



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LYT  
Title : COMPARISON OF RADIATION-INDUCED DECAY AND STRUCTURE  
REFINEMENT FROM X-RAY DATA COLLECTED FROM LYSOZYME  
CRYSTALS AT LOW AND AMBIENT TEMPERATURES  
Authors : Dewan, J.C.; Young, A.C.M.; Tilton, R.F.  
Deposited on : 1992-03-20  
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  
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

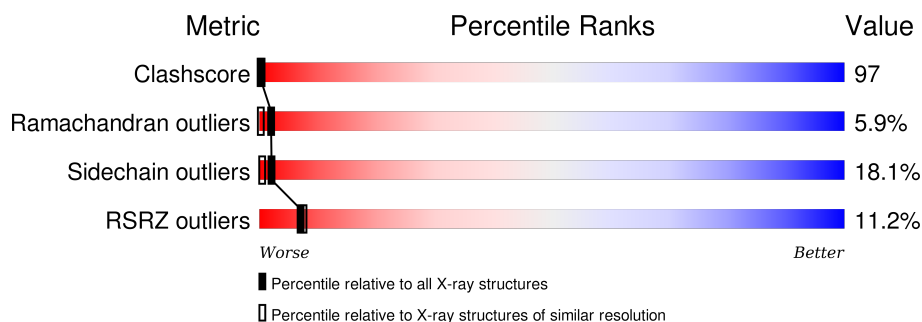
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

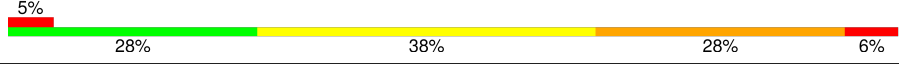

The reported resolution of this entry is 1.90 Å.

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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	
1	B	129	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2408 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			

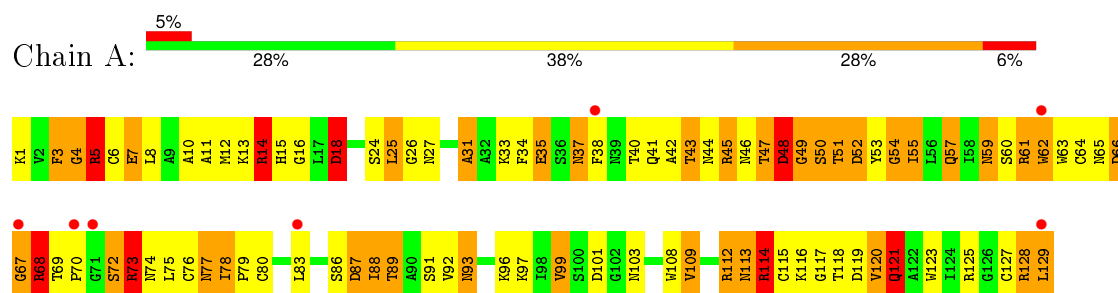
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	0	0
			209	209		
2	B	197	Total	O	0	0
			197	197		

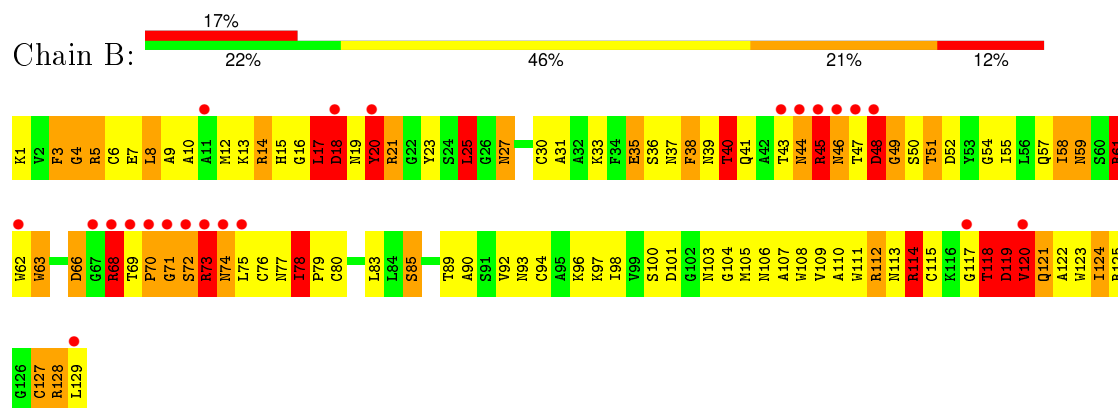
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	27.51Å 62.66Å 59.66Å 90.00° 89.57° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90 17.11 – 1.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 86.8 (17.11-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.99 (at 1.97Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.203 , (Not available) 0.237 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	7.6	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 47.8	EDS
Estimated twinning fraction	0.039 for -h,-l,-k 0.011 for -h,l,k 0.057 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 12514 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	2408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	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 34.23 % 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 7.0490e-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, 0.375 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	1.55	5/1021 (0.5%)	2.33	49/1379 (3.6%)
1	B	1.56	7/1021 (0.7%)	2.18	44/1379 (3.2%)
All	All	1.56	12/2042 (0.6%)	2.26	93/2758 (3.4%)

