



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:44 PM UTC

PDB ID : 1O6V / pdb_00001o6v
Title : Internalin (INLA, *Listeria monocytogenes*) - functional domain, uncomplexed
Authors : Schubert, W.-D.; Urbanke, C.; Ziehm, T.; Beier, V.; Machner, M.P.; Domann, E.; Wehland, J.; Chakraborty, T.; Heinz, D.W.
Deposited on : 2002-10-16
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

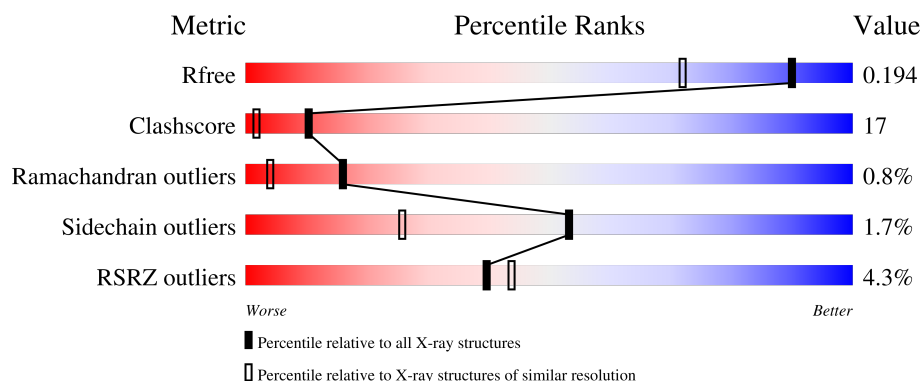
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	466	4% 85% 13% ..
1	B	466	5% 80% 15% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10809 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 INTERNALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	137	2
			4696	2902	800	992	2			
1	B	461	Total	C	N	O	S	0	123	1
			4571	2833	774	962	2			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

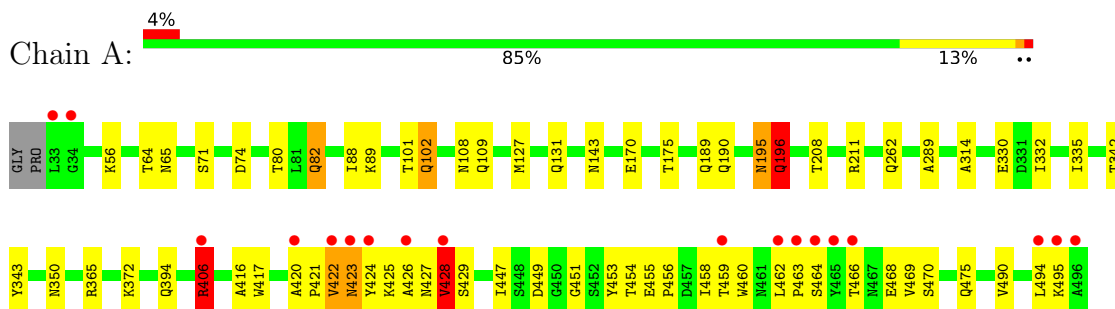
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	793	Total	O	0	0
			793	793		
3	B	747	Total	O	0	0
			747	747		

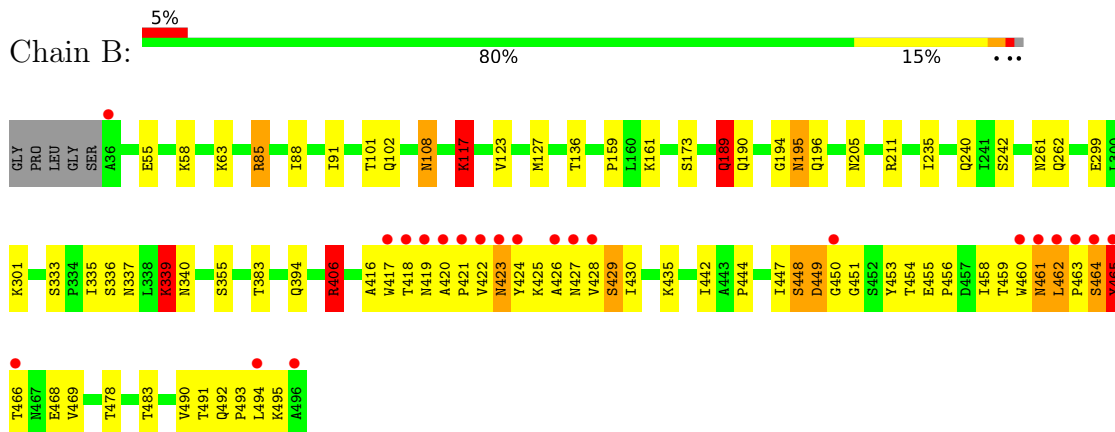
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: INTERNALIN A



• Molecule 1: INTERNALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.59Å 67.91Å 154.25Å 90.00° 103.48° 90.00°	Depositor
Resolution (Å)	158.11 – 1.50 150.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (158.11-1.50) 89.1 (150.00-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.22 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.145 , 0.184 0.159 , 0.194	Depositor DCC
R_{free} test set	6192 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10809	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 40.35 % 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 2.7728e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	1.22	12/4754 (0.3%)	0.89	13/6498 (0.2%)
1	B	2.42	28/4630 (0.6%)	1.37	25/6330 (0.4%)
All	All	1.91	40/9384 (0.4%)	1.15	38/12828 (0.3%)

