



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:38 PM GMT

PDB ID : 1BRG  
Title : CRYSTALLOGRAPHIC ANALYSIS OF PHE->LEU SUBSTITUTION IN  
THE HYDROPHOBIC CORE OF BARNASE  
Authors : Chen, Y.W.; Fersht, A.R.; Henrick, K.  
Deposited on : 1994-03-30  
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

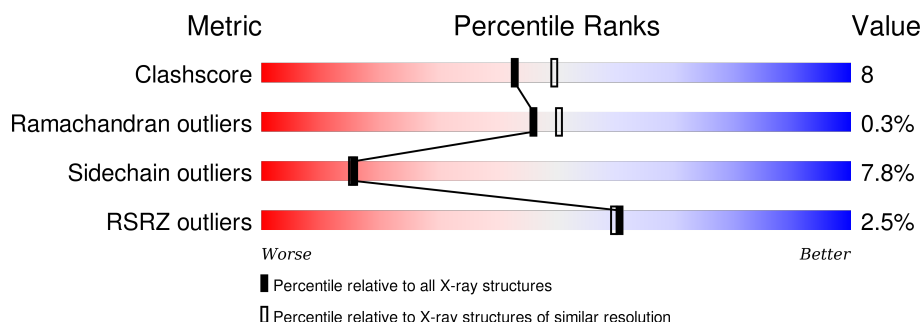
# 1 Overall quality at a glance

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	108	<div> <div>5%</div> <div> <div>53%</div> <div>42%</div> <div>6%</div> </div> </div>
1	B	108	<div> <div>2%</div> <div> <div>54%</div> <div>33%</div> <div>12%</div> </div> </div>
1	C	108	<div> <div>5%</div> <div> <div>55%</div> <div>40%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2752 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
			840	533	142	165			
1	B	108	Total	C	N	O	0	0	0
			843	533	145	165			
1	C	108	Total	C	N	O	0	0	0
			843	533	144	166			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LEU	PHE	CONFLICT	UNP P00648
B	7	LEU	PHE	CONFLICT	UNP P00648
C	7	LEU	PHE	CONFLICT	UNP P00648

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		

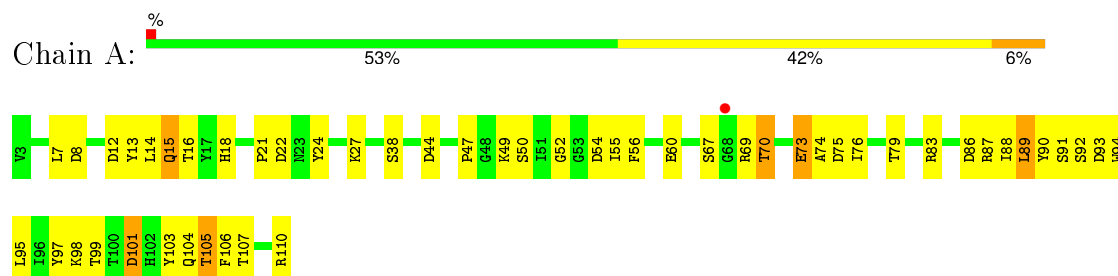
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	77	Total	O	0	0
			77	77		
3	C	79	Total	O	0	0
			79	79		

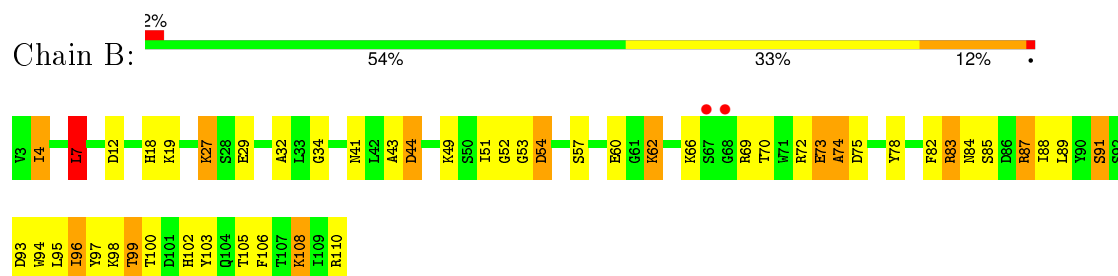
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