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
1	B	0	3
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	GLU	CD-OE2	8.80	1.35	1.25
1	B	73	ARG	N-CA	-7.13	1.32	1.46
1	A	114	ARG	CD-NE	-6.02	1.36	1.46
1	B	114	ARG	CD-NE	-5.98	1.36	1.46
1	A	112	ARG	NE-CZ	-5.96	1.25	1.33
1	A	112	ARG	CZ-NH2	5.71	1.40	1.33
1	B	21	ARG	CZ-NH2	-5.43	1.25	1.33
1	A	53	TYR	CG-CD2	5.30	1.46	1.39
1	B	35	GLU	CD-OE1	-5.27	1.19	1.25
1	A	7	GLU	CD-OE2	5.16	1.31	1.25
1	B	4	GLY	CA-C	5.08	1.59	1.51
1	B	72	SER	CA-C	-5.05	1.39	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	CD-NE-CZ	28.30	163.22	123.60
1	A	114	ARG	CD-NE-CZ	13.97	143.16	123.60
1	A	114	ARG	NE-CZ-NH1	13.71	127.16	120.30
1	B	112	ARG	NE-CZ-NH2	12.86	126.73	120.30
1	B	20	TYR	CB-CG-CD1	-12.13	113.72	121.00
1	B	45	ARG	CG-CD-NE	11.75	136.47	111.80
1	B	21	ARG	NE-CZ-NH1	-11.50	114.55	120.30
1	B	46	ASN	CA-CB-CG	11.42	138.53	113.40
1	B	25	LEU	CA-CB-CG	11.15	140.94	115.30
1	A	14	ARG	NE-CZ-NH1	-10.89	114.85	120.30
1	A	45	ARG	CD-NE-CZ	10.56	138.39	123.60
1	B	46	ASN	CB-CA-C	-10.56	89.27	110.40
1	A	128	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	B	120	VAL	C-N-CA	10.21	147.22	121.70
1	B	114	ARG	CD-NE-CZ	9.58	137.01	123.60
1	B	45	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	14	ARG	NE-CZ-NH2	9.38	124.99	120.30
1	A	66	ASP	CB-CG-OD1	8.70	126.12	118.30
1	A	112	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	B	112	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	B	48	ASP	CB-CG-OD1	8.25	125.73	118.30
1	B	72	SER	O-C-N	8.18	135.78	122.70
1	B	20	TYR	CB-CG-CD2	8.11	125.87	121.00
1	B	61	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	A	68	ARG	CD-NE-CZ	7.60	134.25	123.60
1	B	40	THR	CB-CA-C	7.52	131.90	111.60
1	A	7	GLU	CA-CB-CG	7.50	129.90	113.40
1	A	61	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	B	5	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	B	78	ILE	N-CA-CB	-7.15	94.36	110.80
1	A	53	TYR	CB-CG-CD1	7.12	125.27	121.00
1	B	45	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
1	B	73	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	B	68	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	119	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	125	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	B	20	TYR	CA-CB-CG	-6.75	100.57	113.40
1	B	35	GLU	CG-CD-OE1	6.68	131.67	118.30
1	A	52	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	B	18	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	87	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	112	ARG	NH1-CZ-NH2	-6.52	112.22	119.40
1	A	87	ASP	CB-CG-OD1	-6.30	112.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	SER	CA-C-N	-6.27	103.41	117.20
1	A	128	ARG	C-N-CA	6.21	137.24	121.70
1	A	114	ARG	CG-CD-NE	6.17	124.76	111.80
1	A	66	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	128	ARG	CA-C-O	6.10	132.90	120.10
1	A	43	THR	O-C-N	6.06	132.40	122.70
1	B	38	PHE	CA-CB-CG	5.92	128.11	113.90
1	A	50	SER	O-C-N	5.89	132.12	122.70
1	B	35	GLU	CA-CB-CG	5.86	126.30	113.40
1	B	18	ASP	N-CA-CB	5.86	121.15	110.60
1	B	14	ARG	CD-NE-CZ	5.83	131.77	123.60
1	A	61	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	A	119	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	31	ALA	CB-CA-C	5.74	118.71	110.10
1	A	67	GLY	C-N-CA	5.68	135.91	121.70
1	A	51	THR	N-CA-CB	-5.67	99.52	110.30
1	A	37	ASN	N-CA-CB	5.64	120.76	110.60
1	A	72	SER	C-N-CA	5.64	135.80	121.70
1	A	87	ASP	CB-CA-C	5.63	121.67	110.40
1	B	4	GLY	N-CA-C	-5.59	99.11	113.10
1	A	125	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	B	78	ILE	N-CA-C	5.57	126.03	111.00
1	A	5	ARG	CG-CD-NE	5.55	123.45	111.80
1	A	48	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	72	SER	N-CA-CB	5.53	118.80	110.50
1	A	128	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	A	121	GLN	CA-CB-CG	5.50	125.49	113.40
1	A	18	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	3	PHE	CB-CG-CD1	-5.45	116.98	120.80
1	A	73	ARG	N-CA-CB	5.41	120.34	110.60
1	B	17	LEU	CB-CA-C	5.40	120.45	110.20
1	B	17	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	40	THR	N-CA-CB	-5.36	100.11	110.30
1	A	5	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	61	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	B	58	ILE	CB-CA-C	5.32	122.25	111.60
1	B	127	CYS	CA-C-N	-5.32	105.50	117.20
1	B	3	PHE	O-C-N	5.31	132.22	123.20
1	A	4	GLY	N-CA-C	-5.28	99.91	113.10
1	B	66	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	14	ARG	CD-NE-CZ	5.25	130.95	123.60
1	B	63	TRP	N-CA-C	5.22	125.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	3	PHE	O-C-N	5.14	131.94	123.20
1	A	54	GLY	N-CA-C	5.13	125.92	113.10
1	A	18	ASP	CB-CA-C	5.13	120.65	110.40
1	A	68	ARG	CG-CD-NE	5.08	122.47	111.80
1	B	46	ASN	O-C-N	5.06	130.79	122.70
1	A	87	ASP	N-CA-CB	5.04	119.68	110.60
1	B	85	SER	N-CA-CB	5.02	118.03	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	61	ARG	Sidechain
1	B	68	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	961	173	0
1	B	1001	0	962	202	0
2	A	209	0	0	76	0
2	B	197	0	0	73	1
All	All	2408	0	1923	373	1

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 97.

