WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 08:10 pm BST

PDB ID	:	1O6V
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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
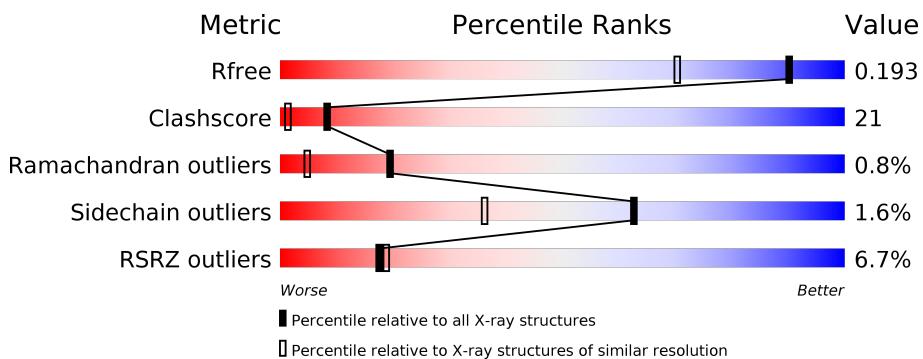
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
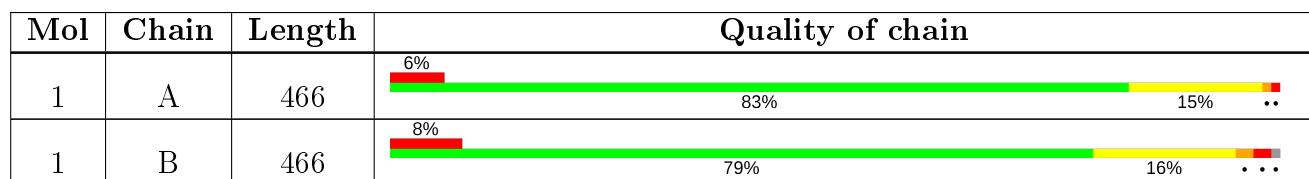
The reported resolution of this entry is 1.50 Å.

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	Percentile Ranks	Value
Rfree		0.193
Clashscore		21
Ramachandran outliers		0.8%
Sidechain outliers		1.6%
RSRZ outliers		6.7%

Worse ← → Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 on 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 <=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	6% / 83% / 15% / ••
1	B	466	8% / 79% / 16% / • • •

2 Entry composition (i)

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 4696	C 2902	N 800	O 992	S 2	0	137	2
1	B	461	Total 4571	C 2833	N 774	O 962	S 2	0	123	1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0
2	A	1	Total 1	Ca 1	0	0
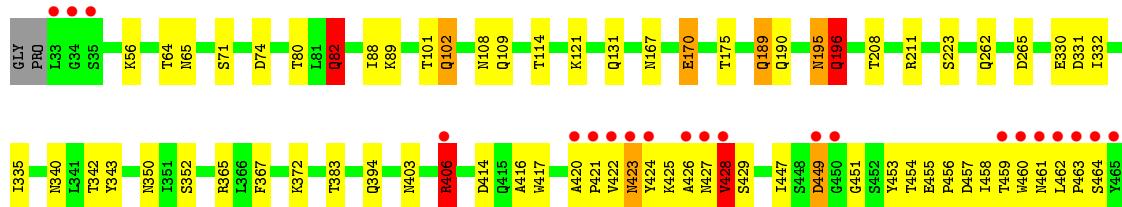
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	793	Total 793	O 793	0	0
3	B	747	Total 747	O 747	0	0
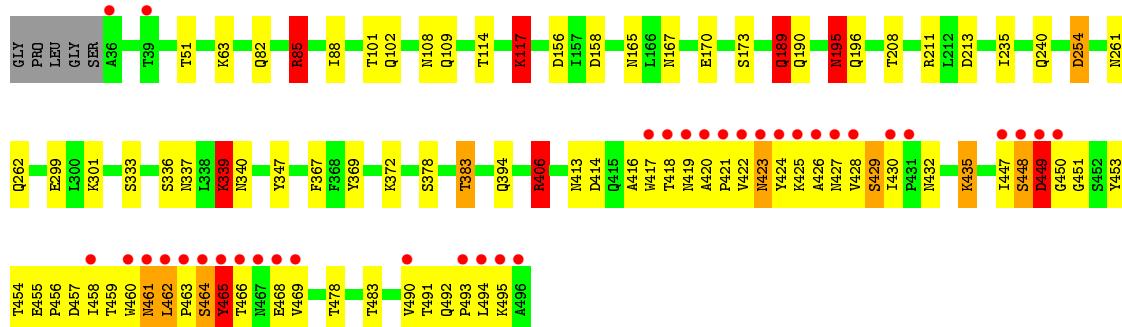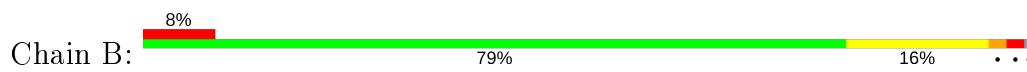
3 Residue-property plots ⓘ

