
1	C	18	HIS
1	C	31	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 carbohydrates 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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.