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	5
1	B	1	7
All	All	1	12

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406[A]	ARG	CZ-NH2	71.33	2.26	1.33
1	B	406[B]	ARG	CZ-NH2	71.33	2.26	1.33
1	B	406[C]	ARG	CZ-NH2	71.33	2.26	1.33
1	B	465[A]	TYR	C-N	-30.34	0.95	1.33
1	B	465[B]	TYR	C-N	-30.34	0.95	1.33
1	B	189[A]	GLN	C-N	-19.05	1.06	1.33
1	B	189[B]	GLN	C-N	-19.05	1.06	1.33
1	B	189[C]	GLN	C-N	-19.05	1.06	1.33
1	B	117[A]	LYS	CG-CD	15.64	1.99	1.52
1	B	117[B]	LYS	CG-CD	15.64	1.99	1.52
1	B	117[C]	LYS	CG-CD	15.64	1.99	1.52
1	B	339[A]	LYS	CG-CD	-15.54	1.05	1.52
1	B	339[B]	LYS	CG-CD	-15.54	1.05	1.52
1	B	339[C]	LYS	CG-CD	-15.54	1.05	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196[A]	GLN	CG-CD	-9.80	1.27	1.52
1	A	196[B]	GLN	CG-CD	-9.80	1.27	1.52
1	A	196[C]	GLN	CG-CD	-9.80	1.27	1.52
1	A	127	MET	SD-CE	-8.16	1.59	1.79
1	B	161	LYS	C-O	-7.04	1.15	1.24
1	A	195[A]	ASN	C-N	6.88	1.42	1.33
1	A	195[B]	ASN	C-N	6.88	1.42	1.33
1	A	475	GLN	C-O	-6.21	1.20	1.25
1	B	195[A]	ASN	C-N	6.07	1.42	1.33
1	B	195[B]	ASN	C-N	6.07	1.42	1.33
1	B	136[A]	THR	C-O	-5.86	1.19	1.24
1	B	136[B]	THR	C-O	-5.86	1.19	1.24
1	B	444	PRO	C-O	5.83	1.30	1.23
1	A	289	ALA	C-O	-5.66	1.19	1.24
1	A	314	ALA	CA-CB	-5.63	1.44	1.53
1	B	127	MET	SD-CE	-5.57	1.65	1.79
1	B	205	ASN	CG-ND2	-5.50	1.21	1.33
1	B	442	ILE	CA-CB	5.49	1.60	1.54
1	B	242	SER	C-O	-5.47	1.16	1.24
1	A	143	ASN	C-O	-5.46	1.16	1.24
1	B	355	SER	C-O	-5.40	1.19	1.24
1	B	91	ILE	CA-CB	5.27	1.60	1.54
1	A	428[A]	VAL	CA-CB	5.18	1.62	1.54
1	A	428[B]	VAL	CA-CB	5.18	1.62	1.54
1	B	159	PRO	C-O	-5.14	1.17	1.24
1	B	108	ASN	CA-CB	5.01	1.61	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406[A]	ARG	NE-CZ-NH2	-42.26	81.16	119.20
1	B	406[B]	ARG	NE-CZ-NH2	-42.26	81.16	119.20
1	B	406[C]	ARG	NE-CZ-NH2	-42.26	81.16	119.20
1	A	406[A]	ARG	CD-NE-CZ	17.88	149.44	124.40
1	A	406[B]	ARG	CD-NE-CZ	17.88	149.44	124.40
1	B	117[A]	LYS	CG-CD-CE	-15.28	76.16	111.30
1	B	117[B]	LYS	CG-CD-CE	-15.28	76.16	111.30
1	B	117[C]	LYS	CG-CD-CE	-15.28	76.16	111.30
1	B	406[A]	ARG	CD-NE-CZ	14.34	144.47	124.40
1	B	406[B]	ARG	CD-NE-CZ	14.34	144.47	124.40
1	B	406[C]	ARG	CD-NE-CZ	14.34	144.47	124.40
1	B	189[A]	GLN	O-C-N	13.14	138.38	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189[B]	GLN	O-C-N	13.14	138.38	122.48
1	B	189[C]	GLN	O-C-N	13.14	138.38	122.48
1	B	406[A]	ARG	CG-CD-NE	11.77	137.89	112.00
1	B	406[B]	ARG	CG-CD-NE	11.77	137.89	112.00
1	B	406[C]	ARG	CG-CD-NE	11.77	137.89	112.00
1	A	196[A]	GLN	CG-CD-NE2	-11.74	98.79	116.40
1	A	196[B]	GLN	CG-CD-NE2	-11.74	98.79	116.40
1	A	196[C]	GLN	CG-CD-NE2	-11.74	98.79	116.40
1	B	117[A]	LYS	CB-CG-CD	-10.97	86.06	111.30
1	B	117[B]	LYS	CB-CG-CD	-10.97	86.06	111.30
1	B	117[C]	LYS	CB-CG-CD	-10.97	86.06	111.30
1	A	196[A]	GLN	CB-CG-CD	10.61	130.64	112.60
1	A	196[B]	GLN	CB-CG-CD	10.61	130.64	112.60
1	A	196[C]	GLN	CB-CG-CD	10.61	130.64	112.60
1	A	406[A]	ARG	CG-CD-NE	8.63	130.98	112.00
1	A	406[B]	ARG	CG-CD-NE	8.63	130.98	112.00
1	A	196[A]	GLN	CG-CD-OE1	8.31	137.41	120.80
1	A	196[B]	GLN	CG-CD-OE1	8.31	137.41	120.80
1	A	196[C]	GLN	CG-CD-OE1	8.31	137.41	120.80
1	B	465[A]	TYR	CA-C-N	-7.29	111.25	122.62
1	B	465[A]	TYR	C-N-CA	-7.29	111.25	122.62
1	B	465[B]	TYR	CA-C-N	-7.29	111.25	122.62
1	B	465[B]	TYR	C-N-CA	-7.29	111.25	122.62
1	B	339[A]	LYS	CB-CG-CD	-6.67	95.97	111.30
1	B	339[B]	LYS	CB-CG-CD	-6.67	95.97	111.30
1	B	339[C]	LYS	CB-CG-CD	-6.67	95.97	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	462[B]	LEU	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170[A]	GLU	Sidechain
1	A	196[A]	GLN	Mainchain
1	A	196[C]	GLN	Mainchain
1	A	406[A]	ARG	Sidechain
1	A	82[A]	GLN	Sidechain
1	B	189[A]	GLN	Sidechain
1	B	406[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	461[B]	ASN	Peptide
1	B	465[B]	TYR	Mainchain
1	B	85[A]	ARG	Sidechain,Mainchain
1	B	85[B]	ARG	Mainchain

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	4696	0	4621	103	0
1	B	4571	0	4504	214	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	793	0	0	6	0
3	B	747	0	0	13	0
All	All	10809	0	9125	317	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 17.