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: INTERNALIN A

- Molecule 1: INTERNALIN A

4   Data and refinement statistics (i)

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 19.58 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (158.11-1.50) 88.8 (19.58-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.22 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.145 , 0.184 0.159 , 0.193	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)	0.34 , 43.5	EDS
L-test for twinning[2]	$< |L| > = 0.53$, $< L^2 > = 0.36$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	1.73	26/4754 (0.5%)	1.30	39/6498 (0.6%)
1	B	4.27	44/4630 (1.0%)	3.47	68/6330 (1.1%)
All	All	3.24	70/9384 (0.7%)	2.61	107/12828 (0.8%)

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 (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	406[A]	ARG	CZ-NH2	108.99	2.74	1.33
1	B	406[B]	ARG	CZ-NH2	108.99	2.74	1.33
1	B	406[C]	ARG	CZ-NH2	108.99	2.74	1.33
1	B	85[A]	ARG	NE-CZ	71.60	2.26	1.33
1	B	85[B]	ARG	NE-CZ	71.60	2.26	1.33
1	B	85[C]	ARG	NE-CZ	71.60	2.26	1.33
1	B	85[A]	ARG	CG-CD	56.71	2.93	1.51
1	B	85[B]	ARG	CG-CD	56.71	2.93	1.51
1	B	85[C]	ARG	CG-CD	56.71	2.93	1.51
1	B	85[A]	ARG	CZ-NH2	49.39	1.97	1.33
1	B	85[B]	ARG	CZ-NH2	49.39	1.97	1.33
1	B	85[C]	ARG	CZ-NH2	49.39	1.97	1.33
1	B	339[A]	LYS	CG-CD	45.47	3.07	1.52
1	B	339[B]	LYS	CG-CD	45.47	3.07	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	339[C]	LYS	CG-CD	45.47	3.07	1.52
1	A	82[A]	GLN	CD-NE2	37.54	2.26	1.32
1	A	82[B]	GLN	CD-NE2	37.54	2.26	1.32
1	A	82[C]	GLN	CD-NE2	37.54	2.26	1.32
1	B	465[A]	TYR	C-N	23.91	1.89	1.34
1	B	465[B]	TYR	C-N	23.91	1.89	1.34
1	A	170[A]	GLU	CD-OE1	-22.17	1.01	1.25
1	A	170[B]	GLU	CD-OE1	-22.17	1.01	1.25
1	A	170[C]	GLU	CD-OE1	-22.17	1.01	1.25
