



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 05:02 AM EST

PDB ID : 4LYT  
Title : COMPARISON OF RADIATION-INDUCED DECAY AND STRUCTURE  
REFINEMENT FROM X-RAY DATA COLLECTED FROM LYSOZYME  
CRYSTALS AT LOW AND AMBIENT TEMPERATURES  
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Deposited on : unknown  
Resolution : 1.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

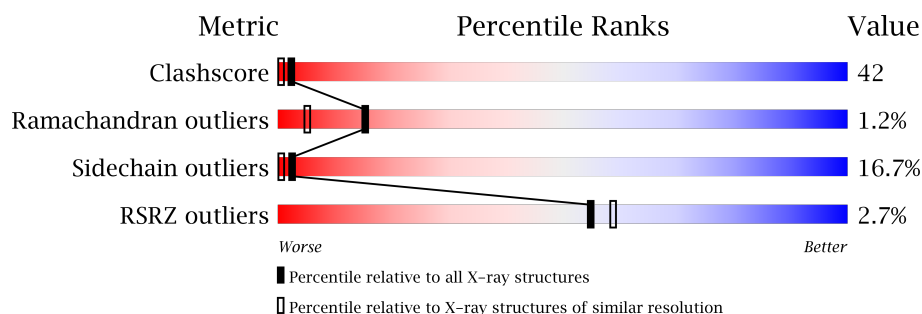
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	129	 3% 38% 40% 16% 6%
1	B	129	 2% 51% 33% 11% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2193 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 HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			
1	B	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

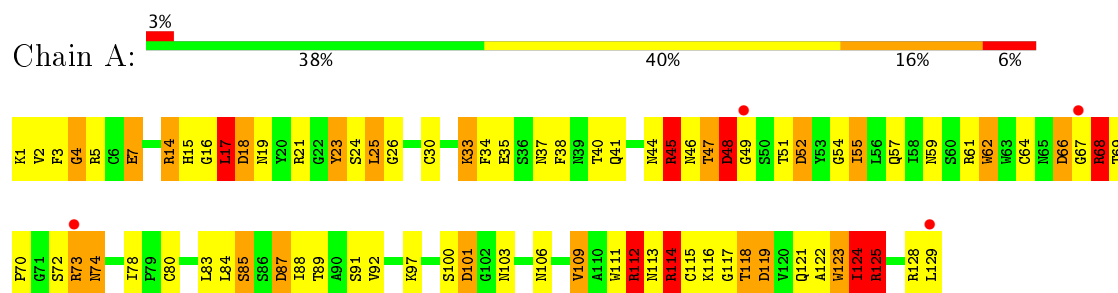
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	105	Total	O	0	0
			105	105		

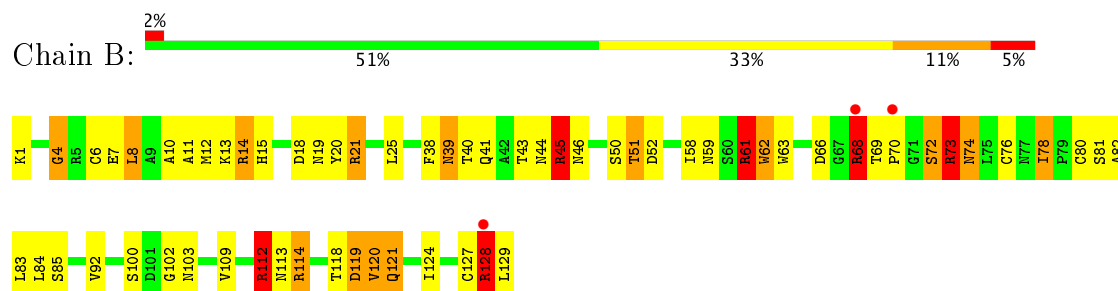
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: HEN EGG WHITE LYSOZYME