All (317) 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:189[B]:GLN:CG	1:B:189[B]:GLN:CD	1.77	1.53
1:B:195[A]:ASN:C	1:B:196[A]:GLN:N	1.68	1.50
1:A:195[A]:ASN:C	1:A:196[A]:GLN:N	1.73	1.47
1:B:435[A]:LYS:CD	1:B:435[A]:LYS:CG	1.92	1.44
1:B:419[B]:ASN:CB	1:B:491[B]:THR:O	1.67	1.41
1:B:117[C]:LYS:CD	1:B:117[C]:LYS:CG	1.99	1.40
1:B:464[B]:SER:C	1:B:465[B]:TYR:N	1.81	1.38
1:A:406[B]:ARG:CZ	1:A:406[B]:ARG:NH2	1.84	1.37
1:B:85[A]:ARG:NH1	1:B:85[A]:ARG:NH2	1.73	1.35
1:A:82[B]:GLN:NE2	1:A:82[B]:GLN:OE1	1.57	1.34
1:A:82[A]:GLN:OE1	1:A:82[A]:GLN:NE2	1.58	1.32
1:B:117[A]:LYS:CG	1:B:117[A]:LYS:CD	2.09	1.30
1:B:465[A]:TYR:C	1:B:466[A]:THR:N	1.89	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196[C]:GLN:CB	1:B:196[C]:GLN:CG	2.09	1.30
1:B:339[B]:LYS:CG	1:B:339[B]:LYS:CB	2.11	1.28
1:B:85[A]:ARG:NH2	1:B:85[A]:ARG:CZ	1.97	1.25
1:A:56[B]:LYS:NZ	1:A:82[B]:GLN:O	1.69	1.24
1:B:419[B]:ASN:O	1:B:493[B]:PRO:CD	1.88	1.20
1:B:422[B]:VAL:O	1:B:494[B]:LEU:HA	1.41	1.19
1:B:117[B]:LYS:CD	1:B:117[B]:LYS:CG	2.26	1.14
1:A:469[B]:VAL:HG13	1:A:494[B]:LEU:HD11	1.29	1.12
1:B:419[B]:ASN:O	1:B:493[B]:PRO:CG	1.98	1.11
1:B:339[C]:LYS:CG	1:B:339[C]:LYS:CB	2.30	1.09
1:B:190[B]:GLN:HE21	1:B:211[B]:ARG:NH2	1.50	1.09
1:A:429[B]:SER:HB2	1:A:459[B]:THR:HG22	1.30	1.08
1:B:419[B]:ASN:HB2	1:B:491[B]:THR:O	1.34	1.08
1:B:190[B]:GLN:HE21	1:B:211[B]:ARG:CZ	1.67	1.07
1:B:117[C]:LYS:CD	1:B:117[C]:LYS:CB	2.33	1.07
1:B:418[B]:THR:HA	1:B:491[B]:THR:HB	1.09	1.06
1:B:85[A]:ARG:NH2	1:B:85[A]:ARG:HH11	1.40	1.05
1:B:420[B]:ALA:O	1:B:492[B]:GLN:NE2	1.91	1.04
1:A:423[B]:ASN:HB2	1:A:495[B]:LYS:HZ2	1.23	1.03
1:B:406[C]:ARG:NE	1:B:406[C]:ARG:CD	2.20	1.03
1:B:339[A]:LYS:CD	1:B:339[A]:LYS:HB3	1.90	1.01
1:B:419[B]:ASN:N	1:B:491[B]:THR:O	1.91	1.01
1:A:423[B]:ASN:HB2	1:A:495[B]:LYS:NZ	1.76	1.00
1:B:85[A]:ARG:CZ	1:B:85[A]:ARG:NE	2.26	0.99
1:B:406[B]:ARG:NH2	1:B:406[B]:ARG:CZ	2.26	0.99
1:B:422[B]:VAL:O	1:B:494[B]:LEU:CA	2.09	0.99
1:B:419[B]:ASN:CA	1:B:491[B]:THR:O	2.11	0.98
1:B:418[B]:THR:HG23	1:B:491[B]:THR:CG2	1.93	0.98
1:B:85[A]:ARG:NE	1:B:85[A]:ARG:CG	2.27	0.97
1:B:418[B]:THR:HA	1:B:491[B]:THR:CB	1.95	0.96
1:B:423[A]:ASN:ND2	3:B:2666:HOH:O	1.97	0.96
1:B:419[B]:ASN:O	1:B:493[B]:PRO:HD3	1.64	0.95
1:B:117[B]:LYS:CG	1:B:117[B]:LYS:CE	2.43	0.95
1:B:429[A]:SER:HB2	1:B:459[A]:THR:HG22	1.48	0.95
1:B:337[B]:ASN:ND2	3:B:2548:HOH:O	1.97	0.95
1:B:417[B]:TRP:CZ2	1:B:490[B]:VAL:HG22	2.01	0.95
1:B:422[B]:VAL:O	1:B:494[B]:LEU:HB3	1.67	0.94
1:B:406[C]:ARG:NE	1:B:406[C]:ARG:CG	2.30	0.94
1:B:117[A]:LYS:CD	1:B:117[A]:LYS:CB	2.45	0.94
1:B:419[B]:ASN:HD22	1:B:420[B]:ALA:N	1.66	0.93
1:B:339[B]:LYS:HB2	1:B:339[B]:LYS:CD	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:CD	2.26	0.92
1:B:85[B]:ARG:CD	1:B:85[B]:ARG:HB3	1.99	0.92
1:B:494[B]:LEU:O	1:B:495[B]:LYS:HG3	1.69	0.92
1:A:189[C]:GLN:HE21	1:A:211[C]:ARG:HH22	1.18	0.91
1:B:419[B]:ASN:HB3	1:B:491[B]:THR:O	1.69	0.91
1:B:190[B]:GLN:CD	1:B:211[B]:ARG:HE	1.81	0.89
1:A:427[B]:ASN:HA	1:A:460[B]:TRP:O	1.72	0.88
1:B:419[B]:ASN:HD22	1:B:420[B]:ALA:H	0.89	0.88
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:NE	2.22	0.88
1:B:339[B]:LYS:CG	1:B:339[B]:LYS:CA	2.51	0.87
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:HG2	1.90	0.87
1:A:406[B]:ARG:NH1	1:A:406[B]:ARG:HH21	1.71	0.87
1:A:82[B]:GLN:NE2	1:A:82[B]:GLN:CD	2.32	0.86
1:A:423[A]:ASN:O	1:A:424[A]:TYR:O	1.93	0.86
1:B:418[B]:THR:HG23	1:B:491[B]:THR:HG21	1.54	0.86
1:B:419[B]:ASN:O	1:B:493[B]:PRO:HG2	1.75	0.86
1:B:435[A]:LYS:CD	1:B:435[A]:LYS:CB	2.54	0.86
1:B:419[B]:ASN:ND2	1:B:420[B]:ALA:H	1.72	0.85
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:NH2	2.24	0.85
1:A:80[B]:THR:OG1	1:A:102[B]:GLN:NE2	2.08	0.85
1:A:429[B]:SER:CB	1:A:459[B]:THR:HG22	2.05	0.85
1:B:419[B]:ASN:HB3	1:B:492[B]:GLN:HA	1.58	0.85
1:B:422[B]:VAL:O	1:B:494[B]:LEU:CB	2.24	0.85
1:A:425[A]:LYS:HB2	1:A:428[A]:VAL:HG13	1.57	0.84