1	A	170[A]	GLU	CD-OE2	21.59	1.49	1.25
1	A	170[B]	GLU	CD-OE2	21.59	1.49	1.25
1	A	170[C]	GLU	CD-OE2	21.59	1.49	1.25
1	A	195[A]	ASN	C-N	17.17	1.73	1.34
1	A	195[B]	ASN	C-N	17.17	1.73	1.34
1	B	117[A]	LYS	CG-CD	16.68	2.09	1.52
1	B	117[B]	LYS	CG-CD	16.68	2.09	1.52
1	B	117[C]	LYS	CG-CD	16.68	2.09	1.52
1	B	195[A]	ASN	C-N	15.12	1.68	1.34
1	B	195[B]	ASN	C-N	15.12	1.68	1.34
1	B	189[A]	GLN	C-N	13.34	1.64	1.34
1	B	189[B]	GLN	C-N	13.34	1.64	1.34
1	B	189[C]	GLN	C-N	13.34	1.64	1.34
1	B	435[A]	LYS	CG-CD	11.75	1.92	1.52
1	B	435[B]	LYS	CG-CD	11.75	1.92	1.52
1	B	435[C]	LYS	CG-CD	11.75	1.92	1.52
1	A	196[A]	GLN	CG-CD	-10.22	1.27	1.51
1	A	196[B]	GLN	CG-CD	-10.22	1.27	1.51
1	A	196[C]	GLN	CG-CD	-10.22	1.27	1.51
1	A	406[A]	ARG	CD-NE	10.10	1.63	1.46
1	A	406[B]	ARG	CD-NE	10.10	1.63	1.46
1	B	406[A]	ARG	CD-NE	-8.02	1.32	1.46
1	B	406[B]	ARG	CD-NE	-8.02	1.32	1.46
1	B	406[C]	ARG	CD-NE	-8.02	1.32	1.46
1	B	170[A]	GLU	CG-CD	-7.90	1.40	1.51
1	B	170[B]	GLU	CG-CD	-7.90	1.40	1.51
1	B	170[C]	GLU	CG-CD	-7.90	1.40	1.51
1	A	196[A]	GLN	C-O	7.30	1.37	1.23
1	A	196[B]	GLN	C-O	7.30	1.37	1.23
1	A	196[C]	GLN	C-O	7.30	1.37	1.23
1	A	352[A]	SER	CA-CB	-6.05	1.43	1.52
1	A	352[B]	SER	CA-CB	-6.05	1.43	1.52
1	A	352[C]	SER	CA-CB	-6.05	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	TYR	CE1-CZ	-6.04	1.30	1.38
1	B	170[A]	GLU	CB-CG	-5.57	1.41	1.52
1	B	170[B]	GLU	CB-CG	-5.57	1.41	1.52
1	B	170[C]	GLU	CB-CG	-5.57	1.41	1.52
1	A	223	SER	CB-OG	-5.54	1.35	1.42
1	B	347	TYR	CE2-CZ	-5.28	1.31	1.38
1	B	378	SER	CB-OG	-5.22	1.35	1.42
1	B	383[A]	THR	CA-CB	5.08	1.66	1.53
1	B	383[B]	THR	CA-CB	5.08	1.66	1.53
1	B	383[C]	THR	CA-CB	5.08	1.66	1.53
1	B	347	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	189[A]	GLN	CG-CD	5.01	1.62	1.51
1	A	189[B]	GLN	CG-CD	5.01	1.62	1.51
1	A	189[C]	GLN	CG-CD	5.01	1.62	1.51