#### • Molecule 1: HEN EGG WHITE LYSOZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	27.99Å 62.92Å 60.48Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90 14.72 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 75.6 (14.72-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.31 (at 1.97Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.179 , (Not available) (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-l,-k 0.014 for -h,l,k 0.065 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2193	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.96 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.2841e-04.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1.53	8/1021 (0.8%)	2.08	34/1379 (2.5%)
1	B	1.47	4/1021 (0.4%)	1.91	23/1379 (1.7%)
All	All	1.50	12/2042 (0.6%)	2.00	57/2758 (2.1%)

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	1	2
1	B	0	4
All	All	1	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	ASP	N-CA	12.71	1.71	1.46
1	A	17	LEU	CA-CB	-12.02	1.26	1.53
1	A	17	LEU	N-CA	8.55	1.63	1.46
1	A	35	GLU	CD-OE2	6.88	1.33	1.25
1	B	73	ARG	NE-CZ	-6.35	1.24	1.33
1	A	7	GLU	CD-OE1	6.33	1.32	1.25
1	B	73	ARG	CD-NE	-6.14	1.36	1.46
1	B	72	SER	C-N	-6.05	1.20	1.34
1	A	23	TYR	CE1-CZ	5.71	1.46	1.38
1	A	4	GLY	N-CA	5.59	1.54	1.46
1	A	123	TRP	NE1-CE2	-5.14	1.30	1.37
1	B	62	TRP	CA-CB	5.03	1.65	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLY	C-N-CA	17.16	164.61	121.70
1	A	17	LEU	CA-CB-CG	17.01	154.41	115.30
1	A	112	ARG	NE-CZ-NH2	-12.23	114.19	120.30
1	B	128	ARG	CD-NE-CZ	11.37	139.52	123.60
1	A	18	ASP	N-CA-CB	-11.04	90.73	110.60
1	B	45	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	B	128	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	17	LEU	CB-CA-C	10.32	129.81	110.20
1	A	66	ASP	CB-CG-OD1	10.23	127.50	118.30
1	B	73	ARG	CD-NE-CZ	9.88	137.44	123.60
1	A	5	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	21	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	21	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	B	128	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	B	20	TYR	CB-CG-CD1	-8.71	115.78	121.00
1	B	21	ARG	CD-NE-CZ	8.67	135.73	123.60
1	A	114	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	17	LEU	C-N-CA	-8.32	100.91	121.70
1	A	14	ARG	CD-NE-CZ	8.00	134.79	123.60
1	A	73	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	A	101	ASP	CB-CG-OD2	7.44	124.99	118.30
1	B	73	ARG	CG-CD-NE	-7.35	96.36	111.80
1	A	125	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	17	LEU	N-CA-C	-7.31	91.27	111.00
1	A	112	ARG	NH1-CZ-NH2	7.24	127.37	119.40
1	A	74	ASN	CB-CA-C	6.89	124.17	110.40
1	A	68	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	45	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	A	87	ASP	CB-CA-C	6.72	123.84	110.40
1	B	73	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	45	ARG	CA-CB-CG	6.26	127.16	113.40
1	A	4	GLY	N-CA-C	-6.18	97.66	113.10
1	B	72	SER	CA-C-O	6.15	133.01	120.10
1	B	61	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	B	21	ARG	CA-C-O	6.10	132.90	120.10
1	A	119	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	B	4	GLY	N-CA-C	-5.99	98.12	113.10
1	A	128	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	B	120	VAL	CB-CA-C	5.92	122.65	111.40
1	B	102	GLY	N-CA-C	5.88	127.80	113.10
1	B	112	ARG	CA-CB-CG	5.86	126.30	113.40
1	A	5	ARG	NH1-CZ-NH2	5.69	125.66	119.40
1	A	52	ASP	CB-CG-OD2	-5.59	113.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	A	23	TYR	CB-CG-CD2	5.54	124.32	121.00
1	A	118	THR	N-CA-CB	-5.53	99.79	110.30
1	A	66	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	A	52	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	48	ASP	CB-CA-C	5.36	121.12	110.40
1	B	68	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	18	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	120	VAL	N-CA-CB	-5.16	100.16	111.50
1	B	112	ARG	CB-CG-CD	5.11	124.89	111.60
1	A	34	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	A	124	ILE	CA-CB-CG2	5.05	121.00	110.90
1	A	68	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	62	TRP	N-CA-C	5.01	124.52	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	17	LEU	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	73	ARG	Sidechain
1	B	112	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	68	ARG	Sidechain
1	B	73	ARG	Sidechain

## 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	1001	0	958	90	0
1	B	1001	0	961	73	1
2	A	86	0	0	23	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	105	0	0	16	0
All	All	2193	0	1919	161	2

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 42.

