



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:32 PM GMT

PDB ID : 1BAN  
Title : THE CONTRIBUTION OF BURIED HYDROGEN BONDS TO PROTEIN STABILITY: THE CRYSTAL STRUCTURES OF TWO BARNASE MUTANTS  
Authors : Chen, Y.W.; Fersht, A.R.; Henrick, K.  
Deposited on : 1993-05-19  
Resolution : 2.20 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

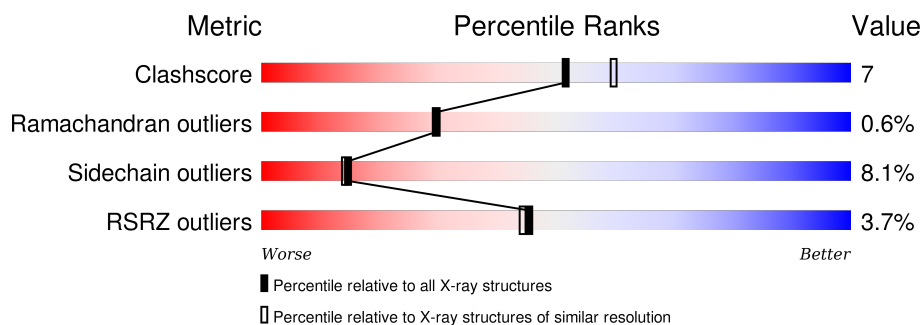
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	110	<div> <div>2%</div> <div>55%</div> <div>35%</div> <div>6%</div> <div>..</div> </div>
1	B	110	<div> <div>7%</div> <div>51%</div> <div>37%</div> <div>8%</div> <div>..</div> </div>
1	C	110	<div> <div>2%</div> <div>56%</div> <div>35%</div> <div>5%</div> <div>..</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2825 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	0	0	0
			839	535	144	160			
1	B	108	Total	C	N	O	0	0	0
			850	541	147	162			
1	C	109	Total	C	N	O	0	0	0
			870	551	151	168			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ALA	SER	CONFLICT	UNP P00648
B	91	ALA	SER	CONFLICT	UNP P00648
C	91	ALA	SER	CONFLICT	UNP P00648

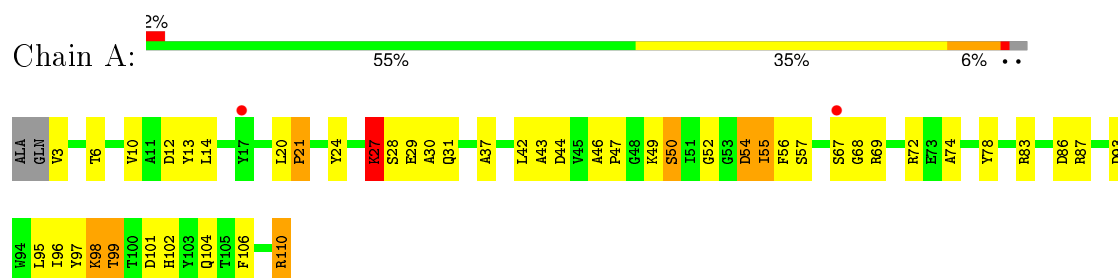
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	91	Total	O	0	0
			91	91		
2	C	102	Total	O	0	0
			102	102		

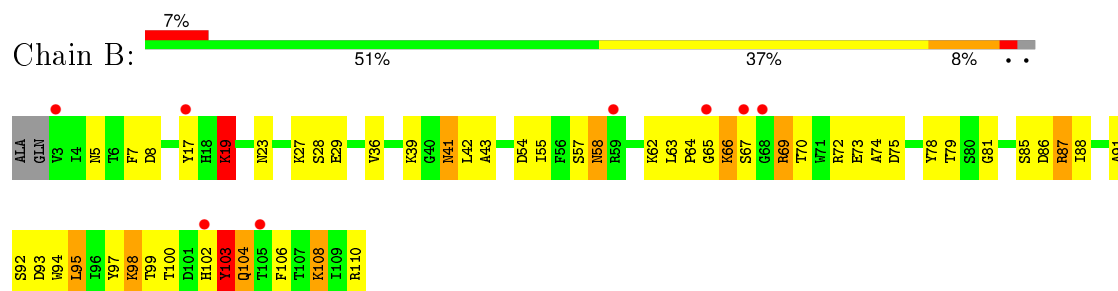
### 3 Residue-property plots [i](#)

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.