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85[A]	ARG	NE-CZ-NH2	-107.70	66.45	120.30
1	B	85[B]	ARG	NE-CZ-NH2	-107.70	66.45	120.30
1	B	85[C]	ARG	NE-CZ-NH2	-107.70	66.45	120.30
1	B	406[A]	ARG	NE-CZ-NH2	-78.61	81.00	120.30
1	B	406[B]	ARG	NE-CZ-NH2	-78.61	81.00	120.30
1	B	406[C]	ARG	NE-CZ-NH2	-78.61	81.00	120.30
1	B	85[A]	ARG	NH1-CZ-NH2	-54.33	59.64	119.40
1	B	85[B]	ARG	NH1-CZ-NH2	-54.33	59.64	119.40
1	B	85[C]	ARG	NH1-CZ-NH2	-54.33	59.64	119.40
1	A	82[A]	GLN	OE1-CD-NE2	-34.49	42.56	121.90
1	A	82[B]	GLN	OE1-CD-NE2	-34.49	42.56	121.90
1	A	82[C]	GLN	OE1-CD-NE2	-34.49	42.56	121.90
1	B	85[A]	ARG	CG-CD-NE	-29.69	49.44	111.80
1	B	85[B]	ARG	CG-CD-NE	-29.69	49.44	111.80
1	B	85[C]	ARG	CG-CD-NE	-29.69	49.44	111.80
1	A	406[A]	ARG	CD-NE-CZ	22.69	155.37	123.60
1	A	406[B]	ARG	CD-NE-CZ	22.69	155.37	123.60
1	B	339[A]	LYS	CB-CG-CD	-20.81	57.49	111.60
1	B	339[B]	LYS	CB-CG-CD	-20.81	57.49	111.60
1	B	339[C]	LYS	CB-CG-CD	-20.81	57.49	111.60
1	B	85[A]	ARG	CB-CG-CD	-18.95	62.33	111.60
1	B	85[B]	ARG	CB-CG-CD	-18.95	62.33	111.60
1	B	85[C]	ARG	CB-CG-CD	-18.95	62.33	111.60
1	A	82[A]	GLN	CG-CD-NE2	-16.14	77.97	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82[B]	GLN	CG-CD-NE2	-16.14	77.97	116.70
1	A	82[C]	GLN	CG-CD-NE2	-16.14	77.97	116.70
1	B	406[A]	ARG	CD-NE-CZ	14.91	144.47	123.60
1	B	406[B]	ARG	CD-NE-CZ	14.91	144.47	123.60
1	B	406[C]	ARG	CD-NE-CZ	14.91	144.47	123.60
1	B	406[A]	ARG	CG-CD-NE	14.14	141.49	111.80
1	B	406[B]	ARG	CG-CD-NE	14.14	141.49	111.80
1	B	406[C]	ARG	CG-CD-NE	14.14	141.49	111.80
1	B	85[A]	ARG	CD-NE-CZ	-13.75	104.36	123.60
1	B	85[B]	ARG	CD-NE-CZ	-13.75	104.36	123.60
1	B	85[C]	ARG	CD-NE-CZ	-13.75	104.36	123.60
1	B	117[A]	LYS	CG-CD-CE	13.02	150.96	111.90
1	B	117[B]	LYS	CG-CD-CE	13.02	150.96	111.90
1	B	117[C]	LYS	CG-CD-CE	13.02	150.96	111.90
1	B	189[A]	GLN	CG-CD-OE1	-11.98	97.64	121.60
1	B	189[B]	GLN	CG-CD-OE1	-11.98	97.64	121.60
1	B	189[C]	GLN	CG-CD-OE1	-11.98	97.64	121.60
1	B	117[A]	LYS	CB-CG-CD	-11.08	82.78	111.60
1	B	117[B]	LYS	CB-CG-CD	-11.08	82.78	111.60
1	B	117[C]	LYS	CB-CG-CD	-11.08	82.78	111.60
1	B	189[A]	GLN	O-C-N	-10.29	106.24	122.70
1	B	189[B]	GLN	O-C-N	-10.29	106.24	122.70
1	B	189[C]	GLN	O-C-N	-10.29	106.24	122.70
1	B	170[A]	GLU	CG-CD-OE1	-9.15	100.00	118.30
1	B	170[B]	GLU	CG-CD-OE1	-9.15	100.00	118.30
1	B	170[C]	GLU	CG-CD-OE1	-9.15	100.00	118.30
1	A	406[A]	ARG	CG-CD-NE	9.13	130.98	111.80
1	A	406[B]	ARG	CG-CD-NE	9.13	130.98	111.80
1	A	170[A]	GLU	CG-CD-OE1	9.02	136.33	118.30
1	A	170[B]	GLU	CG-CD-OE1	9.02	136.33	118.30
1	A	170[C]	GLU	CG-CD-OE1	9.02	136.33	118.30
1	B	170[A]	GLU	CG-CD-OE2	8.84	135.99	118.30