All (373) 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:55:ILE:HG12	2:A:143:HOH:O	1.28	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HB	2:B:341:HOH:O	1.12	1.29
1:B:37:ASN:HB2	2:B:172:HOH:O	1.25	1.25
1:A:113:ASN:HB3	2:A:197:HOH:O	1.30	1.25
1:A:35:GLU:O	2:A:416:HOH:O	1.52	1.24
1:A:12:MET:HA	2:A:378:HOH:O	1.33	1.23
1:A:3:PHE:CE2	2:A:290:HOH:O	1.91	1.22
1:A:55:ILE:HD13	1:A:88:ILE:HG13	1.21	1.19
1:B:59:ASN:HB3	2:B:459:HOH:O	1.43	1.18
1:B:114:ARG:HG3	2:B:404:HOH:O	1.45	1.16
1:B:46:ASN:O	2:B:476:HOH:O	1.61	1.14
1:A:3:PHE:HE2	2:A:290:HOH:O	1.21	1.13
1:A:114:ARG:HD2	2:A:197:HOH:O	1.48	1.13
1:B:1:LYS:N	1:B:40:THR:HG23	1.64	1.12
1:B:61:ARG:HA	1:B:69:THR:HG21	1.14	1.11
1:A:120:VAL:HB	2:A:250:HOH:O	1.51	1.09
1:B:7:GLU:OE2	2:B:449:HOH:O	1.70	1.07
1:A:41:GLN:HG2	2:A:496:HOH:O	1.54	1.06
1:A:41:GLN:HB3	2:A:496:HOH:O	1.55	1.06
1:B:14:ARG:HB3	2:B:205:HOH:O	1.56	1.06
1:A:117:GLY:HA3	1:B:78:ILE:HD11	1.36	1.05
1:B:124:ILE:O	1:B:127:CYS:HB2	1.58	1.02
1:A:121:GLN:CD	2:A:352:HOH:O	1.97	1.02
1:B:45:ARG:HA	1:B:51:THR:HB	1.42	1.01
1:B:69:THR:HB	1:B:72:SER:HB2	1.38	1.01
1:B:15:HIS:HB3	1:B:92:VAL:HG11	1.43	0.99
1:A:120:VAL:CB	2:A:250:HOH:O	2.07	0.98
1:B:75:LEU:HG	2:B:417:HOH:O	1.64	0.97
1:B:71:GLY:HA3	1:B:73:ARG:HH21	1.28	0.97
1:B:120:VAL:HA	2:B:406:HOH:O	1.63	0.96
1:A:33:LYS:HG2	1:A:38:PHE:CZ	2.01	0.96
1:A:65:ASN:HB3	2:A:178:HOH:O	1.66	0.95
1:B:61:ARG:HA	1:B:69:THR:CG2	1.98	0.94
1:B:57:GLN:CB	2:B:282:HOH:O	2.14	0.94
1:A:59:ASN:HD22	1:A:61:ARG:H	1.08	0.94
1:A:121:GLN:NE2	2:A:352:HOH:O	2.00	0.93
1:A:112:ARG:HD2	1:A:116:LYS:HD3	1.49	0.92
1:B:37:ASN:CB	2:B:172:HOH:O	1.94	0.92
1:B:35:GLU:O	1:B:57:GLN:NE2	2.03	0.91
1:A:55:ILE:CD1	1:A:88:ILE:HG13	2.00	0.91
1:B:1:LYS:H3	1:B:40:THR:HG23	1.30	0.90
1:A:88:ILE:CG2	1:A:92:VAL:HG13	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD12	2:A:142:HOH:O	1.69	0.89
1:B:107:ALA:CA	2:B:307:HOH:O	2.18	0.89
1:A:49:GLY:O	2:A:488:HOH:O	1.91	0.89
1:B:69:THR:CB	1:B:72:SER:HB2	2.02	0.89
1:A:41:GLN:CG	2:A:496:HOH:O	2.12	0.89
1:B:118:THR:HG21	2:B:425:HOH:O	1.71	0.89
1:B:1:LYS:H2	1:B:40:THR:HG23	1.38	0.88
1:B:57:GLN:HB2	2:B:282:HOH:O	1.69	0.88
1:B:46:ASN:ND2	1:B:59:ASN:OD1	2.07	0.88
1:B:107:ALA:N	2:B:307:HOH:O	2.06	0.88
1:B:97:LYS:HB3	2:B:417:HOH:O	1.71	0.88
1:A:47:THR:HG21	2:A:327:HOH:O	1.72	0.87
1:A:33:LYS:NZ	2:A:171:HOH:O	1.66	0.86
1:B:44:ASN:C	1:B:45:ARG:HD2	1.95	0.86
1:A:45:ARG:NH2	1:A:49:GLY:HA2	1.91	0.85
1:A:55:ILE:HG22	2:A:348:HOH:O	1.77	0.85
1:B:71:GLY:HA3	1:B:73:ARG:NH2	1.92	0.84
1:A:60:SER:HB2	2:A:365:HOH:O	1.77	0.84
1:A:63:TRP:O	1:A:76:CYS:HB2	1.78	0.84
1:A:3:PHE:HD1	1:A:7:GLU:HG3	1.40	0.84
1:A:113:ASN:CB	2:A:197:HOH:O	1.98	0.84
1:A:41:GLN:NE2	2:A:471:HOH:O	2.09	0.83
1:A:8:LEU:HD22	2:A:348:HOH:O	1.76	0.83
1:A:120:VAL:HG12	2:A:250:HOH:O	1.78	0.83
1:A:34:PHE:HA	2:A:495:HOH:O	1.78	0.83
1:B:100:SER:HA	2:B:428:HOH:O	1.78	0.82
1:B:74:ASN:ND2	1:B:74:ASN:O	2.12	0.82
1:B:69:THR:HG22	1:B:70:PRO:HD2	1.60	0.82
1:A:88:ILE:HG23	1:A:92:VAL:HG13	1.61	0.82
1:A:4:GLY:H	1:A:7:GLU:HG2	1.44	0.82
1:A:115:CYS:O	1:A:118:THR:HB	1.79	0.82