All (161) 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:18:ASP:N	1:A:18:ASP:CA	1.71	1.52
1:B:25:LEU:HD22	1:B:124:ILE:HD11	1.22	1.09
1:A:129:LEU:HA	2:A:234:HOH:O	1.55	1.06
1:A:33:LYS:NZ	1:A:33:LYS:HB2	1.73	1.03
1:A:17:LEU:C	1:A:18:ASP:CA	2.34	0.96
1:A:18:ASP:N	1:A:18:ASP:CB	2.29	0.94
1:B:72:SER:O	2:B:284:HOH:O	1.86	0.94
1:A:117:GLY:HA3	1:B:78:ILE:HD11	1.50	0.93
1:A:48:ASP:HB2	2:A:164:HOH:O	1.70	0.90
1:A:116:LYS:O	2:A:137:HOH:O	1.91	0.89
1:A:113:ASN:HB3	1:A:114:ARG:HH21	1.38	0.88
1:A:59:ASN:HD21	1:A:61:ARG:HB2	1.36	0.87
1:B:68:ARG:O	1:B:68:ARG:HG2	1.74	0.87
1:B:13:LYS:HA	2:B:185:HOH:O	1.75	0.86
1:A:88:ILE:HG23	1:A:92:VAL:HG13	1.58	0.85
1:B:114:ARG:NH2	2:B:257:HOH:O	2.11	0.84
1:B:25:LEU:CD2	1:B:124:ILE:HD11	2.07	0.83
1:A:89:THR:HB	2:A:155:HOH:O	1.79	0.83
1:A:33:LYS:HZ2	1:A:33:LYS:HB2	1.40	0.82
1:A:33:LYS:HZ3	1:A:33:LYS:HB2	1.46	0.81
1:A:48:ASP:HB2	1:A:61:ARG:HH12	1.46	0.78
1:A:67:GLY:O	1:A:69:THR:N	2.13	0.78
1:A:45:ARG:HD2	1:A:46:ASN:N	2.00	0.77
1:A:113:ASN:CB	1:A:114:ARG:HH21	1.98	0.77
1:A:45:ARG:HG2	1:A:51:THR:OG1	1.85	0.76
1:A:59:ASN:ND2	1:A:61:ARG:HB2	2.01	0.76
1:B:74:ASN:HD21	1:B:78:ILE:H	1.33	0.75
1:B:13:LYS:HE3	2:B:307:HOH:O	1.85	0.75
1:A:61:ARG:NH1	2:A:164:HOH:O	2.03	0.74
1:B:11:ALA:HA	1:B:14:ARG:HE	1.53	0.74
1:B:15:HIS:HB3	1:B:92:VAL:HG11	1.70	0.73
1:A:3:PHE:HD2	1:A:7:GLU:HG3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASN:OD1	2:B:262:HOH:O	2.06	0.72
1:A:59:ASN:ND2	1:A:61:ARG:H	1.86	0.72
1:B:7:GLU:HG3	2:B:197:HOH:O	1.89	0.72
1:B:61:ARG:HG3	1:B:62:TRP:CD1	2.25	0.71
1:A:47:THR:C	1:A:49:GLY:H	1.93	0.71
1:A:26:GLY:HA3	2:A:175:HOH:O	1.90	0.71
1:A:119:ASP:HA	2:A:247:HOH:O	1.92	0.70
1:B:112:ARG:HH12	1:B:113:ASN:HD21	1.40	0.69
1:A:74:ASN:HD21	1:A:78:ILE:H	1.38	0.69
1:B:21:ARG:HB2	1:B:21:ARG:CZ	2.22	0.69
1:A:113:ASN:HB3	1:A:114:ARG:NH2	2.08	0.67
1:A:66:ASP:OD1	1:A:68:ARG:HG3	1.93	0.67
1:A:101:ASP:OD1	2:A:281:HOH:O	2.11	0.67
1:B:25:LEU:HD22	1:B:124:ILE:CD1	2.14	0.66
1:A:122:ALA:O	1:A:125:ARG:HB2	1.97	0.65
1:B:118:THR:O	2:B:246:HOH:O	2.15	0.65
1:B:21:ARG:NH2	1:B:100:SER:OG	2.30	0.64
1:B:4:GLY:HA3	2:B:195:HOH:O	1.95	0.64
1:B:69:THR:HG23	1:B:70:PRO:HD2	1.78	0.64
1:B:39:ASN:HD22	1:B:40:THR:N	1.96	0.64
1:A:17:LEU:O	1:A:18:ASP:CA	2.46	0.63