1	B	170[B]	GLU	CG-CD-OE2	8.84	135.99	118.30
1	B	170[C]	GLU	CG-CD-OE2	8.84	135.99	118.30
1	A	196[A]	GLN	CG-CD-OE1	7.91	137.41	121.60
1	A	196[B]	GLN	CG-CD-OE1	7.91	137.41	121.60
1	A	196[C]	GLN	CG-CD-OE1	7.91	137.41	121.60
1	A	170[A]	GLU	CG-CD-OE2	-7.54	103.22	118.30
1	A	170[B]	GLU	CG-CD-OE2	-7.54	103.22	118.30
1	A	170[C]	GLU	CG-CD-OE2	-7.54	103.22	118.30
1	A	196[A]	GLN	CG-CD-NE2	-7.46	98.79	116.70
1	A	196[B]	GLN	CG-CD-NE2	-7.46	98.79	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196[C]	GLN	CG-CD-NE2	-7.46	98.79	116.70
1	B	189[A]	GLN	CG-CD-NE2	7.43	134.53	116.70
1	B	189[B]	GLN	CG-CD-NE2	7.43	134.53	116.70
1	B	189[C]	GLN	CG-CD-NE2	7.43	134.53	116.70
1	A	196[A]	GLN	CB-CG-CD	7.32	130.64	111.60
1	A	196[B]	GLN	CB-CG-CD	7.32	130.64	111.60
1	A	196[C]	GLN	CB-CG-CD	7.32	130.64	111.60
1	B	435[A]	LYS	CB-CG-CD	-6.86	93.76	111.60
1	B	435[B]	LYS	CB-CG-CD	-6.86	93.76	111.60
1	B	435[C]	LYS	CB-CG-CD	-6.86	93.76	111.60
1	A	352[A]	SER	CB-CA-C	6.81	123.03	110.10
1	A	352[B]	SER	CB-CA-C	6.81	123.03	110.10
1	A	352[C]	SER	CB-CA-C	6.81	123.03	110.10
1	B	189[A]	GLN	CA-C-O	6.70	134.17	120.10
1	B	189[B]	GLN	CA-C-O	6.70	134.17	120.10
1	B	189[C]	GLN	CA-C-O	6.70	134.17	120.10
1	A	265	ASP	CB-CG-OD1	6.23	123.90	118.30
1	B	213	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	85[A]	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	85[B]	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	85[C]	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	B	339[A]	LYS	CG-CD-CE	-6.09	93.64	111.90
1	B	339[B]	LYS	CG-CD-CE	-6.09	93.64	111.90
1	B	339[C]	LYS	CG-CD-CE	-6.09	93.64	111.90
1	B	449[A]	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	449[B]	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	457[A]	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	457[B]	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	196[A]	GLN	O-C-N	-5.73	113.53	122.70
1	A	196[B]	GLN	O-C-N	-5.73	113.53	122.70
1	A	196[C]	GLN	O-C-N	-5.73	113.53	122.70
1	A	414	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	331[A]	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	331[B]	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	449[A]	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	449[B]	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	457[A]	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	457[B]	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	414	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	254[A]	ASP	CB-CG-OD2	5.06	122.86	118.30
1	B	254[B]	ASP	CB-CG-OD2	5.06	122.86	118.30