1:A:33:LYS:CE	2:A:171:HOH:O	2.17	0.82
1:B:35:GLU:OE2	1:B:108:TRP:HB3	1.79	0.81
1:A:62:TRP:HB3	1:A:73:ARG:NH2	1.96	0.81
1:B:63:TRP:O	1:B:76:CYS:HB2	1.80	0.80
1:B:59:ASN:ND2	1:B:61:ARG:HB2	1.98	0.79
1:B:27:ASN:HB2	1:B:111:TRP:HE1	1.45	0.78
1:B:17:LEU:HD23	2:B:462:HOH:O	1.84	0.78
1:B:124:ILE:HD12	2:B:245:HOH:O	1.83	0.78
1:A:112:ARG:HD2	1:A:116:LYS:CD	2.13	0.78
1:B:7:GLU:N	2:B:234:HOH:O	1.78	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:SER:C	2:B:172:HOH:O	2.21	0.78
1:B:33:LYS:NZ	2:B:286:HOH:O	2.16	0.77
1:B:1:LYS:N	1:B:40:THR:CG2	2.46	0.77
1:B:118:THR:CG2	2:B:425:HOH:O	2.27	0.76
1:B:48:ASP:OD1	1:B:48:ASP:N	2.18	0.76
1:B:113:ASN:HB3	1:B:114:ARG:HE	1.50	0.76
1:B:1:LYS:O	1:B:40:THR:HG22	1.86	0.76
1:B:14:ARG:CB	2:B:205:HOH:O	2.22	0.76
1:A:109:VAL:HG22	2:A:405:HOH:O	1.85	0.76
1:A:74:ASN:HD22	1:A:77:ASN:HA	1.49	0.76
1:A:55:ILE:HD13	1:A:88:ILE:CG1	2.12	0.75
1:A:88:ILE:CG2	1:A:92:VAL:CG1	2.64	0.75
1:A:50:SER:HB3	1:A:59:ASN:HD21	1.51	0.75
1:A:45:ARG:O	2:A:220:HOH:O	2.05	0.75
1:A:16:GLY:HA2	2:A:165:HOH:O	1.86	0.75
1:B:69:THR:HB	1:B:72:SER:CB	2.17	0.74
1:B:62:TRP:O	1:B:74:ASN:HA	1.87	0.74
1:A:18:ASP:OD2	2:A:202:HOH:O	2.05	0.74
1:B:63:TRP:CZ3	1:B:75:LEU:HB3	2.23	0.73
1:A:103:ASN:OD1	2:A:226:HOH:O	2.06	0.73
1:A:41:GLN:CD	2:A:471:HOH:O	2.27	0.73
1:A:120:VAL:CG1	2:A:250:HOH:O	2.25	0.72
1:A:35:GLU:C	2:A:416:HOH:O	2.09	0.72
1:B:59:ASN:HD21	1:B:61:ARG:HB2	1.51	0.71
1:B:45:ARG:NH1	2:B:452:HOH:O	2.22	0.71
1:A:34:PHE:O	2:A:495:HOH:O	2.08	0.71
1:B:78:ILE:HG23	1:B:79:PRO:O	1.90	0.70
1:A:45:ARG:HD2	1:A:50:SER:O	1.92	0.70
1:B:57:GLN:HB3	2:B:282:HOH:O	1.82	0.70
1:A:1:LYS:HB3	1:A:40:THR:HG21	1.73	0.70
1:A:31:ALA:HA	2:A:174:HOH:O	1.91	0.70
1:B:69:THR:CG2	1:B:70:PRO:HD2	2.21	0.70
1:A:86:SER:OG	2:A:529:HOH:O	2.10	0.70
1:B:1:LYS:H3	1:B:40:THR:CG2	2.03	0.69
1:A:47:THR:O	1:A:49:GLY:N	2.25	0.69
1:B:74:ASN:HD22	1:B:74:ASN:C	1.95	0.68
1:A:33:LYS:HE3	1:A:123:TRP:HZ3	1.57	0.68
1:A:59:ASN:ND2	1:A:61:ARG:H	1.89	0.68
1:A:33:LYS:O	1:A:37:ASN:HA	1.93	0.68
1:A:41:GLN:CB	2:A:496:HOH:O	2.14	0.68
1:B:107:ALA:HA	2:B:307:HOH:O	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:O	1:A:14:ARG:HD2	1.94	0.68
1:B:14:ARG:HD2	2:B:205:HOH:O	1.95	0.67
1:B:48:ASP:O	1:B:50:SER:N	2.28	0.67
1:A:73:ARG:HG2	2:A:301:HOH:O	1.95	0.67
1:A:67:GLY:O	1:A:69:THR:N	2.26	0.66
1:B:97:LYS:CE	1:B:97:LYS:HA	2.25	0.66
1:A:43:THR:O	1:A:44:ASN:ND2	2.29	0.66
1:A:74:ASN:ND2	1:A:77:ASN:HA	2.09	0.66
1:B:61:ARG:HB2	2:B:331:HOH:O	1.94	0.66
1:B:120:VAL:HG12	1:B:121:GLN:N	2.10	0.66
1:B:7:GLU:CG	2:B:294:HOH:O	2.43	0.66
1:A:52:ASP:HB3	1:A:57:GLN:HB3	1.78	0.66
1:B:44:ASN:HB3	1:B:52:ASP:HB2	1.78	0.66
1:A:117:GLY:CA	1:B:78:ILE:HD11	2.22	0.65
1:B:96:LYS:NZ	2:B:284:HOH:O	2.28	0.65
1:A:8:LEU:CD2	2:A:348:HOH:O	2.41	0.65
1:A:55:ILE:HD11	1:A:91:SER:HB2	1.78	0.65
1:B:33:LYS:HE2	2:B:312:HOH:O	1.95	0.65
1:A:61:ARG:HA	1:A:69:THR:HG21	1.78	0.65
1:B:122:ALA:O	2:B:166:HOH:O	2.14	0.65
1:A:37:ASN:O	2:A:395:HOH:O	2.14	0.64
1:A:113:ASN:ND2	2:A:287:HOH:O	2.21	0.64
1:A:72:SER:C	1:A:73:ARG:HD3	2.18	0.64
1:B:113:ASN:CB	1:B:114:ARG:HE	2.09	0.64