1:A:33:LYS:HZ2	1:A:33:LYS:CB	2.08	0.63
1:A:109:VAL:HG23	2:A:260:HOH:O	1.97	0.63
1:A:88:ILE:HG23	1:A:92:VAL:CG1	2.27	0.63
1:B:13:LYS:NZ	2:B:203:HOH:O	2.22	0.63
1:A:103:ASN:OD1	2:A:143:HOH:O	2.15	0.63
1:B:59:ASN:OD1	1:B:61:ARG:HB3	2.00	0.62
1:B:81:SER:O	1:B:84:LEU:HB2	1.99	0.61
1:B:11:ALA:HA	1:B:14:ARG:NE	2.16	0.61
1:A:41:GLN:NE2	2:A:161:HOH:O	2.34	0.61
1:B:112:ARG:NH1	1:B:113:ASN:HD21	1.98	0.60
1:A:117:GLY:CA	1:B:78:ILE:HD11	2.30	0.60
1:A:24:SER:HB2	2:A:245:HOH:O	2.01	0.60
1:A:59:ASN:ND2	1:A:61:ARG:CB	2.66	0.59
1:B:128:ARG:O	1:B:128:ARG:HD2	2.02	0.59
1:A:87:ASP:HB2	2:A:217:HOH:O	2.01	0.59
1:B:45:ARG:HA	1:B:51:THR:HB	1.85	0.58
1:B:39:ASN:HD22	1:B:39:ASN:C	2.06	0.58
1:B:66:ASP:HB3	1:B:80:CYS:SG	2.43	0.58
1:A:45:ARG:HD2	1:A:46:ASN:H	1.67	0.58
1:A:25:LEU:HD13	1:A:124:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD13	1:A:124:ILE:CD1	2.34	0.57
1:B:109:VAL:CG1	2:B:218:HOH:O	2.51	0.57
1:B:68:ARG:HG3	2:B:315:HOH:O	2.03	0.57
1:B:43:THR:HA	1:B:52:ASP:O	2.05	0.56
1:A:47:THR:O	1:A:49:GLY:N	2.37	0.56
1:A:48:ASP:HB2	1:A:61:ARG:NH1	2.19	0.56
1:A:19:ASN:N	1:A:23:TYR:O	2.36	0.56
1:B:10:ALA:O	1:B:14:ARG:HG3	2.04	0.56
1:A:55:ILE:HD11	1:A:91:SER:CB	2.35	0.56
1:B:68:ARG:O	1:B:68:ARG:CG	2.48	0.56
1:A:109:VAL:HG12	2:A:239:HOH:O	2.05	0.55
1:A:103:ASN:O	1:A:106:ASN:HB2	2.06	0.55
1:B:128:ARG:H	1:B:128:ARG:NE	2.04	0.55
1:B:25:LEU:HD12	2:B:307:HOH:O	2.08	0.54
1:B:46:ASN:N	1:B:50:SER:O	2.34	0.54
1:B:61:ARG:HA	1:B:69:THR:HG21	1.91	0.53
1:B:18:ASP:OD2	2:B:295:HOH:O	2.19	0.53
1:B:45:ARG:HA	1:B:51:THR:HA	1.91	0.53
1:B:8:LEU:HD12	1:B:38:PHE:CD1	2.44	0.52
1:B:69:THR:CG2	1:B:70:PRO:HD2	2.39	0.52
1:A:1:LYS:HG2	1:A:2:VAL:N	2.24	0.52
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.24	0.52
1:A:3:PHE:CD2	1:A:7:GLU:HG3	2.40	0.52
1:B:109:VAL:HG11	2:B:218:HOH:O	2.08	0.52
1:B:58:ILE:HB	1:B:83:LEU:CD1	2.40	0.52
1:A:45:ARG:NH1	1:A:46:ASN:O	2.42	0.51
1:A:33:LYS:NZ	1:A:38:PHE:CZ	2.78	0.51
1:B:21:ARG:HB2	1:B:21:ARG:NH1	2.24	0.50
1:A:129:LEU:HD23	2:A:234:HOH:O	2.10	0.50
1:B:58:ILE:HB	1:B:83:LEU:HD12	1.92	0.50
1:A:40:THR:HB	1:A:85:SER:O	2.12	0.50
1:A:111:TRP:CH2	1:A:116:LYS:HD3	2.48	0.49
1:B:112:ARG:NH1	1:B:113:ASN:ND2	2.61	0.49
1:B:11:ALA:O	1:B:14:ARG:HD2	2.13	0.48