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
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 (i)

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	133	0
1	B	4571	0	4504	259	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	793	0	0	36	0
3	B	747	0	0	62	0
All	All	10809	0	9125	392	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 21.

All (392) 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	1.50
1:B:195[A]:ASN:C	1:B:196[A]:GLN:N	1.68	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435[A]:LYS:CG	1:B:435[A]:LYS:CD	1.92	1.44
1:A:195[A]:ASN:C	1:A:196[A]:GLN:N	1.73	1.42
1:B:419[B]:ASN:CB	1:B:491[B]:THR:O	1.67	1.41
1:B:117[C]:LYS:CG	1:B:117[C]:LYS:CD	1.99	1.40
1:A:406[B]:ARG:NH2	1:A:406[B]:ARG:CZ	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:B:464[B]:SER:C	1:B:465[B]:TYR:N	1.81	1.34
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:OE1	1.58	1.32
1:B:117[A]:LYS:CD	1:B:117[A]:LYS:CG	2.09	1.30
1:B:196[C]:GLN:CB	1:B:196[C]:GLN:CG	2.09	1.30
1:B:339[B]:LYS:CB	1:B:339[B]:LYS:CG	2.11	1.28
1:B:406[B]:ARG:CZ	3:B:2646:HOH:O	1.75	1.27
1:A:211[C]:ARG:NH1	3:A:2388:HOH:O	1.59	1.26
1:B:85[A]:ARG:CZ	1:B:85[A]:ARG:NH2	1.97	1.25
1:A:383[C]:THR:HB	3:A:2647:HOH:O	1.08	1.25
1:B:465[A]:TYR:C	1:B:466[A]:THR:N	1.89	1.25
1:B:337[B]:ASN:HB2	3:B:2544:HOH:O	1.33	1.24
1:A:56[B]:LYS:NZ	1:A:82[B]:GLN:O	1.69	1.24
1:B:208[A]:THR:OG1	3:B:2366:HOH:O	1.52	1.22
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:A:82[B]:GLN:NE2	3:A:2121:HOH:O	1.74	1.18
1:B:262[C]:GLN:NE2	3:B:2427:HOH:O	1.76	1.17
1:B:420[B]:ALA:CB	3:B:2664:HOH:O	1.92	1.17
1:B:417[B]:TRP:O	3:B:2659:HOH:O	1.61	1.15
1:B:165[A]:ASN:OD1	3:B:2300:HOH:O	1.62	1.14
1:B:117[B]:LYS:CD	1:B:117[B]:LYS:CG	2.26	1.14
1:A:406[B]:ARG:NH2	3:A:2683:HOH:O	1.79	1.13
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:A:417[A]:TRP:O	3:A:2697:HOH:O	1.70	1.10
1:B:339[C]:LYS:CB	1:B:339[C]:LYS:CG	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:158[B]:ASP:OD1	3:B:2274:HOH:O	1.73	1.05
1:B:85[A]:ARG:HH11	1:B:85[A]:ARG:NH2	1.40	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420[B]:ALA:O	3:B:2663:HOH:O	1.73	1.03
1:B:406[C]:ARG:CD	1:B:406[C]:ARG:NE	2.20	1.03
1:B:420[B]:ALA:C	3:B:2663:HOH:O	1.95	1.03
1:B:339[A]:LYS:HB3	1:B:339[A]:LYS:CD	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:156[B]:ASP:OD2	3:B:2269:HOH:O	1.77	0.99
1:B:85[A]:ARG:NE	1:B:85[A]:ARG:CZ	2.26	0.99
1:B:406[B]:ARG:CZ	1:B:406[B]:ARG:NH2	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:372[A]:LYS:NZ	3:B:2588:HOH:O	1.82	0.97
1:A:208[A]:THR:OG1	3:A:2382:HOH:O	1.83	0.96
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:CE	1:B:117[B]:LYS:CG	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:114[A]:THR:CG2	3:B:2191:HOH:O	2.14	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:82[A]:GLN:OE1	3:B:2120:HOH:O	1.85	0.93
1:B:419[B]:ASN:HD22	1:B:420[B]:ALA:N	1.66	0.93
1:B:339[B]:LYS:CD	1:B:339[B]:LYS:HB2	1.99	0.93
1:A:367[B]:PHE:CE2	3:A:2613:HOH:O	2.22	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:367[B]:PHE:CE2	3:B:2203:HOH:O	2.23	0.91
1:B:419[B]:ASN:HB3	1:B:491[B]:THR:O	1.69	0.91
1:B:158[B]:ASP:OD1	3:B:2276:HOH:O	1.88	0.90
1:A:427[B]:ASN:HA	1:A:460[B]:TRP:O	1.72	0.88
1:A:114[C]:THR:CG2	3:A:2200:HOH:O	2.20	0.88