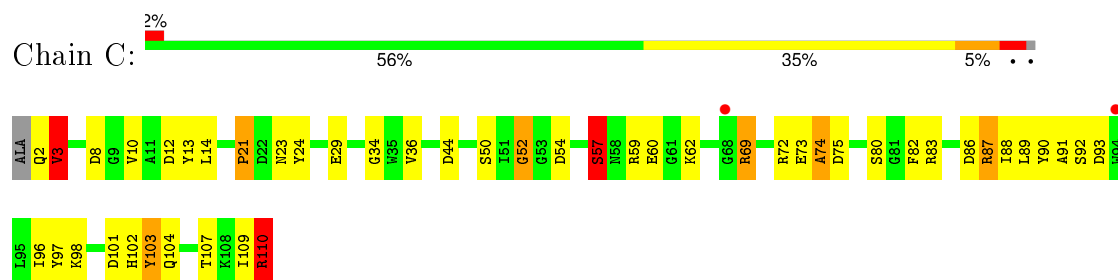
#### • Molecule 1: BARNASE



#### • Molecule 1: BARNASE



#### • Molecule 1: BARNASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.53 Å 59.53 Å 82.65 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.20 28.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 98.0 (28.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.20 Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.176 , (Not available) 0.170 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 94.5	EDS
Estimated twinning fraction	0.028 for -h,-k,l 0.085 for h,-h-k,-l 0.055 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 16275 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2825	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.14	0/860	2.52	50/1166 (4.3%)
1	B	1.15	0/871	2.35	40/1180 (3.4%)
1	C	1.20	0/891	2.62	58/1206 (4.8%)
All	All	1.17	0/2622	2.50	148/3552 (4.2%)

There are no bond length outliers.