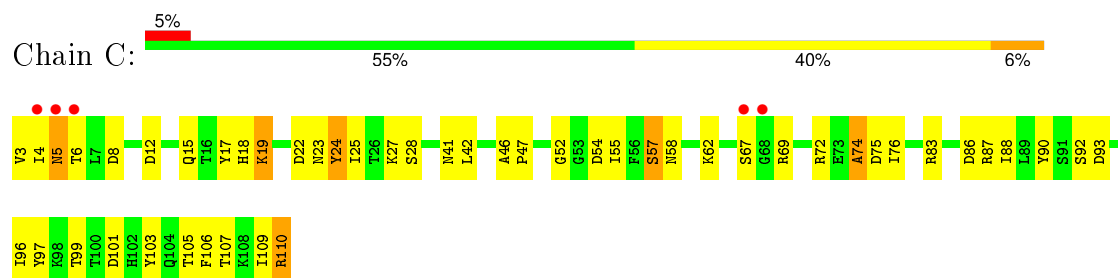
#### • Molecule 1: BARNASE



#### • Molecule 1: BARNASE



#### • Molecule 1: BARNASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.72Å 58.72Å 82.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.20 25.43 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 94.8 (25.43-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.20Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.168 , (Not available) 0.167 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 95.2	EDS
Estimated twinning fraction	0.016 for -h,-k,l 0.056 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15097 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.04	1/860 (0.1%)	2.47	49/1166 (4.2%)
1	B	1.10	3/863 (0.3%)	2.48	50/1170 (4.3%)
1	C	1.06	0/863	2.79	53/1173 (4.5%)
All	All	1.07	4/2586 (0.2%)	2.58	152/3509 (4.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	ARG	CZ-NH2	-5.99	1.25	1.33
1	A	50	SER	CB-OG	-5.40	1.35	1.42
1	B	87	ARG	NE-CZ	5.13	1.39	1.33
1	B	94	TRP	CA-CB	5.02	1.65	1.53