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:HE	1.75	0.82
1:B:189[B]:GLN:CG	1:B:189[B]:GLN:NE2	2.42	0.81
1:B:301[B]:LYS:NZ	3:B:2484:HOH:O	2.12	0.81
1:B:117[A]:LYS:CD	1:B:117[A]:LYS:HB2	2.11	0.81
1:A:190[B]:GLN:HE21	1:A:211[B]:ARG:HE	1.27	0.81
1:A:424[A]:TYR:O	1:A:425[A]:LYS:HG3	1.80	0.81
1:B:418[B]:THR:HG23	1:B:491[B]:THR:HG22	1.63	0.81
1:B:117[C]:LYS:HD2	1:B:117[C]:LYS:HB3	1.63	0.81
1:B:189[B]:GLN:CD	1:B:189[B]:GLN:CB	2.54	0.80
1:B:339[A]:LYS:CD	1:B:339[A]:LYS:CB	2.59	0.80
1:B:85[A]:ARG:HB2	1:B:85[A]:ARG:CD	2.11	0.80
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:CG	2.45	0.79
1:A:80[A]:THR:HG22	1:A:102[A]:GLN:HE21	1.48	0.79
1:A:343[B]:TYR:CE1	1:A:365[B]:ARG:HD3	2.18	0.78
1:A:406[B]:ARG:NH1	1:A:406[B]:ARG:HE	1.81	0.78
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:HH21	1.80	0.78
1:B:406[C]:ARG:NE	1:B:406[C]:ARG:HG2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235[B]:ILE:HD13	3:B:2136:HOH:O	1.84	0.78
1:A:428[B]:VAL:CG2	1:A:460[B]:TRP:HB2	2.14	0.78
1:A:406[B]:ARG:NH2	1:A:406[B]:ARG:NH1	2.32	0.77
1:B:85[A]:ARG:NH2	1:B:85[A]:ARG:NE	2.33	0.77
1:B:85[A]:ARG:CD	1:B:85[A]:ARG:CB	2.61	0.77
1:B:339[B]:LYS:CB	1:B:339[B]:LYS:CD	2.62	0.77
1:A:406[B]:ARG:NH2	1:A:406[B]:ARG:NE	2.33	0.77
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:CZ	2.46	0.77
1:B:190[B]:GLN:HG2	1:B:211[B]:ARG:NE	2.00	0.77
1:B:339[C]:LYS:CB	1:B:339[C]:LYS:CD	2.63	0.76
1:B:117[A]:LYS:HB2	1:B:117[A]:LYS:HD2	1.66	0.76
1:B:423[B]:ASN:HB2	1:B:495[B]:LYS:HD2	1.68	0.76
1:A:423[B]:ASN:HA	1:A:495[B]:LYS:HG2	1.68	0.76
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:HE	1.98	0.76
1:B:117[C]:LYS:CB	1:B:117[C]:LYS:HD2	2.16	0.75
1:A:189[C]:GLN:HE21	1:A:211[C]:ARG:NH2	1.83	0.74
1:B:190[B]:GLN:HG3	1:B:211[B]:ARG:HH21	1.51	0.74
1:B:406[B]:ARG:NH2	1:B:406[B]:ARG:HE	1.86	0.74
1:A:64[B]:THR:HG23	1:A:65[B]:ASN:ND2	2.01	0.74
1:B:196[C]:GLN:CG	1:B:196[C]:GLN:CA	2.66	0.74
1:B:117[A]:LYS:CB	1:B:117[A]:LYS:HD2	2.16	0.74
1:A:428[B]:VAL:HG23	1:A:460[B]:TRP:HE3	1.54	0.73
1:B:448[B]:SER:O	1:B:450[B]:GLY:N	2.21	0.73
1:B:418[B]:THR:CA	1:B:491[B]:THR:HB	2.05	0.73
1:B:422[B]:VAL:C	1:B:494[B]:LEU:HA	2.13	0.73
1:A:102[B]:GLN:OE1	3:A:2172:HOH:O	2.05	0.73
1:B:419[B]:ASN:C	1:B:493[B]:PRO:CD	2.60	0.73
1:B:190[B]:GLN:HE21	1:B:211[B]:ARG:NE	1.83	0.72
1:B:117[B]:LYS:CD	1:B:117[B]:LYS:CB	2.67	0.72
1:A:406[B]:ARG:NH1	1:A:406[B]:ARG:NE	2.37	0.72
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:HH21	2.03	0.72
1:B:435[A]:LYS:CG	1:B:435[A]:LYS:CE	2.66	0.72
1:B:190[B]:GLN:HE21	1:B:211[B]:ARG:HH21	1.34	0.71
1:B:419[B]:ASN:H	1:B:491[B]:THR:C	1.97	0.71
1:A:428[A]:VAL:HG23	1:A:460[A]:TRP:HB2	1.70	0.71
1:A:424[A]:TYR:CG	1:A:425[A]:LYS:N	2.59	0.71
1:B:117[B]:LYS:CG	1:B:117[B]:LYS:HE3	2.21	0.70
1:B:190[B]:GLN:HG2	1:B:211[B]:ARG:HE	1.55	0.70
1:A:428[B]:VAL:HG23	1:A:460[B]:TRP:CE3	2.26	0.70
1:A:423[B]:ASN:CB	1:A:495[B]:LYS:NZ	2.53	0.70
1:B:428[B]:VAL:HB	1:B:460[B]:TRP:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449[B]:ASP:O	3:B:2689:HOH:O	2.08	0.69
1:B:85[B]:ARG:CG	1:B:85[B]:ARG:NE	2.56	0.69
1:B:101:THR:OG1	1:B:102[B]:GLN:NE2	2.27	0.68
1:B:419[B]:ASN:C	1:B:493[B]:PRO:HD3	2.18	0.68
1:B:417[B]:TRP:NE1	1:B:490[B]:VAL:HG13	2.09	0.68
1:B:190[B]:GLN:HG3	1:B:211[B]:ARG:NH2	2.09	0.67
1:B:85[A]:ARG:NH1	1:B:85[A]:ARG:HH22	1.85	0.66
1:B:117[B]:LYS:CD	1:B:117[B]:LYS:HB2	2.25	0.66
1:A:343[B]:TYR:CE2	1:A:365[B]:ARG:NH1	2.64	0.66
1:A:175:THR:HA	1:A:196[C]:GLN:HE22	1.59	0.65
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:NE	2.59	0.65
1:B:406[B]:ARG:NH2	1:B:406[B]:ARG:NE	2.44	0.65
1:B:339[C]:LYS:CB	1:B:339[C]:LYS:HD2	2.27	0.64
1:B:428[B]:VAL:O	1:B:460[B]:TRP:N	2.31	0.64
1:B:423[B]:ASN:HD22	1:B:495[B]:LYS:HB2	1.62	0.64
1:B:85[B]:ARG:CD	1:B:85[B]:ARG:CB	2.76	0.63
1:A:131[B]:GLN:CD	3:A:2236:HOH:O	2.40	0.63
1:B:422[B]:VAL:N	1:B:493[B]:PRO:O	2.31	0.63
1:A:429[B]:SER:HB2	1:A:459[B]:THR:CG2	2.19	0.62