1:A:112:ARG:HH21	1:A:116:LYS:NZ	1.96	0.64
1:B:6:CYS:N	2:B:234:HOH:O	2.30	0.63
1:B:114:ARG:CG	2:B:404:HOH:O	2.20	0.63
1:A:33:LYS:HE2	2:A:171:HOH:O	1.89	0.63
1:B:112:ARG:NH1	2:B:437:HOH:O	2.30	0.63
1:A:33:LYS:HG2	1:A:38:PHE:CE1	2.33	0.63
1:A:12:MET:CA	2:A:378:HOH:O	2.13	0.63
1:B:1:LYS:HA	2:B:319:HOH:O	1.99	0.63
1:B:112:ARG:HB2	2:B:439:HOH:O	1.98	0.63
1:B:120:VAL:HG12	1:B:121:GLN:HG3	1.80	0.62
1:A:128:ARG:HG2	2:A:338:HOH:O	1.99	0.62
1:B:5:ARG:NH2	1:B:125:ARG:O	2.31	0.62
1:B:40:THR:OG1	1:B:85:SER:O	2.16	0.62
1:A:44:ASN:HB2	2:A:252:HOH:O	1.99	0.62
1:B:61:ARG:NH1	1:B:70:PRO:HG2	2.15	0.62
1:B:94:CYS:O	1:B:98:ILE:HG13	1.99	0.62
1:B:17:LEU:HD13	1:B:96:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:O	1:A:73:ARG:HD3	1.98	0.62
1:A:59:ASN:O	1:A:62:TRP:O	2.17	0.62
1:B:124:ILE:O	1:B:127:CYS:CB	2.43	0.62
1:B:33:LYS:HE2	2:B:336:HOH:O	1.99	0.62
1:A:1:LYS:O	1:A:40:THR:HG23	2.00	0.62
1:B:63:TRP:HZ3	1:B:75:LEU:HB3	1.63	0.61
1:B:123:TRP:CZ3	2:B:340:HOH:O	2.51	0.61
1:B:114:ARG:O	2:B:324:HOH:O	2.16	0.61
1:A:24:SER:O	1:A:27:ASN:HB2	2.00	0.61
1:B:105:MET:HE2	1:B:111:TRP:CE2	2.36	0.61
1:B:59:ASN:CB	2:B:459:HOH:O	2.19	0.60
1:B:31:ALA:HB2	1:B:111:TRP:CD1	2.36	0.60
1:B:10:ALA:O	1:B:14:ARG:HG3	2.01	0.60
1:B:44:ASN:ND2	2:B:469:HOH:O	2.33	0.60
1:A:67:GLY:HA2	2:A:492:HOH:O	2.01	0.60
1:B:118:THR:HG22	1:B:119:ASP:H	1.67	0.60
1:B:31:ALA:HB2	1:B:111:TRP:HD1	1.67	0.59
1:A:55:ILE:CG1	2:A:143:HOH:O	2.10	0.59
1:B:66:ASP:HB3	1:B:80:CYS:SG	2.41	0.59
1:A:5:ARG:HE	1:A:33:LYS:HE3	1.67	0.59
1:A:5:ARG:NH1	2:A:247:HOH:O	2.35	0.59
1:A:43:THR:CG2	2:A:354:HOH:O	2.50	0.59
1:B:37:ASN:N	2:B:172:HOH:O	2.34	0.59
1:B:54:GLY:O	1:B:57:GLN:HG2	2.02	0.59
1:B:68:ARG:O	1:B:72:SER:HB3	2.03	0.59
1:B:89:THR:HG22	1:B:93:ASN:ND2	2.18	0.59
1:B:7:GLU:HG3	2:B:294:HOH:O	2.00	0.58
1:B:59:ASN:ND2	1:B:61:ARG:H	2.01	0.58
1:B:23:TYR:HE2	2:B:357:HOH:O	1.85	0.58
1:B:7:GLU:HG2	2:B:294:HOH:O	2.02	0.58
1:B:45:ARG:CA	1:B:51:THR:HB	2.27	0.58
1:B:33:LYS:HE3	1:B:37:ASN:OD1	2.04	0.58
1:A:1:LYS:HB3	1:A:40:THR:CG2	2.33	0.58
1:B:92:VAL:O	1:B:96:LYS:HG3	2.04	0.58
1:B:117:GLY:O	1:B:118:THR:O	2.22	0.57
1:B:44:ASN:O	1:B:45:ARG:HD2	2.04	0.57
1:A:73:ARG:HB3	2:A:361:HOH:O	2.04	0.57
1:A:11:ALA:O	1:A:15:HIS:ND1	2.38	0.57
1:A:43:THR:HG21	2:A:354:HOH:O	2.05	0.57
1:A:47:THR:CG2	2:A:327:HOH:O	2.43	0.56
1:A:6:CYS:SG	1:A:127:CYS:HA	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD23	2:A:383:HOH:O	2.04	0.56
1:B:21:ARG:NH2	2:B:532:HOH:O	2.31	0.56
1:A:35:GLU:CG	1:A:57:GLN:HB2	2.36	0.56
1:B:47:THR:HB	1:B:48:ASP:OD1	2.04	0.56
1:A:35:GLU:HG2	1:A:57:GLN:HB2	1.86	0.55
1:A:112:ARG:HH21	1:A:116:LYS:HZ3	1.55	0.55
1:B:89:THR:HG22	1:B:93:ASN:HD21	1.71	0.55
1:B:45:ARG:HA	1:B:51:THR:CB	2.27	0.55
2:A:402:HOH:O	1:B:79:PRO:HG2	2.07	0.55
1:B:8:LEU:O	1:B:9:ALA:C	2.45	0.55
1:A:65:ASN:O	1:A:79:PRO:HA	2.07	0.55
1:A:75:LEU:HD21	2:A:391:HOH:O	2.05	0.55
1:A:33:LYS:CG	1:A:38:PHE:CZ	2.85	0.54
1:A:33:LYS:HE3	1:A:123:TRP:CZ3	2.39	0.54
1:B:61:ARG:O	1:B:72:SER:HA	2.08	0.54
1:B:61:ARG:CA	1:B:69:THR:HG21	2.09	0.54
1:A:93:ASN:ND2	2:A:355:HOH:O	2.39	0.54