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ARG	NE-CZ-NH1	-21.15	109.72	120.30
1	C	72	ARG	NE-CZ-NH1	20.64	130.62	120.30
1	B	87	ARG	NE-CZ-NH1	20.35	130.47	120.30
1	C	110	ARG	NE-CZ-NH2	18.53	129.56	120.30
1	C	8	ASP	CB-CG-OD1	18.48	134.93	118.30
1	B	54	ASP	CB-CG-OD2	15.52	132.26	118.30
1	A	110	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	C	17	TYR	CB-CG-CD1	-15.14	111.92	121.00
1	C	87	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	C	83	ARG	NE-CZ-NH2	14.71	127.66	120.30
1	B	72	ARG	NE-CZ-NH2	-14.25	113.17	120.30
1	C	69	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	C	17	TYR	CB-CG-CD2	13.13	128.88	121.00
1	A	69	ARG	NE-CZ-NH2	-12.98	113.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	A	110	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	C	69	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	86	ASP	CB-CG-OD1	12.24	129.31	118.30
1	B	87	ARG	NH1-CZ-NH2	-11.77	106.46	119.40
1	C	90	TYR	CB-CG-CD2	-11.72	113.97	121.00
1	B	12	ASP	CB-CG-OD2	11.54	128.68	118.30
1	A	105	THR	OG1-CB-CG2	-11.29	84.03	110.00
1	A	54	ASP	CB-CG-OD2	11.10	128.29	118.30
1	B	83	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	72	ARG	CD-NE-CZ	10.50	138.30	123.60
1	C	86	ASP	CB-CG-OD2	9.95	127.25	118.30
1	C	72	ARG	NH1-CZ-NH2	-9.87	108.54	119.40
1	C	12	ASP	CB-CG-OD2	-9.72	109.55	118.30
1	C	54	ASP	CB-CG-OD2	9.65	126.98	118.30
1	B	108	LYS	CG-CD-CE	9.48	140.34	111.90
1	A	103	TYR	CB-CG-CD1	-9.39	115.37	121.00
1	C	105	THR	CA-CB-CG2	9.17	125.24	112.40
1	A	87	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	B	78	TYR	CB-CG-CD1	-9.11	115.54	121.00
1	C	110	ARG	CA-C-O	9.04	139.09	120.10
1	A	97	TYR	CB-CG-CD2	-9.00	115.60	121.00
1	B	93	ASP	CB-CG-OD2	8.95	126.36	118.30
1	A	103	TYR	CB-CG-CD2	8.78	126.27	121.00
1	C	69	ARG	CD-NE-CZ	8.67	135.74	123.60
1	B	54	ASP	CB-CG-OD1	-8.66	110.51	118.30
1	B	110	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	A	105	THR	CB-CA-C	8.27	133.92	111.60
1	A	27	LYS	CD-CE-NZ	8.21	130.57	111.70
1	A	44	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	A	90	TYR	CB-CG-CD1	8.06	125.83	121.00
1	C	62	LYS	O-C-N	-8.03	109.85	122.70
1	C	24	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	A	101	ASP	CB-CG-OD1	8.00	125.50	118.30
1	C	86	ASP	OD1-CG-OD2	-7.95	108.19	123.30
1	A	56	PHE	CB-CG-CD2	-7.94	115.24	120.80
1	A	24	TYR	CB-CG-CD2	-7.91	116.26	121.00
1	A	90	TYR	CB-CG-CD2	-7.83	116.31	121.00
1	A	99	THR	N-CA-CB	7.71	124.96	110.30
1	B	75	ASP	CB-CG-OD2	7.56	125.10	118.30
1	C	93	ASP	CB-CG-OD1	7.50	125.05	118.30
1	C	72	ARG	CD-NE-CZ	7.43	134.00	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	99	THR	N-CA-CB	7.30	124.17	110.30
1	C	8	ASP	OD1-CG-OD2	-7.30	109.44	123.30
1	A	12	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	60	GLU	CG-CD-OE2	7.25	132.80	118.30
1	B	72	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	C	83	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	B	78	TYR	O-C-N	7.15	134.14	122.70
1	B	27	LYS	N-CA-CB	-7.01	97.98	110.60
1	B	69	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	C	86	ASP	CB-CG-OD1	6.92	124.52	118.30
1	A	105	THR	O-C-N	-6.90	111.66	122.70
1	C	93	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	83	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	73	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	B	41	ASN	N-CA-CB	-6.65	98.63	110.60
1	A	24	TYR	CB-CG-CD1	6.64	124.98	121.00
1	C	41	ASN	N-CA-C	6.64	128.92	111.00