1:A:56[B]:LYS:NZ	1:A:82[B]:GLN:C	2.57	0.62
1:B:240:GLN:HA	1:B:262[C]:GLN:HE22	1.65	0.62
1:B:196[C]:GLN:CB	1:B:196[C]:GLN:CD	2.72	0.62
1:B:461[B]:ASN:O	1:B:462[B]:LEU:HD23	1.98	0.62
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:NH2	2.63	0.62
1:A:422[B]:VAL:O	1:A:494[B]:LEU:HA	2.00	0.62
1:A:460[B]:TRP:HB3	1:A:462[B]:LEU:HD21	1.82	0.62
1:A:343[B]:TYR:CZ	1:A:365[B]:ARG:HD3	2.35	0.61
1:B:417[B]:TRP:HE1	1:B:490[B]:VAL:HG13	1.64	0.61
1:A:423[A]:ASN:O	1:A:424[A]:TYR:C	2.44	0.61
1:B:447[B]:ILE:HD11	1:B:453[B]:TYR:HB2	1.81	0.61
1:B:463[B]:PRO:O	1:B:464[B]:SER:HB2	1.99	0.61
1:A:428[B]:VAL:HG22	1:A:460[B]:TRP:HB2	1.82	0.60
1:A:82[A]:GLN:HG2	1:A:82[A]:GLN:HE21	1.66	0.60
1:A:447[B]:ILE:CG2	1:A:451[B]:GLY:HA3	2.31	0.60
1:A:406[B]:ARG:NH2	1:A:406[B]:ARG:HE	1.99	0.59
1:B:424[B]:TYR:CE1	1:B:462[B]:LEU:CD1	2.85	0.59
1:A:425[A]:LYS:HB2	1:A:428[A]:VAL:CG1	2.29	0.59
1:A:262[B]:GLN:NE2	3:A:2444:HOH:O	2.35	0.59
1:A:423[B]:ASN:CB	1:A:495[B]:LYS:HZ1	2.16	0.59
1:B:421[B]:PRO:HA	1:B:493[B]:PRO:HB2	1.85	0.59
1:B:195[A]:ASN:C	1:B:196[A]:GLN:CA	2.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383[C]:THR:HG21	3:B:2638:HOH:O	2.02	0.59
1:B:299:GLU:OE1	3:B:2484:HOH:O	2.17	0.59
1:A:424[A]:TYR:O	1:A:425[A]:LYS:CG	2.51	0.58
1:B:85[A]:ARG:NE	1:B:85[A]:ARG:HH21	2.00	0.58
1:B:420[B]:ALA:O	1:B:493[B]:PRO:HD2	2.03	0.58
1:A:423[A]:ASN:C	1:A:424[A]:TYR:O	2.44	0.58
1:A:425[B]:LYS:O	1:A:462[B]:LEU:HD12	2.03	0.58
1:B:339[B]:LYS:CG	1:B:339[B]:LYS:HA	2.31	0.58
1:B:85[B]:ARG:CG	1:B:85[B]:ARG:HE	2.17	0.57
1:A:423[B]:ASN:HA	1:A:495[B]:LYS:CG	2.32	0.57
1:A:82[B]:GLN:NE2	1:A:82[B]:GLN:CG	2.67	0.57
1:A:109[A]:GLN:HA	1:A:131[A]:GLN:OE1	2.04	0.57
1:B:85[A]:ARG:HH11	1:B:85[A]:ARG:HH22	1.42	0.57
1:B:190[B]:GLN:CD	1:B:211[B]:ARG:HH21	2.13	0.57
1:B:465[A]:TYR:C	1:B:466[A]:THR:CA	2.77	0.57
1:B:428[B]:VAL:HG23	1:B:462[B]:LEU:HD11	1.87	0.56
1:B:453[B]:TYR:OH	1:B:455[B]:GLU:HB2	2.03	0.56
1:A:423[B]:ASN:HB2	1:A:495[B]:LYS:HZ1	1.68	0.56
1:A:447[B]:ILE:HG22	1:A:451[B]:GLY:HA3	1.85	0.56
1:B:429[A]:SER:CB	1:B:459[A]:THR:HG22	2.30	0.56
1:B:460[B]:TRP:NE1	1:B:469[B]:VAL:HB	2.20	0.56
1:B:339[A]:LYS:CE	3:B:2547:HOH:O	2.52	0.56
1:A:101:THR:OG1	1:A:102[A]:GLN:NE2	2.39	0.56
1:B:424[B]:TYR:CE1	1:B:462[B]:LEU:HD12	2.40	0.56
1:B:419[B]:ASN:O	1:B:493[B]:PRO:HD2	2.00	0.56
1:B:460[B]:TRP:CE2	1:B:469[B]:VAL:HB	2.41	0.55
1:B:465[B]:TYR:CG	1:B:466[B]:THR:N	2.68	0.55
1:B:424[B]:TYR:CZ	1:B:425[B]:LYS:O	2.61	0.54
1:A:427[B]:ASN:OD1	3:A:2709:HOH:O	2.18	0.54
1:B:339[A]:LYS:HB3	1:B:339[A]:LYS:HD3	1.85	0.54
1:B:196[C]:GLN:CG	1:B:196[C]:GLN:HA	2.37	0.54
1:B:459[B]:THR:HG22	1:B:460[B]:TRP:N	2.23	0.54
1:B:419[B]:ASN:ND2	3:B:2664:HOH:O	2.40	0.54
1:B:417[B]:TRP:CE2	1:B:490[B]:VAL:HG22	2.42	0.53
1:B:85[B]:ARG:CD	1:B:85[B]:ARG:CG	2.86	0.53
1:A:195[A]:ASN:C	1:A:196[A]:GLN:CA	2.76	0.53
1:B:261:ASN:C	1:B:262[C]:GLN:HE21	2.15	0.53
1:B:426[B]:ALA:O	1:B:462[B]:LEU:HA	2.08	0.53
1:B:453[B]:TYR:CZ	1:B:455[B]:GLU:HB2	2.45	0.52
1:A:428[B]:VAL:HG23	1:A:460[B]:TRP:HB2	1.90	0.51
1:A:454[B]:THR:O	1:A:455[B]:GLU:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428[B]:VAL:HG11	1:B:469[B]:VAL:HG21	1.91	0.51
1:A:189[B]:GLN:HG2	1:A:208[B]:THR:HG22	1.92	0.51
1:A:447[B]:ILE:HD11	1:A:453[B]:TYR:HB2	1.92	0.51
1:A:71[B]:SER:OG	1:A:74[B]:ASP:OD2	2.28	0.51
1:A:80[A]:THR:CG2	1:A:102[A]:GLN:HE21	2.22	0.51
1:A:425[A]:LYS:O	1:A:426[A]:ALA:C	2.54	0.51
1:B:88:ILE:H	1:B:108:ASN:HD22	1.59	0.51
1:B:339[B]:LYS:NZ	1:B:340[B]:ASN:HD21	2.09	0.50
1:B:454:THR:O	1:B:455[A]:GLU:C	2.54	0.50
1:B:465[B]:TYR:CE1	1:B:466[B]:THR:O	2.65	0.50
1:B:417[B]:TRP:CZ2	1:B:490[B]:VAL:CG2	2.85	0.50
1:B:419[B]:ASN:C	1:B:493[B]:PRO:HD2	2.36	0.49
1:B:420[B]:ALA:C	1:B:493[B]:PRO:HD2	2.38	0.49
1:B:337[A]:ASN:ND2	3:B:2545:HOH:O	2.45	0.49
1:B:406[A]:ARG:CZ	1:B:406[A]:ARG:NH2	2.74	0.49
1:B:189[A]:GLN:NE2	3:B:2336:HOH:O	2.46	0.49
1:A:394:GLN:HG2	1:A:416[B]:ALA:O	2.13	0.49
