Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BNJ
Title	:	BARNASE WILDTYPE STRUCTURE AT PH 9.0
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 (i) symbol.

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

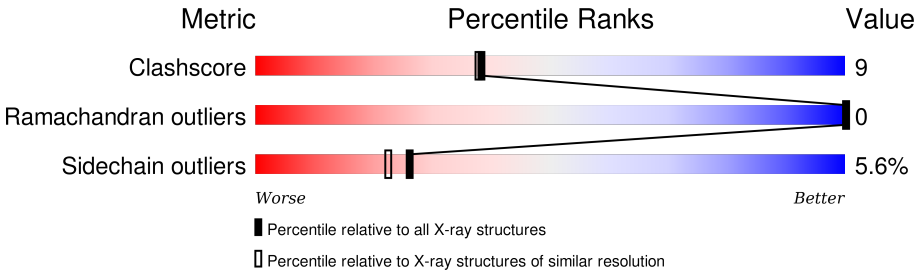
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	51% 36% 11%
1	B	110	48% 45%
1	C	110	59% 35%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2800 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	109	Total	C	N	O	8	1	1
			863	548	151	164			
1	B	108	Total	C	N	O	2	1	0
			858	545	147	166			
1	C	107	Total	C	N	O	5	1	0
			860	545	150	165			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	78	Total	O	0	0
			78	78		
2	C	80	Total	O	0	0
			80	80		

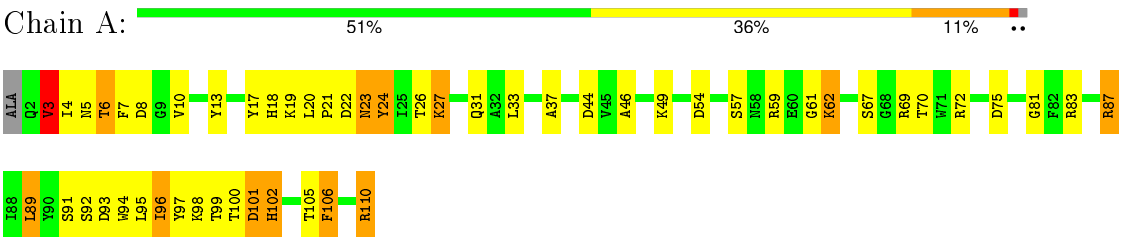
3 Residue-property plots (i)

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.

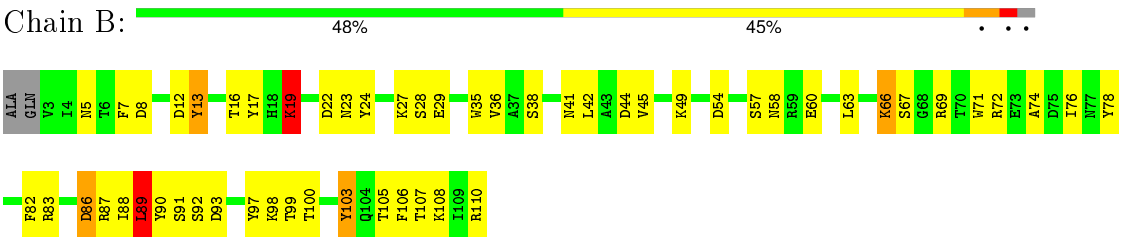
- Molecule 1: BARNASE

Chain A:



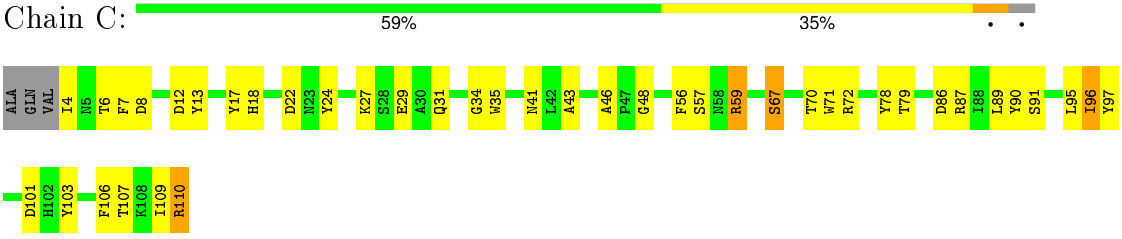
- Molecule 1: BARNASE

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	59.53Å 59.53Å 81.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	83.7 (10.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2800	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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	1.17	2/890 (0.2%)	2.54	54/1204 (4.5%)
1	B	1.26	1/884 (0.1%)	2.48	58/1196 (4.8%)
1	C	1.19	1/886 (0.1%)	2.43	48/1198 (4.0%)
All	All	1.21	4/2660 (0.2%)	2.48	160/3598 (4.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	LYS	CE-NZ	-14.48	1.12	1.49
1	C	59	ARG	CG-CD	-10.15	1.26	1.51
1	A	59	ARG	CB-CG	-6.10	1.36	1.52
1	A	19	LYS	CE-NZ	5.82	1.63	1.49