1	B	97	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	C	15	GLN	OE1-CD-NE2	-6.54	106.85	121.90
1	C	97	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	A	15	GLN	O-C-N	6.52	133.13	122.70
1	C	83	ARG	CD-NE-CZ	6.51	132.71	123.60
1	C	87	ARG	CD-NE-CZ	6.49	132.68	123.60
1	C	90	TYR	CB-CG-CD1	6.48	124.89	121.00
1	A	8	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	32	ALA	CB-CA-C	-6.43	100.45	110.10
1	C	42	LEU	O-C-N	6.41	132.96	122.70
1	B	57	SER	N-CA-CB	6.35	120.02	110.50
1	A	56	PHE	CB-CA-C	6.34	123.08	110.40
1	C	74	ALA	N-CA-CB	6.30	118.93	110.10
1	B	94	TRP	CA-CB-CG	-6.24	101.84	113.70
1	C	97	TYR	CB-CG-CD2	6.21	124.73	121.00
1	C	75	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	12	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	105	THR	C-N-CA	6.07	136.86	121.70
1	B	110	ARG	N-CA-CB	6.05	121.49	110.60
1	C	107	THR	O-C-N	6.05	132.38	122.70
1	C	6	THR	N-CA-CB	6.02	121.74	110.30
1	A	105	THR	CA-CB-OG1	5.98	121.55	109.00
1	C	110	ARG	CD-NE-CZ	5.93	131.90	123.60
1	B	100	THR	CA-CB-CG2	5.93	120.70	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ILE	CA-C-O	-5.91	107.70	120.10
1	B	108	LYS	CB-CG-CD	5.90	126.95	111.60
1	A	56	PHE	CG-CD1-CE1	-5.88	114.33	120.80
1	A	107	THR	N-CA-CB	5.88	121.46	110.30
1	A	22	ASP	CB-CG-OD2	5.87	123.59	118.30
1	B	82	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	A	38	SER	O-C-N	5.82	132.01	122.70
1	B	12	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	C	87	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	C	27	LYS	O-C-N	5.78	131.95	122.70
1	A	76	ILE	C-N-CA	5.75	136.09	121.70
1	C	99	THR	N-CA-CB	5.73	121.18	110.30
1	B	53	GLY	CA-C-O	-5.70	110.34	120.60
1	C	69	ARG	O-C-N	5.67	131.78	122.70
1	A	55	ILE	CB-CA-C	-5.66	100.28	111.60
1	B	74	ALA	CB-CA-C	5.66	118.58	110.10
1	B	75	ASP	OD1-CG-OD2	-5.63	112.59	123.30
1	C	101	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	75	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	55	ILE	C-N-CA	5.57	135.61	121.70
1	B	7	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	38	SER	N-CA-CB	5.55	118.82	110.50
1	B	49	LYS	CD-CE-NZ	-5.54	98.95	111.70
1	B	87	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	C	18	HIS	CA-CB-CG	-5.53	104.20	113.60
1	C	5	ASN	O-C-N	5.52	131.53	122.70
1	B	84	ASN	CA-C-O	5.50	131.65	120.10
1	B	83	ARG	CG-CD-NE	5.50	123.34	111.80
1	A	13	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	B	108	LYS	CA-CB-CG	5.48	125.46	113.40
1	C	17	TYR	N-CA-C	5.42	125.64	111.00
1	B	78	TYR	CB-CG-CD2	5.37	124.22	121.00
1	B	62	LYS	O-C-N	-5.37	114.11	122.70
1	B	62	LYS	CA-C-O	5.30	131.24	120.10
1	B	19	LYS	CA-C-N	-5.30	105.55	117.20
1	B	34	GLY	O-C-N	5.28	131.14	122.70
1	C	41	ASN	N-CA-CB	-5.25	101.14	110.60
1	B	96	ILE	O-C-N	5.23	131.07	122.70
1	B	91	SER	CA-C-N	-5.20	105.77	117.20
1	C	106	PHE	CB-CG-CD1	-5.18	117.18	120.80
1	A	13	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	A	55	ILE	O-C-N	5.15	130.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	HIS	CA-CB-CG	-5.11	104.91	113.60
1	B	75	ASP	O-C-N	5.11	130.88	122.70
1	A	79	THR	N-CA-CB	5.11	120.01	110.30
1	A	16	THR	O-C-N	5.11	130.87	122.70
1	B	29	GLU	CG-CD-OE1	5.10	128.49	118.30
1	A	56	PHE	CD1-CE1-CZ	5.09	126.21	120.10
1	A	21	PRO	C-N-CA	5.08	134.41	121.70
1	A	95	LEU	CA-CB-CG	5.05	126.92	115.30
1	C	19	LYS	CD-CE-NZ	5.03	123.26	111.70
1	B	44	ASP	CA-CB-CG	-5.02	102.35	113.40
1	B	95	LEU	N-CA-CB	5.02	120.44	110.40
1	A	22	ASP	OD1-CG-OD2	-5.01	113.78	123.30