1:B:21:ARG:CB	1:B:21:ARG:CZ	2.89	0.48
1:A:33:LYS:NZ	1:A:38:PHE:CE2	2.82	0.48
1:A:62:TRP:HZ3	2:A:189:HOH:O	1.96	0.48
1:B:69:THR:HB	1:B:72:SER:HB2	1.96	0.47
1:B:128:ARG:H	1:B:128:ARG:CD	2.27	0.47
1:B:44:ASN:O	1:B:51:THR:HA	2.14	0.47
1:A:66:ASP:HB3	1:A:80:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ARG:CB	1:B:21:ARG:NH1	2.78	0.47
1:A:41:GLN:HA	1:A:84:LEU:HD22	1.97	0.47
1:A:61:ARG:O	1:A:72:SER:HA	2.15	0.46
1:B:119:ASP:OD1	1:B:121:GLN:OE1	2.33	0.46
1:A:17:LEU:O	1:A:18:ASP:HA	2.15	0.46
1:B:45:ARG:NH2	1:B:51:THR:HG21	2.31	0.46
1:A:109:VAL:HG21	2:A:191:HOH:O	2.15	0.46
1:B:61:ARG:HG3	1:B:62:TRP:NE1	2.30	0.46
1:A:52:ASP:HB3	1:A:57:GLN:HB3	1.99	0.45
1:B:128:ARG:C	1:B:128:ARG:HD2	2.36	0.45
1:A:46:ASN:O	1:A:49:GLY:N	2.50	0.45
1:A:109:VAL:CG1	2:A:239:HOH:O	2.65	0.45
1:A:33:LYS:HG2	1:A:123:TRP:CH2	2.51	0.45
1:A:48:ASP:CB	1:A:61:ARG:NH1	2.79	0.44
1:A:83:LEU:HA	2:A:212:HOH:O	2.17	0.44
1:B:6:CYS:HB3	1:B:128:ARG:HH12	1.81	0.44
1:B:8:LEU:HD22	1:B:12:MET:HG3	1.98	0.44
1:B:41:GLN:HA	1:B:84:LEU:HD22	1.99	0.43
1:A:44:ASN:HB2	1:A:57:GLN:HE22	1.83	0.43
1:A:66:ASP:O	1:A:68:ARG:HG2	2.18	0.43
1:B:74:ASN:C	1:B:74:ASN:HD22	2.22	0.43
1:B:6:CYS:CB	1:B:127:CYS:SG	3.05	0.43
1:B:19:ASN:O	1:B:21:ARG:N	2.52	0.43
1:B:63:TRP:O	1:B:76:CYS:HB2	2.19	0.43
1:B:82:ALA:C	1:B:84:LEU:H	2.22	0.43
1:A:15:HIS:HD2	2:A:237:HOH:O	2.01	0.43
1:A:4:GLY:H	1:A:7:GLU:HG2	1.84	0.43
1:A:14:ARG:HG3	2:A:184:HOH:O	2.18	0.42
1:A:30:CYS:HB2	1:A:123:TRP:CD1	2.53	0.42
1:B:1:LYS:O	1:B:40:THR:HG23	2.19	0.42
1:A:112:ARG:HE	1:A:116:LYS:HE2	1.84	0.42
1:A:89:THR:O	1:A:92:VAL:HG22	2.20	0.42
1:A:45:ARG:NH1	1:A:46:ASN:C	2.73	0.42
1:A:19:ASN:CA	1:A:23:TYR:O	2.68	0.42
1:A:111:TRP:CD1	1:A:115:CYS:HB2	2.55	0.42
1:B:39:ASN:C	1:B:39:ASN:ND2	2.73	0.41
1:A:64:CYS:HA	1:A:74:ASN:ND2	2.36	0.41
1:A:106:ASN:HD21	1:A:116:LYS:NZ	2.17	0.41
1:A:44:ASN:HB2	1:A:57:GLN:NE2	2.36	0.41
1:B:44:ASN:O	1:B:52:ASP:N	2.50	0.41
1:B:70:PRO:HA	2:B:287:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:NH1	2:B:275:HOH:O	2.54	0.41
1:A:48:ASP:CB	1:A:61:ARG:HH12	2.23	0.41
1:A:123:TRP:HZ2	2:A:317:HOH:O	2.04	0.40
1:A:45:ARG:HG2	1:A:51:THR:HG1	1.81	0.40
1:A:54:GLY:HA2	2:A:160:HOH:O	2.20	0.40
1:A:59:ASN:ND2	1:A:61:ARG:N	2.64	0.40