1:B:90:ALA:HB3	2:B:280:HOH:O	2.07	0.54
1:B:59:ASN:ND2	2:B:331:HOH:O	2.41	0.54
1:B:39:ASN:OD1	1:B:41:GLN:HB2	2.08	0.54
1:B:8:LEU:HD22	1:B:12:MET:HG3	1.90	0.54
1:A:54:GLY:O	1:A:57:GLN:OE1	2.26	0.53
1:A:70:PRO:HG3	2:A:270:HOH:O	2.08	0.53
1:B:107:ALA:HB2	2:B:307:HOH:O	2.08	0.53
1:B:8:LEU:CD2	1:B:12:MET:HG3	2.39	0.53
1:B:75:LEU:CG	2:B:417:HOH:O	2.40	0.53
1:B:110:ALA:O	1:B:114:ARG:HD2	2.09	0.53
1:A:26:GLY:C	1:A:120:VAL:HG13	2.28	0.53
1:A:27:ASN:N	1:A:120:VAL:HG13	2.24	0.53
1:A:128:ARG:NE	2:A:338:HOH:O	2.42	0.53
1:A:10:ALA:O	1:A:14:ARG:HB2	2.09	0.53
1:B:128:ARG:NH1	2:B:241:HOH:O	2.07	0.53
1:A:112:ARG:NH2	1:A:116:LYS:HZ3	2.06	0.53
1:A:64:CYS:C	1:A:74:ASN:HB3	2.30	0.53
1:B:80:CYS:O	1:B:83:LEU:HB2	2.08	0.52
1:A:33:LYS:CE	1:A:123:TRP:HZ3	2.22	0.52
1:A:45:ARG:CZ	1:A:49:GLY:HA2	2.38	0.52
1:B:6:CYS:O	1:B:9:ALA:HB3	2.10	0.52
1:B:35:GLU:OE1	2:B:474:HOH:O	2.18	0.52
1:B:45:ARG:HA	1:B:51:THR:HA	1.91	0.52
1:A:112:ARG:NE	1:A:116:LYS:HZ3	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HE2	1:B:111:TRP:CD2	2.43	0.52
1:B:14:ARG:HB3	1:B:14:ARG:HH11	1.75	0.52
1:A:120:VAL:CA	2:A:250:HOH:O	2.50	0.51
1:B:61:ARG:HH11	1:B:70:PRO:HG2	1.75	0.51
1:A:88:ILE:HG22	1:A:92:VAL:HG13	1.88	0.51
1:B:17:LEU:HD22	1:B:92:VAL:HG13	1.91	0.51
1:B:69:THR:C	1:B:71:GLY:H	2.12	0.51
1:B:1:LYS:H2	1:B:40:THR:CG2	2.14	0.51
1:A:74:ASN:HD22	1:A:77:ASN:CA	2.22	0.51
1:B:128:ARG:H	1:B:128:ARG:NE	2.09	0.51
1:A:33:LYS:HE2	1:A:38:PHE:CE2	2.46	0.51
1:B:31:ALA:O	1:B:35:GLU:N	2.37	0.51
1:B:19:ASN:N	1:B:23:TYR:O	2.43	0.51
1:B:77:ASN:O	1:B:78:ILE:HD12	2.10	0.51
1:A:112:ARG:CD	1:A:116:LYS:HD3	2.31	0.51
1:B:107:ALA:CB	2:B:307:HOH:O	2.55	0.51
1:A:129:LEU:CB	2:A:422:HOH:O	2.59	0.51
1:B:76:CYS:SG	1:B:94:CYS:HA	2.51	0.51
1:A:78:ILE:HD13	1:A:83:LEU:HD13	1.93	0.50
1:B:12:MET:O	1:B:17:LEU:HB2	2.11	0.50
1:A:34:PHE:C	2:A:495:HOH:O	2.50	0.50
1:A:8:LEU:HD23	1:A:38:PHE:CE1	2.46	0.50
1:B:9:ALA:O	1:B:25:LEU:HD21	2.12	0.50
1:B:114:ARG:N	1:B:114:ARG:HD2	2.27	0.50
1:B:121:GLN:HB2	2:B:366:HOH:O	2.12	0.50
1:B:62:TRP:CZ3	1:B:73:ARG:HD2	2.46	0.50
1:B:5:ARG:NH1	1:B:125:ARG:O	2.44	0.50
1:B:14:ARG:CG	2:B:205:HOH:O	2.54	0.49
1:B:101:ASP:O	1:B:101:ASP:OD1	2.29	0.49
1:A:108:TRP:HA	2:A:405:HOH:O	2.12	0.49
1:A:4:GLY:N	1:A:7:GLU:HG2	2.22	0.49
1:B:30:CYS:CB	1:B:115:CYS:SG	3.00	0.49
1:A:47:THR:O	1:A:48:ASP:C	2.50	0.49
1:B:120:VAL:CG1	1:B:121:GLN:N	2.75	0.49
1:A:78:ILE:CD1	1:A:83:LEU:HD13	2.43	0.49
1:B:25:LEU:HD23	2:B:432:HOH:O	2.13	0.49
1:B:114:ARG:HA	2:B:404:HOH:O	2.12	0.48
1:B:4:GLY:C	2:B:234:HOH:O	2.51	0.48
1:A:76:CYS:SG	1:A:97:LYS:HE2	2.52	0.48
1:A:37:ASN:O	1:A:38:PHE:HB2	2.13	0.48
1:B:75:LEU:CD2	2:B:417:HOH:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:O	1:B:45:ARG:N	2.46	0.48
1:B:45:ARG:NH1	2:B:150:HOH:O	2.47	0.48
1:B:119:ASP:HB2	2:B:221:HOH:O	2.13	0.48
1:B:18:ASP:N	2:B:432:HOH:O	2.46	0.48
1:A:6:CYS:SG	1:A:127:CYS:CA	3.02	0.47
1:B:77:ASN:C	1:B:78:ILE:HD12	2.34	0.47
1:B:128:ARG:HA	2:B:232:HOH:O	2.14	0.47
1:B:43:THR:HA	1:B:52:ASP:O	2.14	0.47
1:B:109:VAL:O	1:B:110:ALA:C	2.53	0.47
1:A:68:ARG:NH2	2:A:490:HOH:O	2.48	0.47