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	840	0	792	10	0
1	B	843	0	795	16	0
1	C	843	0	790	14	0
2	C	1	0	0	0	0
3	A	69	0	0	1	0
3	B	77	0	0	4	0
3	C	79	0	0	2	0
All	All	2752	0	2377	40	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 8.

All (40) 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:7:LEU:HD21	1:B:98:LYS:HD3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD13	1:A:106:PHE:HE2	1.55	0.70
1:A:89:LEU:HD13	1:A:106:PHE:CE2	2.34	0.61
1:B:27:LYS:HD2	3:B:182:HOH:O	2.04	0.58
1:A:7:LEU:HD21	1:A:98:LYS:HD3	1.86	0.57
1:B:89:LEU:HD13	1:B:106:PHE:HE2	1.69	0.57
1:B:87:ARG:HB2	1:B:99:THR:HG22	1.87	0.56
1:C:19:LYS:HE3	3:C:165:HOH:O	2.08	0.54
1:C:3:VAL:O	1:C:4:ILE:HG13	2.08	0.54
1:C:76:ILE:HD11	1:C:88:ILE:HG21	1.91	0.53
1:A:52:GLY:HA2	1:A:74:ALA:HA	1.92	0.51
1:C:96:ILE:HB	1:C:110:ARG:HB2	1.92	0.51
1:B:85:SER:HB3	1:B:102:HIS:CE1	2.46	0.51
1:A:47:PRO:HA	3:A:144:HOH:O	2.09	0.50
1:C:46:ALA:N	1:C:47:PRO:HD3	2.27	0.50
1:B:43:ALA:HA	3:B:170:HOH:O	2.11	0.49
1:B:7:LEU:HD21	1:B:98:LYS:CD	2.37	0.48
1:A:14:LEU:O	1:A:18:HIS:HA	2.15	0.47
1:C:74:ALA:O	1:C:88:ILE:HG22	2.14	0.47
1:B:27:LYS:HB2	1:B:54:ASP:OD2	2.14	0.47
1:B:89:LEU:HD13	1:B:106:PHE:CE2	2.49	0.47
1:C:76:ILE:HD11	1:C:88:ILE:CG2	2.45	0.47
1:C:109:ILE:O	1:C:110:ARG:NH1	2.41	0.46
1:A:101:ASP:O	1:A:104:GLN:HG3	2.15	0.46
1:A:70:THR:O	1:A:91:SER:HA	2.15	0.45
1:B:51:ILE:HG13	1:B:83:ARG:HD2	1.98	0.45
1:A:73:GLU:HA	1:A:88:ILE:O	2.17	0.45
1:C:3:VAL:HG22	1:C:23:ASN:HB3	1.99	0.44
1:C:57:SER:O	1:C:58:ASN:HB3	2.18	0.44
1:C:5:ASN:C	1:C:5:ASN:OD1	2.54	0.44
1:B:70:THR:O	1:B:91:SER:HA	2.18	0.44
1:C:24:TYR:CD1	1:C:52:GLY:HA3	2.54	0.43
1:B:52:GLY:HA2	1:B:74:ALA:HA	2.01	0.42
1:C:92:SER:HA	3:C:169:HOH:O	2.18	0.41
1:B:60:GLU:HG3	3:B:140:HOH:O	2.20	0.41
1:B:4:ILE:HA	3:B:163:HOH:O	2.21	0.41
1:B:85:SER:CB	1:B:102:HIS:CE1	3.04	0.41
1:B:73:GLU:HA	1:B:88:ILE:O	2.21	0.41
1:C:74:ALA:HB3	1:C:88:ILE:CG2	2.52	0.40
1:A:15:GLN:HG2	1:A:94:TRP:HB3	2.04	0.40

There are no symmetry-related clashes.

## 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	106/108 (98%)	98 (92%)	8 (8%)	0	100	100
1	B	106/108 (98%)	98 (92%)	7 (7%)	1 (1%)	21	19
1	C	106/108 (98%)	98 (92%)	8 (8%)	0	100	100
All	All	318/324 (98%)	294 (92%)	23 (7%)	1 (0%)	46	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	LYS

### 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	85/91 (93%)	79 (93%)	6 (7%)	18	19
1	B	86/91 (94%)	78 (91%)	8 (9%)	11	10
1	C	86/91 (94%)	80 (93%)	6 (7%)	19	19
All	All	257/273 (94%)	237 (92%)	20 (8%)	16	15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	67	SER

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Mol	Chain	Res	Type
1	A	70	THR
1	A	89	LEU
1	A	92	SER
1	A	105	THR
1	B	7	LEU
1	B	44	ASP
1	B	62	LYS
1	B	73	GLU
1	B	96	ILE
1	B	103	TYR
1	B	105	THR
1	B	108	LYS
1	C	22	ASP
1	C	25	ILE
1	C	28	SER
1	C	57	SER
1	C	67	SER
1	C	103	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	31	GLN
1	A	77	ASN
1	B	102	HIS
1	B	104	GLN
1	C	31	GLN
1	C	102	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	108/108 (100%)	-0.06	1 (0%) 85 85	3, 15, 31, 39	1 (0%)
1	B	108/108 (100%)	-0.20	2 (1%) 70 68	3, 15, 36, 45	0
1	C	108/108 (100%)	-0.12	5 (4%) 36 35	6, 15, 32, 44	0
All	All	324/324 (100%)	-0.13	8 (2%) 61 60	3, 15, 33, 45	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	GLY	3.5
1	C	67	SER	3.3
1	B	67	SER	3.2
1	C	4	ILE	2.5
1	C	5	ASN	2.5
1	A	68	GLY	2.4
1	C	6	THR	2.2
1	C	68	GLY	2.2

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	1	1/1	1.00	0.03	-3.78	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.