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH2	-24.82	107.89	120.30
1	B	13	TYR	CB-CG-CD2	-16.08	111.35	121.00
1	B	8	ASP	CB-CG-OD1	14.59	131.43	118.30
1	A	17	TYR	CB-CG-CD1	-13.64	112.82	121.00
1	A	93	ASP	CB-CG-OD1	13.50	130.45	118.30
1	C	72	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	B	13	TYR	CB-CG-CD1	13.16	128.90	121.00
1	C	13	TYR	CB-CG-CD2	-12.96	113.22	121.00
1	B	19	LYS	CD-CE-NZ	12.81	141.17	111.70
1	A	110	ARG	NE-CZ-NH2	12.67	126.64	120.30
1	B	72	ARG	NE-CZ-NH1	-12.11	114.24	120.30
1	C	90	TYR	CB-CG-CD1	12.06	128.24	121.00
1	A	75	ASP	CB-CG-OD1	11.76	128.89	118.30
1	A	17	TYR	CB-CG-CD2	11.71	128.02	121.00
1	C	72	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	66	LYS	CD-CE-NZ	11.00	137.01	111.70
1	C	110	ARG	NE-CZ-NH1	-10.83	114.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	59	ARG	CB-CG-CD	10.81	139.71	111.60
1	A	72	ARG	NH1-CZ-NH2	10.69	131.16	119.40
1	B	54	ASP	CB-CG-OD1	10.26	127.53	118.30
1	B	86	ASP	CB-CG-OD1	10.25	127.53	118.30
1	A	110	ARG	NE-CZ-NH1	-10.15	115.23	120.30
1	C	87	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	C	87	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	B	90	TYR	CG-CD2-CE2	-9.92	113.36	121.30
1	C	90	TYR	CB-CG-CD2	-9.86	115.08	121.00
1	B	12	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	C	86	ASP	CB-CG-OD1	9.55	126.90	118.30
1	C	17	TYR	CB-CG-CD2	-9.36	115.38	121.00
1	C	22	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	A	101	ASP	CB-CG-OD1	8.72	126.15	118.30
1	C	86	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	B	22	ASP	CB-CG-OD1	8.53	125.97	118.30
1	A	93	ASP	CB-CG-OD2	-8.51	110.65	118.30
1	B	83	ARG	CD-NE-CZ	-8.37	111.88	123.60
1	C	78	TYR	CB-CG-CD1	-8.19	116.09	121.00
1	A	87	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	C	29	GLU	CG-CD-OE1	7.99	134.29	118.30
1	C	8	ASP	CB-CG-OD2	7.93	125.43	118.30
1	B	17	TYR	CA-CB-CG	-7.75	98.67	113.40
1	B	97	TYR	CB-CG-CD1	-7.66	116.40	121.00
1	C	22	ASP	CB-CG-OD1	7.63	125.17	118.30
1	C	101	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	57	SER	N-CA-CB	-7.55	99.18	110.50
1	A	83	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	C	13	TYR	CB-CG-CD1	7.54	125.52	121.00
1	A	22	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	45	VAL	CG1-CB-CG2	-7.51	98.89	110.90
1	B	93	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	59	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	B	12	ASP	CB-CG-OD1	7.40	124.96	118.30
1	C	90	TYR	CD1-CE1-CZ	7.33	126.40	119.80
1	C	29	GLU	OE1-CD-OE2	-7.17	114.69	123.30
1	B	108	LYS	CA-C-N	7.09	132.79	117.20
1	B	8	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	44	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	71	TRP	CH2-CZ2-CE2	-6.94	110.46	117.40
1	B	17	TYR	CB-CG-CD1	-6.91	116.85	121.00
1	C	59	ARG	NE-CZ-NH2	6.88	123.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	SER	CB-CA-C	6.87	123.15	110.10
1	C	34	GLY	CA-C-O	-6.79	108.37	120.60
1	A	3	VAL	N-CA-CB	6.76	126.38	111.50
1	C	56	PHE	CA-C-O	6.74	134.24	120.10
1	A	61	GLY	CA-C-O	-6.70	108.54	120.60
1	C	35	TRP	CG-CD2-CE3	-6.70	127.87	133.90
1	B	71	TRP	O-C-N	6.66	133.36	122.70
1	B	38	SER	N-CA-CB	6.64	120.47	110.50
1	B	110	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	A	97	TYR	CD1-CE1-CZ	-6.61	113.85	119.80
1	B	24	TYR	CB-CG-CD1	6.61	124.97	121.00
1	A	61	GLY	CA-C-N	6.56	131.63	117.20
1	B	110	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	13	TYR	CD1-CE1-CZ	-6.51	113.94	119.80
1	C	6	THR	O-C-N	6.50	133.10	122.70
1	A	17	TYR	CA-CB-CG	-6.50	101.05	113.40
1	A	81	GLY	CA-C-O	6.46	132.24	120.60
1	B	72	ARG	O-C-N	6.46	133.04	122.70
1	B	97	TYR	CD1-CE1-CZ	-6.37	114.07	119.80
1	A	72	ARG	CD-NE-CZ	-6.36	114.70	123.60