1:A:129:LEU:HB2	2:A:422:HOH:O	2.13	0.47
1:B:103:ASN:O	1:B:106:ASN:HB2	2.15	0.47
1:B:43:THR:C	1:B:52:ASP:O	2.52	0.47
1:B:68:ARG:NH1	2:B:179:HOH:O	2.46	0.47
1:A:112:ARG:HG3	1:A:112:ARG:O	2.15	0.47
1:A:99:VAL:HG13	1:A:108:TRP:HZ3	1.80	0.47
1:A:35:GLU:OE1	1:A:108:TRP:CD1	2.68	0.47
1:B:68:ARG:HB3	1:B:69:THR:H	1.40	0.46
1:A:112:ARG:CZ	1:A:116:LYS:HZ3	2.28	0.46
1:A:50:SER:CB	1:A:59:ASN:HD21	2.24	0.46
1:A:33:LYS:NZ	2:A:525:HOH:O	2.47	0.46
1:A:88:ILE:HG23	1:A:92:VAL:CG1	2.34	0.46
1:A:112:ARG:NH2	1:A:116:LYS:NZ	2.61	0.46
1:A:114:ARG:HA	1:A:114:ARG:NE	2.30	0.46
1:B:128:ARG:N	1:B:128:ARG:NE	2.64	0.46
1:B:128:ARG:HH21	1:B:129:LEU:CD2	2.29	0.45
1:A:46:ASN:HB3	2:A:442:HOH:O	2.17	0.45
1:B:50:SER:HB3	1:B:69:THR:HG23	1.98	0.45
1:B:128:ARG:N	1:B:128:ARG:HE	2.15	0.45
1:B:38:PHE:HE2	2:B:347:HOH:O	1.97	0.45
1:B:33:LYS:O	1:B:37:ASN:HA	2.17	0.45
1:A:96:LYS:HE3	2:A:464:HOH:O	2.16	0.45
1:A:66:ASP:HB3	1:A:80:CYS:SG	2.57	0.45
1:A:86:SER:O	1:A:87:ASP:OD1	2.35	0.45
1:A:129:LEU:CD2	2:A:383:HOH:O	2.61	0.45
1:A:3:PHE:CD1	1:A:7:GLU:HG3	2.33	0.45
1:B:118:THR:HG22	1:B:119:ASP:N	2.31	0.45
1:A:112:ARG:CD	1:A:116:LYS:HZ3	2.30	0.45
1:A:88:ILE:O	1:A:89:THR:C	2.54	0.44
1:B:1:LYS:HE2	1:B:3:PHE:CD2	2.52	0.44
1:A:114:ARG:HE	1:A:114:ARG:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG22	1:A:120:VAL:HG23	1.99	0.44
1:B:104:GLY:N	2:B:259:HOH:O	2.49	0.44
1:A:42:ALA:HA	2:A:423:HOH:O	2.17	0.44
1:B:73:ARG:O	1:B:74:ASN:HB3	2.17	0.44
1:A:4:GLY:H	1:A:7:GLU:CG	2.23	0.44
1:A:44:ASN:CB	2:A:252:HOH:O	2.62	0.44
1:B:111:TRP:O	1:B:115:CYS:HB2	2.18	0.43
1:B:33:LYS:CE	1:B:37:ASN:OD1	2.66	0.43
1:B:97:LYS:HA	1:B:97:LYS:HZ2	1.83	0.43
1:A:69:THR:HA	1:A:70:PRO:HD3	1.81	0.43
1:B:27:ASN:HB2	1:B:111:TRP:NE1	2.24	0.43
1:B:112:ARG:HD2	2:B:439:HOH:O	2.18	0.43
1:A:13:LYS:HB2	1:A:25:LEU:HD11	1.99	0.43
1:B:103:ASN:ND2	2:B:431:HOH:O	2.50	0.43
1:A:50:SER:OG	1:A:69:THR:HG21	2.17	0.43
1:A:31:ALA:O	1:A:35:GLU:HB2	2.19	0.43
1:B:108:TRP:O	1:B:111:TRP:HB3	2.19	0.42
1:A:48:ASP:O	1:A:50:SER:N	2.52	0.42
1:B:114:ARG:CA	2:B:404:HOH:O	2.67	0.42
1:B:30:CYS:O	1:B:33:LYS:HB3	2.19	0.42
1:B:78:ILE:HA	1:B:79:PRO:HD3	1.84	0.42
1:A:62:TRP:O	1:A:63:TRP:HB2	2.20	0.42
1:B:114:ARG:CB	2:B:404:HOH:O	2.58	0.42
1:B:58:ILE:HA	2:B:394:HOH:O	2.19	0.42
1:A:129:LEU:HG	2:A:383:HOH:O	2.19	0.42
1:B:48:ASP:O	1:B:49:GLY:C	2.57	0.42
1:A:31:ALA:CA	2:A:174:HOH:O	2.62	0.42
1:B:44:ASN:O	1:B:45:ARG:HB2	2.20	0.42
1:B:61:ARG:HB3	1:B:62:TRP:CD1	2.55	0.42
1:B:69:THR:OG1	1:B:72:SER:HB2	2.19	0.41
1:A:120:VAL:N	2:A:250:HOH:O	2.53	0.41
1:A:42:ALA:O	1:A:54:GLY:N	2.49	0.41
1:B:35:GLU:HB3	1:B:57:GLN:HG3	2.01	0.41
1:B:8:LEU:HD22	1:B:12:MET:SD	2.61	0.41
1:A:35:GLU:HG2	1:A:57:GLN:CB	2.50	0.41
1:A:24:SER:OG	1:A:27:ASN:ND2	2.54	0.41
1:B:46:ASN:ND2	1:B:52:ASP:OD1	2.54	0.41
1:A:89:THR:HB	2:A:148:HOH:O	2.21	0.41
1:A:8:LEU:CD2	1:A:38:PHE:CD1	3.04	0.41
1:B:14:ARG:NH1	1:B:14:ARG:HB3	2.36	0.40
1:B:16:GLY:O	1:B:20:TYR:CD1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:LYS:HE2	1:B:3:PHE:CE2	2.56	0.40
1:A:50:SER:C	1:A:51:THR:OG1	2.60	0.40
1:B:36:SER:CB	1:B:55:ILE:HA	2.51	0.40