All (2) 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)
1:B:103:ASN:ND2	1:B:128:ARG:NH2[2_847]	1.81	0.39
2:A:133:HOH:O	2:A:198:HOH:O[2_756]	1.83	0.37

## 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	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	7	1
1	B	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
All	All	254/258 (98%)	234 (92%)	17 (7%)	3 (1%)	15	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	48	ASP
1	A	70	PRO

### 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	105/105 (100%)	86 (82%)	19 (18%)	2	0
1	B	105/105 (100%)	89 (85%)	16 (15%)	3	1
All	All	210/210 (100%)	175 (83%)	35 (17%)	2	0

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	25	LEU
1	A	33	LYS
1	A	37	ASN
1	A	45	ARG
1	A	47	THR
1	A	48	ASP
1	A	55	ILE
1	A	62	TRP
1	A	85	SER
1	A	97	LYS
1	A	100	SER
1	A	109	VAL
1	A	112	ARG
1	A	114	ARG
1	A	118	THR
1	A	121	GLN
1	A	124	ILE
1	A	125	ARG
1	B	8	LEU
1	B	14	ARG
1	B	39	ASN
1	B	51	THR
1	B	61	ARG
1	B	68	ARG
1	B	73	ARG
1	B	74	ASN

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Mol	Chain	Res	Type
1	B	78	ILE
1	B	85	SER
1	B	114	ARG
1	B	119	ASP
1	B	120	VAL
1	B	121	GLN
1	B	128	ARG
1	B	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	37	ASN
1	A	41	GLN
1	A	59	ASN
1	A	74	ASN
1	A	93	ASN
1	A	103	ASN
1	A	106	ASN
1	A	113	ASN
1	A	121	GLN
1	B	39	ASN
1	B	46	ASN
1	B	74	ASN
1	B	93	ASN
1	B	113	ASN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	72:SER	C	73:ARG	N	1.20

## 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	129/129 (100%)	0.27	4 (3%) 49 53	8, 17, 29, 36	0
1	B	129/129 (100%)	0.17	3 (2%) 61 64	6, 15, 29, 32	0
All	All	258/258 (100%)	0.22	7 (2%) 55 59	6, 16, 30, 36	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	ARG	3.8
1	A	129	LEU	3.1
1	A	73	ARG	3.0
1	B	68	ARG	2.6
1	A	49	GLY	2.2
1	B	70	PRO	2.2
1	A	67	GLY	2.1

### 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.