1	B	93	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	B	103	TYR	CB-CG-CD1	-6.32	117.20	121.00
1	B	78	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	B	8	ASP	C-N-CA	-6.32	109.03	122.30
1	A	8	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	75	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	97	TYR	CB-CG-CD2	6.24	124.75	121.00
1	B	72	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	C	67	SER	N-CA-CB	6.12	119.69	110.50
1	C	79	THR	CA-CB-CG2	6.10	120.95	112.40
1	B	5	ASN	CB-CG-ND2	6.06	131.24	116.70
1	C	18	HIS	CA-CB-CG	-6.06	103.30	113.60
1	B	60	GLU	CG-CD-OE1	6.05	130.41	118.30
1	A	6	THR	N-CA-CB	6.05	121.80	110.30
1	A	13	TYR	N-CA-CB	-6.03	99.74	110.60
1	A	20	LEU	O-C-N	6.00	132.50	121.10
1	A	95	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	A	13	TYR	CZ-CE2-CD2	-5.97	114.42	119.80
1	C	34	GLY	O-C-N	5.93	132.19	122.70
1	C	101	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	35	TRP	CG-CD1-NE1	5.90	116.00	110.10
1	B	89	LEU	CA-CB-CG	-5.87	101.80	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	SER	CA-C-O	5.84	132.35	120.10
1	B	78	TYR	CG-CD2-CE2	-5.81	116.65	121.30
1	C	35	TRP	CD1-NE1-CE2	-5.81	103.77	109.00
1	B	82	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	C	107	THR	CA-CB-CG2	5.78	120.50	112.40
1	A	24	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	B	90	TYR	CZ-CE2-CD2	5.77	124.99	119.80
1	A	37	ALA	CB-CA-C	5.74	118.71	110.10
1	A	72	ARG	CG-CD-NE	-5.72	99.78	111.80
1	B	82	PHE	CB-CG-CD2	5.70	124.79	120.80
1	A	102	HIS	CA-CB-CG	-5.70	103.91	113.60
1	A	44	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	12	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	22	ASP	O-C-N	5.66	131.75	122.70
1	B	76	ILE	O-C-N	5.63	131.71	122.70
1	A	22	ASP	CB-CA-C	-5.63	99.14	110.40
1	B	41	ASN	N-CA-CB	-5.61	100.51	110.60
1	C	24	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	A	7	PHE	O-C-N	5.60	131.66	122.70
1	A	33	LEU	CB-CA-C	-5.59	99.57	110.20
1	A	100	THR	N-CA-CB	5.55	120.84	110.30
1	B	22	ASP	CA-C-O	-5.54	108.46	120.10
1	A	8	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	C	110	ARG	N-CA-CB	5.53	120.56	110.60
1	C	46	ALA	CB-CA-C	5.51	118.36	110.10
1	B	74	ALA	CB-CA-C	5.50	118.35	110.10
1	C	35	TRP	CD1-CG-CD2	-5.44	101.95	106.30
1	A	7	PHE	CB-CG-CD1	-5.43	117.00	120.80
1	C	110	ARG	CA-CB-CG	5.42	125.33	113.40
1	A	17	TYR	O-C-N	5.42	131.37	122.70
1	B	88	ILE	O-C-N	-5.42	114.03	122.70
1	C	110	ARG	CD-NE-CZ	5.41	131.17	123.60
1	A	96	ILE	CA-CB-CG1	5.40	121.26	111.00
1	A	7	PHE	CA-C-O	-5.38	108.79	120.10
1	C	41	ASN	CA-C-O	-5.38	108.81	120.10
1	B	36	VAL	CA-CB-CG1	5.36	118.94	110.90
1	A	4	ILE	O-C-N	5.36	131.27	122.70
1	A	3	VAL	O-C-N	5.35	131.26	122.70
1	B	22	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	16	THR	N-CA-CB	5.27	120.32	110.30
1	A	105	THR	CA-C-O	5.27	131.17	120.10
1	A	106	PHE	CB-CG-CD2	-5.27	117.11	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	C	41	ASN	OD1-CG-ND2	-5.26	109.80	121.90
1	B	60	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	23	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	B	105	THR	CA-CB-CG2	5.17	119.64	112.40
1	C	7	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	B	28	SER	CA-CB-OG	-5.16	97.26	111.20
1	A	33	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	B	107	THR	CA-CB-CG2	5.11	119.56	112.40
1	C	48	GLY	O-C-N	-5.10	114.53	122.70
1	C	97	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	89	LEU	CB-CA-C	5.04	119.79	110.20
1	B	71	TRP	CA-C-N	-5.04	106.10	117.20
1	C	103	TYR	CG-CD1-CE1	5.03	125.33	121.30
1	B	29	GLU	CG-CD-OE1	5.03	128.36	118.30
1	A	6	THR	O-C-N	5.03	130.74	122.70
1	B	24	TYR	CG-CD1-CE1	5.00	125.30	121.30