All (1) 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)
2:B:295:HOH:O	2:B:397:HOH:O[2_857]	2.18	0.02

## 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	127/129 (98%)	109 (86%)	11 (9%)	7 (6%)	2	0
1	B	127/129 (98%)	97 (76%)	22 (17%)	8 (6%)	2	0
All	All	254/258 (98%)	206 (81%)	33 (13%)	15 (6%)	2	0

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	A	48	ASP
1	A	68	ARG
1	B	44	ASN
1	B	118	THR
1	B	121	GLN
1	A	49	GLY
1	A	89	THR
1	A	113	ASN
1	B	49	GLY

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Mol	Chain	Res	Type
1	B	120	VAL
1	B	18	ASP
1	A	57	GLN
1	B	70	PRO
1	B	71	GLY

### 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%)	86 (82%)	19 (18%)	2	0
All	All	210/210 (100%)	172 (82%)	38 (18%)	2	0

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	18	ASP
1	A	25	LEU
1	A	35	GLU
1	A	55	ILE
1	A	59	ASN
1	A	62	TRP
1	A	73	ARG
1	A	77	ASN
1	A	78	ILE
1	A	88	ILE
1	A	93	ASN
1	A	99	VAL
1	A	101	ASP
1	A	109	VAL
1	A	114	ARG
1	A	120	VAL
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	129	LEU
1	B	8	LEU
1	B	13	LYS
1	B	17	LEU
1	B	20	TYR
1	B	25	LEU
1	B	27	ASN
1	B	40	THR
1	B	48	ASP
1	B	51	THR
1	B	59	ASN
1	B	61	ARG
1	B	73	ARG
1	B	74	ASN
1	B	78	ILE
1	B	114	ARG
1	B	118	THR
1	B	119	ASP
1	B	124	ILE
1	B	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	41	GLN
1	A	59	ASN
1	A	65	ASN
1	A	74	ASN
1	A	93	ASN
1	A	103	ASN
1	A	121	GLN
1	B	27	ASN
1	B	46	ASN
1	B	59	ASN
1	B	113	ASN

### 5.3.3 RNA ⓘ

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

### 6.1 Protein, DNA and RNA chains

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%)	0.89	7 (5%) 29 33	1, 6, 14, 17	0
1	B	129/129 (100%)	1.01	22 (17%) 2 2	1, 7, 22, 23	0
All	All	258/258 (100%)	0.95	29 (11%) 7 7	1, 7, 19, 23	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	TRP	6.0
1	A	129	LEU	5.0
1	B	70	PRO	3.9
1	A	83	LEU	3.6
1	B	120	VAL	3.3
1	A	71	GLY	3.2
1	B	46	ASN	3.2
1	B	20	TYR	2.9
1	A	67	GLY	2.8
1	B	74	ASN	2.8
1	B	48	ASP	2.8
1	B	45	ARG	2.8
1	B	117	GLY	2.8
1	B	75	LEU	2.8
1	B	72	SER	2.7
1	B	69	THR	2.7
1	B	44	ASN	2.7
1	A	70	PRO	2.6
1	B	47	THR	2.6
1	B	11	ALA	2.5
1	B	73	ARG	2.4
1	B	129	LEU	2.4
1	B	67	GLY	2.4
1	A	38	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	2.3
1	B	62	TRP	2.2
1	B	43	THR	2.2
1	B	18	ASP	2.1
1	B	68	ARG	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.