1:B:478:THR:OG1	1:B:483[A]:THR:HG23	2.13	0.49
1:A:131[B]:GLN:NE2	3:A:2236:HOH:O	2.45	0.48
1:B:339[B]:LYS:HZ3	1:B:340[B]:ASN:HD21	1.59	0.48
1:A:454[A]:THR:O	1:A:455[A]:GLU:C	2.55	0.48
1:B:465[A]:TYR:CA	1:B:466[A]:THR:N	2.74	0.48
1:B:430[B]:ILE:HG12	1:B:460[B]:TRP:HZ3	1.78	0.48
1:B:339[C]:LYS:CG	1:B:339[C]:LYS:CA	2.92	0.48
1:B:429[B]:SER:HA	1:B:458[B]:ILE:O	2.14	0.47
1:B:424[B]:TYR:HE1	1:B:462[B]:LEU:CD1	2.28	0.47
1:A:449[B]:ASP:HB2	1:A:460[B]:TRP:HD1	1.80	0.47
1:B:424[B]:TYR:CE1	1:B:462[B]:LEU:HD13	2.49	0.47
1:B:427[A]:ASN:ND2	1:B:461[A]:ASN:OD1	2.46	0.47
1:B:428[B]:VAL:HG12	1:B:460[B]:TRP:CE3	2.50	0.47
1:B:63[B]:LYS:NZ	3:B:2071:HOH:O	2.37	0.47
1:A:330[B]:GLU:HG2	1:A:350[B]:ASN:HB3	1.97	0.46
1:B:459[B]:THR:CG2	1:B:460[B]:TRP:N	2.79	0.46
1:A:88:ILE:H	1:A:108:ASN:ND2	2.14	0.46
1:B:85[A]:ARG:CG	1:B:85[A]:ARG:CD	2.93	0.45
1:A:417[B]:TRP:CZ2	1:A:490[B]:VAL:HG22	2.52	0.45
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:CZ	2.95	0.45
1:B:262[C]:GLN:HE21	1:B:262[C]:GLN:N	2.13	0.45
1:B:418[B]:THR:CG2	1:B:491[B]:THR:HG21	2.37	0.45
1:B:447[B]:ILE:O	1:B:448[B]:SER:O	2.35	0.45
1:B:448[B]:SER:O	1:B:449[B]:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494[B]:LEU:C	1:B:495[B]:LYS:HG3	2.38	0.45
1:B:426[A]:ALA:HA	1:B:462[A]:LEU:O	2.17	0.45
1:B:450[B]:GLY:O	3:B:2690:HOH:O	2.21	0.45
1:A:342[B]:THR:O	1:A:343[B]:TYR:HD1	2.01	0.45
1:B:428[B]:VAL:HB	1:B:460[B]:TRP:CB	2.46	0.44
1:A:423[B]:ASN:CG	1:A:424[B]:TYR:N	2.75	0.44
1:A:425[A]:LYS:CB	1:A:428[A]:VAL:HG13	2.40	0.44
1:B:194:GLY:C	1:B:195[A]:ASN:HD22	2.25	0.44
1:B:455[A]:GLU:HA	1:B:456[A]:PRO:HA	1.72	0.44
1:B:424[B]:TYR:CE1	1:B:425[B]:LYS:O	2.71	0.44
1:B:394:GLN:HG2	1:B:416[A]:ALA:O	2.16	0.44
1:A:88:ILE:H	1:A:108:ASN:HD22	1.64	0.44
1:B:339[B]:LYS:CD	1:B:339[B]:LYS:HB3	2.44	0.44
1:B:430[B]:ILE:HG12	1:B:460[B]:TRP:CZ3	2.53	0.44
1:A:470[B]:SER:HB2	1:A:490[B]:VAL:O	2.18	0.43
1:B:88:ILE:H	1:B:108:ASN:ND2	2.15	0.43
1:A:195[B]:ASN:ND2	3:A:2356:HOH:O	2.50	0.43
1:B:461[B]:ASN:C	1:B:462[B]:LEU:HD23	2.44	0.43
1:B:55:GLU:OE2	1:B:58:LYS:NZ	2.43	0.43
1:B:240:GLN:HA	1:B:262[C]:GLN:NE2	2.33	0.43
1:A:350[B]:ASN:OD1	1:A:372[B]:LYS:HD2	2.18	0.43
1:B:173:SER:H	1:B:195[A]:ASN:HD21	1.66	0.43
1:A:332:ILE:O	1:A:335[A]:ILE:HG12	2.18	0.43
1:B:85[A]:ARG:HH21	1:B:85[A]:ARG:HE	1.67	0.43
1:B:451[B]:GLY:HA2	1:B:459[B]:THR:O	2.19	0.43
1:A:462[A]:LEU:HA	1:A:463[A]:PRO:HD2	1.85	0.42
1:B:428[B]:VAL:CG2	1:B:462[B]:LEU:HD11	2.48	0.42
1:B:117[B]:LYS:CG	1:B:117[B]:LYS:HE2	2.44	0.42
1:B:424[B]:TYR:CD1	1:B:462[B]:LEU:CD1	3.03	0.42
1:A:417[B]:TRP:CE2	1:A:490[B]:VAL:HG22	2.55	0.42
1:A:422[A]:VAL:CG1	1:A:423[A]:ASN:N	2.82	0.42
1:B:447[B]:ILE:C	1:B:448[B]:SER:O	2.62	0.42
1:A:421[A]:PRO:HB2	1:A:495[A]:LYS:HE3	2.02	0.42
1:A:428[B]:VAL:CG2	1:A:460[B]:TRP:CE3	3.01	0.42
1:B:117[B]:LYS:HE3	1:B:117[B]:LYS:HG3	1.98	0.42
1:A:429[B]:SER:HA	1:A:458[B]:ILE:O	2.20	0.41
1:A:460[B]:TRP:HB3	1:A:462[B]:LEU:CD2	2.48	0.41
1:B:463[B]:PRO:O	1:B:464[B]:SER:CB	2.68	0.41
1:A:343[B]:TYR:CD1	1:A:365[B]:ARG:HD3	2.53	0.41
1:B:419[B]:ASN:ND2	1:B:420[B]:ALA:N	2.47	0.41
1:B:333[B]:SER:O	1:B:336[B]:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451[B]:GLY:CA	1:B:459[B]:THR:O	2.69	0.40
1:A:455[A]:GLU:HA	1:A:456[A]:PRO:HA	1.87	0.40
1:A:80[A]:THR:HG22	1:A:102[A]:GLN:HB2	2.03	0.40
1:B:117[C]:LYS:CD	1:B:117[C]:LYS:HB2	2.39	0.40
1:A:420[B]:ALA:HA	1:A:421[B]:PRO:HD3	1.92	0.40
1:A:466[A]:THR:O	1:A:494[A]:LEU:HB2	2.21	0.40
1:A:343[B]:TYR:CE1	1:A:365[B]:ARG:CD	2.99	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	610/466 (131%)	562 (92%)	42 (7%)	6 (1%)	12	2
1	B	593/466 (127%)	542 (91%)	43 (7%)	8 (1%)	9	1
All	All	1203/932 (129%)	1104 (92%)	85 (7%)	14 (1%)	16	2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449[A]	ASP
1	B	449[B]	ASP
1	B	462[A]	LEU
1	B	462[B]	LEU
1	A	423[A]	ASN
1	A	423[B]	ASN
1	B	448[A]	SER
1	B	448[B]	SER
1	B	464[A]	SER
1	B	464[B]	SER
1	A	464[A]	SER