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ARG	NE-CZ-NH2	19.08	129.84	120.30
1	C	72	ARG	NE-CZ-NH2	-15.64	112.48	120.30
1	C	83	ARG	NE-CZ-NH2	15.19	127.90	120.30
1	C	59	ARG	NE-CZ-NH1	13.73	127.17	120.30
1	C	72	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	B	72	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	C	87	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	C	75	ASP	CB-CG-OD1	13.19	130.17	118.30
1	C	69	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	C	13	TYR	CB-CG-CD2	-12.88	113.28	121.00
1	C	86	ASP	CB-CG-OD2	-12.29	107.23	118.30
1	A	86	ASP	CB-CG-OD2	-12.09	107.42	118.30
1	A	97	TYR	CB-CG-CD1	11.66	128.00	121.00
1	C	13	TYR	CB-CG-CD1	11.61	127.97	121.00
1	A	12	ASP	CB-CG-OD2	-11.56	107.90	118.30
1	A	83	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	C	90	TYR	CB-CG-CD2	-11.25	114.25	121.00
1	A	72	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	C	2	GLN	CA-CB-CG	10.77	137.10	113.40
1	A	69	ARG	NE-CZ-NH2	10.75	125.68	120.30
1	C	90	TYR	CB-CG-CD1	10.42	127.25	121.00
1	A	110	ARG	CD-NE-CZ	10.40	138.16	123.60
1	B	110	ARG	NE-CZ-NH2	10.18	125.39	120.30
1	C	83	ARG	NE-CZ-NH1	-10.07	115.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	ASP	CB-CG-OD2	-9.99	109.31	118.30
1	A	44	ASP	CB-CG-OD1	9.97	127.28	118.30
1	A	83	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	C	59	ARG	CD-NE-CZ	9.67	137.14	123.60
1	C	101	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	110	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	B	19	LYS	CA-CB-CG	8.72	132.59	113.40
1	C	110	ARG	CA-CB-CG	8.62	132.36	113.40
1	B	54	ASP	CB-CG-OD2	8.45	125.91	118.30
1	B	95	LEU	CA-CB-CG	8.40	134.61	115.30
1	B	75	ASP	CB-CG-OD2	8.39	125.85	118.30
1	A	97	TYR	CB-CG-CD2	-8.26	116.04	121.00
1	B	100	THR	CA-CB-CG2	8.25	123.95	112.40
1	C	80	SER	N-CA-CB	-8.24	98.14	110.50
1	C	3	VAL	C-N-CA	8.18	142.15	121.70
1	B	110	ARG	CA-CB-CG	8.18	131.39	113.40
1	C	36	VAL	O-C-N	8.16	135.75	122.70
1	B	98	LYS	CA-CB-CG	7.91	130.81	113.40
1	B	8	ASP	CB-CG-OD1	-7.89	111.20	118.30
1	A	99	THR	CA-CB-CG2	7.80	123.31	112.40
1	A	95	LEU	CA-CB-CG	7.79	133.22	115.30
1	A	93	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	C	73	GLU	CG-CD-OE2	7.70	133.70	118.30
1	A	83	ARG	CD-NE-CZ	7.68	134.36	123.60
1	C	29	GLU	OE1-CD-OE2	-7.33	114.50	123.30
1	B	110	ARG	N-CA-CB	7.21	123.58	110.60
1	B	7	PHE	CB-CG-CD2	-7.21	115.75	120.80
1	A	14	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	87	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	52	GLY	CA-C-N	7.09	130.39	116.20
1	A	29	GLU	CA-C-O	7.09	134.98	120.10
1	A	44	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	B	67	SER	N-CA-CB	7.07	121.11	110.50
1	C	82	PHE	CB-CG-CD2	7.07	125.75	120.80
1	A	37	ALA	CB-CA-C	7.03	120.64	110.10
1	C	54	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	B	86	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	93	ASP	CB-CA-C	6.85	124.11	110.40
1	A	54	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	87	ARG	CD-NE-CZ	-6.69	114.23	123.60
1	B	27	LYS	O-C-N	-6.69	112.00	122.70
1	C	91	ALA	CB-CA-C	-6.65	100.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	LYS	CA-C-O	6.58	133.92	120.10
1	B	41	ASN	N-CA-CB	-6.51	98.89	110.60
1	A	93	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	2	GLN	CB-CG-CD	6.48	128.44	111.60
1	B	69	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	97	TYR	OH-CZ-CE2	6.44	137.49	120.10