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	863	0	835	18	0
1	B	858	0	825	20	0
1	C	860	0	833	8	0
2	A	61	0	0	2	0
2	B	78	0	0	0	0
2	C	80	0	0	3	0
All	All	2800	0	2493	46	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 (46) 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:98[A]:LYS:NZ	1:B:100:THR:HG23	1.79	0.96
1:A:89:LEU:HD13	1:A:106:PHE:CE1	2.09	0.88
1:A:89:LEU:HD13	1:A:106:PHE:HE1	1.40	0.87
1:B:98[A]:LYS:HZ3	1:B:100:THR:HG23	1.47	0.79
1:A:18:HIS:HB3	1:A:94:TRP:CZ2	2.26	0.71
1:B:63:LEU:HD11	1:B:89:LEU:HD22	1.80	0.64
1:A:96:ILE:HB	1:A:110:ARG:HB2	1.84	0.60
1:B:89:LEU:HD13	1:B:106:PHE:HE1	1.67	0.59
1:A:87:ARG:HB2	1:A:99:THR:CG2	2.33	0.58
1:B:98[A]:LYS:HZ1	1:B:100:THR:HG23	1.67	0.55
1:A:89:LEU:CD1	1:A:106:PHE:HE1	2.16	0.54
1:A:46:ALA:HB1	1:A:49:LYS:HG3	1.88	0.54
1:A:69:ARG:HG3	1:A:91:SER:HB2	1.90	0.54
1:A:3:VAL:HG12	1:A:23:ASN:CB	2.40	0.52
1:B:7:PHE:CE1	1:B:98[B]:LYS:HB2	2.45	0.52
1:B:98[A]:LYS:NZ	1:B:100:THR:CG2	2.65	0.52
1:B:86:ASP:C	1:B:87:ARG:HG2	2.31	0.51
1:B:87:ARG:HB2	1:B:99:THR:HG22	1.92	0.51
1:C:57:SER:HB2	2:C:129:HOH:O	2.12	0.50
1:C:27:LYS:O	1:C:31:GLN:HG3	2.13	0.49
1:C:89:LEU:HD13	1:C:106:PHE:CE1	2.48	0.48
1:A:62:LYS:HG2	1:A:62:LYS:HZ2	1.56	0.48
1:B:7:PHE:CE1	1:B:98[A]:LYS:HB2	2.49	0.48
1:B:87:ARG:HB2	1:B:99:THR:CG2	2.45	0.47
1:B:35:TRP:CD1	1:B:42:LEU:HB2	2.50	0.47
1:C:27:LYS:HE2	2:C:143:HOH:O	2.15	0.46
1:C:70:THR:O	1:C:91:SER:HA	2.15	0.46
1:B:23:ASN:O	1:B:49:LYS:HA	2.15	0.46
1:A:62:LYS:CD	2:A:129:HOH:O	2.65	0.45
1:A:26:THR:HB	1:A:54:ASP:OD1	2.17	0.45
1:B:13:TYR:HD1	1:B:19:LYS:O	2.01	0.44
1:A:6:THR:O	1:A:10:VAL:HG23	2.16	0.44
1:B:69:ARG:HG3	1:B:91:SER:HB2	2.00	0.44
1:B:66:LYS:HG2	1:B:67:SER:H	1.82	0.43
1:B:89:LEU:HD13	1:B:106:PHE:CE1	2.51	0.43
1:A:101:ASP:O	1:A:102:HIS:HB2	2.18	0.43
1:B:98[A]:LYS:HZ1	1:B:100:THR:CG2	2.31	0.43
1:C:95:LEU:C	1:C:96:ILE:HG12	2.39	0.42
1:A:5:ASN:HB2	2:A:122:HOH:O	2.18	0.42
1:B:27:LYS:HZ2	1:B:27:LYS:HG3	1.68	0.42
1:C:109:ILE:O	1:C:110:ARG:HD3	2.19	0.42
1:B:57:SER:O	1:B:58:ASN:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HE21	1:A:31:GLN:HB2	1.66	0.41
1:C:43:ALA:HA	2:C:154:HOH:O	2.20	0.41
1:A:21:PRO:HD2	1:A:24:TYR:CD2	2.56	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	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
1	B	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
1	C	106/110 (96%)	103 (97%)	3 (3%)	0	100	100
All	All	321/330 (97%)	313 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	91/92 (99%)	83 (91%)	8 (9%)	12	8
1	B	90/92 (98%)	86 (96%)	4 (4%)	35	33
1	C	91/92 (99%)	87 (96%)	4 (4%)	35	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	272/276 (99%)	256 (94%)	16 (6%)	26 20

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	27[A]	LYS
1	A	27[B]	LYS
1	A	62	LYS
1	A	70	THR
1	A	89	LEU
1	A	92	SER
1	A	98	LYS
1	B	19	LYS
1	B	89	LEU
1	B	92	SER
1	B	103	TYR
1	C	4	ILE
1	C	59	ARG
1	C	67	SER
1	C	96	ILE

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

Mol	Chain	Res	Type
1	A	31	GLN
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.