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Mol	Chain	Res	Type
1	A	464[B]	SER
1	A	428[A]	VAL
1	A	428[B]	VAL

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	558/418 (134%)	545 (98%)	13 (2%)	44	16
1	B	542/418 (130%)	523 (96%)	19 (4%)	32	7
All	All	1100/836 (132%)	1068 (97%)	32 (3%)	53	10

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89[A]	LYS
1	A	89[B]	LYS
1	A	102[A]	GLN
1	A	102[B]	GLN
1	A	102[C]	GLN
1	A	406[A]	ARG
1	A	406[B]	ARG
1	A	422[A]	VAL
1	A	422[B]	VAL
1	A	428[A]	VAL
1	A	428[B]	VAL
1	A	468[A]	GLU
1	A	468[B]	GLU
1	B	117[A]	LYS
1	B	117[B]	LYS
1	B	117[C]	LYS
1	B	123[A]	VAL
1	B	123[B]	VAL
1	B	189[A]	GLN
1	B	189[B]	GLN

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Mol	Chain	Res	Type
1	B	189[C]	GLN
1	B	335[A]	ILE
1	B	335[B]	ILE
1	B	339[A]	LYS
1	B	339[B]	LYS
1	B	339[C]	LYS
1	B	423[A]	ASN
1	B	423[B]	ASN
1	B	429[A]	SER
1	B	429[B]	SER
1	B	468[A]	GLU
1	B	468[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	238	ASN
1	A	282	ASN
1	A	370	ASN
1	A	386	ASN
1	A	394	GLN
1	B	108	ASN
1	B	238	ASN
1	B	282	ASN
1	B	370	ASN
1	B	475	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	7
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	465[A]:TYR	C	466[A]:THR	N	1.89
1	B	464[B]:SER	C	465[B]:TYR	N	1.81
1	A	195[A]:ASN	C	196[A]:GLN	N	1.73
1	B	195[A]:ASN	C	196[A]:GLN	N	1.68
1	B	189[A]:GLN	C	190[A]:GLN	N	1.64
1	B	189[B]:GLN	C	190[B]:GLN	N	1.06
1	B	461[B]:ASN	C	462:LEU	N	1.05
1	B	465[B]:TYR	C	466[B]:THR	N	0.95