1	C	97	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	C	44	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	10	VAL	CB-CA-C	6.38	123.52	111.40
1	C	60	GLU	CG-CD-OE2	6.34	130.97	118.30
1	B	69	ARG	CA-C-N	-6.33	103.27	117.20
1	C	75	ASP	OD1-CG-OD2	-6.33	111.28	123.30
1	A	6	THR	CA-CB-CG2	6.25	121.15	112.40
1	B	99	THR	N-CA-CB	6.18	122.04	110.30
1	B	110	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	B	36	VAL	C-N-CA	6.07	136.88	121.70
1	B	54	ASP	OD1-CG-OD2	-6.03	111.84	123.30
1	A	24	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	C	57	SER	CA-CB-OG	-5.93	95.18	111.20
1	B	108	LYS	C-N-CA	5.93	136.52	121.70
1	A	13	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
1	B	87	ARG	CA-CB-CG	5.91	126.39	113.40
1	B	29	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	43	ALA	N-CA-CB	5.87	118.32	110.10
1	C	90	TYR	CB-CA-C	5.87	122.14	110.40
1	C	60	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	A	6	THR	N-CA-CB	5.82	121.36	110.30
1	A	57	SER	CA-CB-OG	-5.82	95.49	111.20
1	B	65	GLY	N-CA-C	5.81	127.62	113.10
1	A	27	LYS	O-C-N	5.80	131.98	122.70
1	A	99	THR	N-CA-CB	5.80	121.31	110.30
1	C	103	TYR	CB-CG-CD1	5.78	124.47	121.00
1	C	86	ASP	OD1-CG-OD2	5.77	134.26	123.30
1	C	103	TYR	CA-CB-CG	5.76	124.35	113.40
1	A	56	PHE	CB-CA-C	5.69	121.77	110.40
1	A	68	GLY	C-N-CA	5.69	135.92	121.70
1	C	82	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	50	SER	O-C-N	5.64	131.73	122.70
1	B	102	HIS	CA-C-O	5.62	131.89	120.10
1	B	23	ASN	N-CA-CB	-5.60	100.52	110.60
1	A	49	LYS	N-CA-CB	5.57	120.62	110.60
1	B	81	GLY	C-N-CA	5.53	135.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	N-CA-CB	5.53	120.56	110.60
1	B	27	LYS	C-N-CA	5.53	135.52	121.70
1	B	85	SER	N-CA-CB	-5.51	102.23	110.50
1	C	89	LEU	O-C-N	5.50	131.50	122.70
1	A	55	ILE	O-C-N	5.50	131.50	122.70
1	C	8	ASP	CA-CB-CG	-5.49	101.33	113.40
1	C	69	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	A	106	PHE	C-N-CA	5.47	135.37	121.70
1	C	80	SER	CA-CB-OG	-5.46	96.46	111.20
1	A	98	LYS	CA-CB-CG	5.43	125.34	113.40
1	A	97	TYR	CE1-CZ-OH	-5.43	105.45	120.10
1	A	21	PRO	O-C-N	-5.39	114.07	122.70
1	C	74	ALA	N-CA-CB	5.37	117.62	110.10
1	A	21	PRO	CA-C-O	5.36	133.07	120.20
1	C	14	LEU	N-CA-CB	-5.34	99.72	110.40
1	B	23	ASN	O-C-N	-5.32	114.18	122.70
1	B	103	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
1	B	104	GLN	CB-CA-C	-5.32	99.76	110.40
1	C	3	VAL	CA-C-O	5.30	131.24	120.10
1	B	72	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	97	TYR	CB-CG-CD1	5.28	124.17	121.00
1	C	91	ALA	O-C-N	5.27	131.13	122.70
1	C	59	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	106	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	C	50	SER	O-C-N	5.20	131.02	122.70
1	C	10	VAL	O-C-N	5.19	131.01	122.70
1	B	73	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	A	43	ALA	O-C-N	5.17	130.97	122.70
1	A	67	SER	CB-CA-C	5.15	119.89	110.10
1	C	107	THR	CA-CB-CG2	5.13	119.59	112.40
1	C	21	PRO	O-C-N	-5.11	114.53	122.70
1	C	73	GLU	CG-CD-OE1	-5.11	108.09	118.30
1	B	66	LYS	CA-CB-CG	5.10	124.62	113.40
1	A	30	ALA	N-CA-CB	5.10	117.24	110.10
1	C	87	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	19	LYS	CB-CA-C	5.06	120.52	110.40
1	A	21	PRO	C-N-CA	5.05	134.32	121.70
1	A	3	VAL	N-CA-CB	-5.04	100.42	111.50
1	A	13	TYR	CG-CD1-CE1	5.02	125.32	121.30
1	C	89	LEU	CA-CB-CG	5.01	126.83	115.30