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, 95th 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 ²)	Q<0.9
1	A	464/466 (99%)	-0.12	18 (3%) 43 47	2, 12, 19, 41	137 (29%)
1	B	461/466 (98%)	-0.04	22 (4%) 35 39	4, 12, 20, 35	123 (26%)
All	All	925/932 (99%)	-0.08	40 (4%) 40 44	2, 12, 19, 41	260 (28%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	ALA	6.1
1	B	420[A]	ALA	5.6
1	A	406[A]	ARG	5.5
1	B	423[A]	ASN	5.4
1	A	34	GLY	5.1
1	A	422[A]	VAL	5.0
1	B	428[A]	VAL	4.8
1	A	494[A]	LEU	4.5
1	B	463[A]	PRO	4.4
1	B	426[A]	ALA	4.2
1	A	466[A]	THR	4.1
1	A	423[A]	ASN	4.1
1	B	494[A]	LEU	4.0
1	A	424[A]	TYR	3.5
1	A	465	TYR	3.5
1	B	422[A]	VAL	3.4
1	B	464[A]	SER	3.3
1	A	464[A]	SER	3.2
1	B	461[A]	ASN	3.1
1	A	33	LEU	3.1
1	B	496	ALA	3.1
1	A	428[A]	VAL	3.0
1	B	418[A]	THR	2.9
1	B	421[A]	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	420[A]	ALA	2.8
1	B	460[A]	TRP	2.7
1	B	424[A]	TYR	2.7
1	A	462[A]	LEU	2.7
1	B	462[A]	LEU	2.7
1	B	36	ALA	2.6
1	B	465[A]	TYR	2.6
1	B	466[A]	THR	2.6
1	A	459[A]	THR	2.5
1	B	427[A]	ASN	2.3
1	A	426[A]	ALA	2.2
1	B	450[A]	GLY	2.1
1	A	463[A]	PRO	2.1
1	B	419[A]	ASN	2.1
1	B	417[A]	TRP	2.1
1	A	495[A]	LYS	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	1497	1/1	1.00	0.02	7,7,7,7	1
2	CA	B	1497	1/1	1.00	0.04	7,7,7,7	1

6.5 Other polymers [i](#)

There are no such residues in this entry.