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	839	0	789	10	0
1	B	850	0	816	15	0
1	C	870	0	833	10	0
2	A	73	0	0	0	0
2	B	91	0	0	2	0
2	C	102	0	0	2	0
All	All	2825	0	2438	34	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 7.

All (34) 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:39:LYS:HG2	1:B:41:ASN:HB3	1.67	0.75
1:C:74:ALA:HB3	1:C:88:ILE:HG22	1.73	0.71
1:C:3:VAL:HG23	1:C:23:ASN:HB3	1.71	0.71
1:C:98:LYS:HD3	1:C:109:ILE:HG21	1.76	0.65
1:A:28:SER:HA	1:A:31:GLN:HE21	1.64	0.63
1:C:96:ILE:HB	1:C:110:ARG:HB2	1.85	0.57
1:A:101:ASP:HB2	1:A:104:GLN:HE21	1.71	0.56
1:C:21:PRO:HD2	1:C:24:TYR:CD2	2.43	0.53
1:A:46:ALA:N	1:A:47:PRO:HD3	2.23	0.53
1:A:96:ILE:HD12	1:A:110:ARG:HB2	1.91	0.53
1:C:87:ARG:HG3	1:C:103:TYR:CE1	2.49	0.48
1:B:69:ARG:HG3	1:B:91:ALA:HB1	1.95	0.48
1:C:52:GLY:HA2	1:C:74:ALA:HA	1.95	0.47
1:B:74:ALA:HB3	1:B:88:ILE:CG2	2.45	0.46
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.99	0.44
1:B:17:TYR:HB3	1:B:19:LYS:HD2	2.00	0.44
1:B:95:LEU:HD22	1:B:108:LYS:HE3	1.99	0.44
1:A:20:LEU:HA	1:A:21:PRO:HD3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:NZ	1:A:54:ASP:OD2	2.50	0.43
1:C:57:SER:HB2	2:C:153:HOH:O	2.17	0.43
1:B:42:LEU:HD23	1:B:78:TYR:CE1	2.53	0.43
1:A:42:LEU:HD23	1:A:78:TYR:CE2	2.53	0.43
1:A:101:ASP:O	1:A:104:GLN:NE2	2.51	0.43
1:A:87:ARG:HB2	1:A:99:THR:CG2	2.49	0.43
1:B:66:LYS:O	1:B:69:ARG:HB3	2.19	0.43
1:B:57:SER:O	1:B:58:ASN:HB3	2.19	0.42
1:B:5:ASN:HB2	2:B:122:HOH:O	2.18	0.42
1:B:64:PRO:HB3	1:C:34:GLY:HA2	2.02	0.41
1:B:103:TYR:HB3	1:B:106:PHE:HZ	1.86	0.41
1:B:93:ASP:O	1:B:94:TRP:HB2	2.20	0.41
1:B:79:THR:HG23	2:B:165:HOH:O	2.21	0.41
1:B:95:LEU:HD13	1:B:97:TYR:HE1	1.86	0.40
1:B:87:ARG:HG3	1:B:103:TYR:CE2	2.57	0.40
1:C:62:LYS:HB2	2:C:130:HOH:O	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	106/110 (96%)	98 (92%)	8 (8%)	0	100	100
1	B	106/110 (96%)	96 (91%)	9 (8%)	1 (1%)	21	19
1	C	107/110 (97%)	102 (95%)	4 (4%)	1 (1%)	21	19
All	All	319/330 (97%)	296 (93%)	21 (7%)	2 (1%)	30	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	VAL

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Mol	Chain	Res	Type
1	B	58	ASN

### 5.3.2 Protein sidechains ⓘ

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	83/91 (91%)	78 (94%)	5 (6%)	24	26
1	B	87/91 (96%)	77 (88%)	10 (12%)	7	6
1	C	90/91 (99%)	84 (93%)	6 (7%)	20	21
All	All	260/273 (95%)	239 (92%)	21 (8%)	15	14

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	50	SER
1	A	55	ILE
1	A	98	LYS
1	A	102	HIS
1	B	19	LYS
1	B	28	SER
1	B	55	ILE
1	B	62	LYS
1	B	63	LEU
1	B	70	THR
1	B	92	SER
1	B	98	LYS
1	B	103	TYR
1	B	104	GLN
1	C	57	SER
1	C	69	ARG
1	C	92	SER
1	C	102	HIS
1	C	104	GLN
1	C	110	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	104	GLN
1	B	31	GLN
1	C	15	GLN
1	C	18	HIS
1	C	31	GLN

### 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 carbohydrates 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	108/110 (98%)	0.17	2 (1%) 70 68	6, 16, 31, 34	0
1	B	108/110 (98%)	0.25	8 (7%) 17 17	2, 12, 35, 45	0
1	C	109/110 (99%)	-0.19	2 (1%) 71 70	2, 11, 23, 32	0
All	All	325/330 (98%)	0.08	12 (3%) 45 44	2, 13, 32, 45	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	SER	4.1
1	B	68	GLY	3.6
1	B	102	HIS	3.5
1	B	3	VAL	3.1
1	A	67	SER	3.1
1	B	17	TYR	2.9
1	B	105	THR	2.4
1	B	59	ARG	2.4
1	B	65	GLY	2.2
1	A	17	TYR	2.2
1	C	94	TRP	2.1
1	C	68	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.