1:B:419[B]:ASN:HD22	1:B:420[B]:ALA:H	0.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167[B]:ASN:OD1	3:A:2321:HOH:O	1.91	0.88
1:B:102[A]:GLN:OE1	3:B:2161:HOH:O	1.90	0.88
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:NE	2.22	0.88
1:B:339[B]:LYS:CA	1:B:339[B]:LYS:CG	2.51	0.87
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:CD	2.26	0.87
1:A:82[A]:GLN:NE2	1:A:82[A]:GLN:HG2	1.90	0.87
1:A:406[B]:ARG:HH21	1:A:406[B]:ARG:NH1	1.71	0.87
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:422[B]:VAL:CG1	3:B:2666:HOH:O	2.23	0.86
1:B:435[A]:LYS:CB	1:B:435[A]:LYS:CD	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:CD	1:B:211[B]:ARG:HE	1.81	0.84
1:B:190[B]:GLN:NE2	1:B:211[B]:ARG:HE	1.75	0.83
1:B:422[B]:VAL:HG12	3:B:2666:HOH:O	1.76	0.83
1:B:420[B]:ALA:HB3	3:B:2664:HOH:O	1.63	0.82
1:A:82[B]:GLN:CD	1:A:82[B]:GLN:NE2	2.32	0.82
1:B:189[B]:GLN:NE2	1:B:189[B]:GLN:CG	2.42	0.81
1:B:383[C]:THR:HG22	3:B:2645:HOH:O	1.80	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:HB3	1:B:117[C]:LYS:HD2	1.63	0.81
1:B:339[A]:LYS:CD	1:B:339[A]:LYS:CB	2.59	0.80
1:B:406[B]:ARG:NH1	3:B:2646:HOH:O	1.94	0.80
1:B:85[A]:ARG:CD	1:B:85[A]:ARG:HB2	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:HG2	1:B:406[C]:ARG:NE	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451[A]:GLY:N	3:B:2692:HOH:O	2.15	0.78
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:CB	1:B:85[A]:ARG:CD	2.61	0.77
1:B:85[A]:ARG:NE	1:B:85[A]:ARG:NH2	2.33	0.77
1:B:339[B]:LYS:CB	1:B:339[B]:LYS:CD	2.62	0.77
1:A:406[B]:ARG:NE	1:A:406[B]:ARG:NH2	2.33	0.77
1:A:406[B]:ARG:CZ	3:A:2649:HOH:O	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:167[A]:ASN:ND2	3:B:2305:HOH:O	1.81	0.76
1:B:339[C]:LYS:CB	1:B:339[C]:LYS:CD	2.63	0.76
1:B:63[A]:LYS:NZ	3:B:2069:HOH:O	2.18	0.76
1:B:117[A]:LYS:HD2	1:B:117[A]:LYS:HB2	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:B:51[B]:THR:CG2	3:B:2045:HOH:O	2.33	0.75
1:A:189[C]:GLN:HE21	1:A:211[C]:ARG:NH2	1.83	0.74
1:A:372[B]:LYS:HE2	3:A:2622:HOH:O	1.86	0.74
1:B:190[B]:GLN:HG3	1:B:211[B]:ARG:HH21	1.51	0.74
1:B:406[B]:ARG:HE	1:B:406[B]:ARG:NH2	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:CA	1:B:196[C]:GLN:CG	2.66	0.74
1:B:420[B]:ALA:HB2	3:B:2664:HOH:O	1.67	0.74
1:B:117[A]:LYS:HD2	1:B:117[A]:LYS:CB	2.16	0.74
1:A:167[B]:ASN:CG	3:A:2321:HOH:O	2.26	0.74
1:B:189[B]:GLN:CD	1:B:189[B]:GLN:CB	2.54	0.73
1:A:428[B]:VAL:HG23	1:A:460[B]:TRP:HE3	1.54	0.73
1:B:254[B]:ASP:OD1	3:B:2416:HOH:O	2.06	0.73
1:B:448[B]:SER:O	1:B:450[B]:GLY:N	2.21	0.73
1:A:367[B]:PHE:HE2	3:A:2613:HOH:O	1.64	0.73
1:B:85[A]:ARG:NH1	3:B:2128:HOH:O	1.73	0.73
1:B:418[B]:THR:CA	1:B:491[B]:THR:HB	2.05	0.73
1:A:102[B]:GLN:OE1	3:A:2172:HOH:O	2.05	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:NE	1:A:406[B]:ARG:NH1	2.37	0.72
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:HH21	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE3	1:B:117[B]:LYS:CG	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:449[B]:ASP:O	3:B:2689:HOH:O	2.08	0.69
1:B:428[B]:VAL:HB	1:B:460[B]:TRP:HB2	1.74	0.69
1:B:85[B]:ARG:CG	1:B:85[B]:ARG:NE	2.56	0.69
1:A:167[B]:ASN:ND2	3:A:2321:HOH:O	2.26	0.69
1:B:426[B]:ALA:HB3	3:B:2667:HOH:O	1.91	0.69
1:B:101:THR:OG1	1:B:102[B]:GLN:NE2	2.27	0.68
1:B:422[B]:VAL:C	1:B:494[B]:LEU:HA	2.13	0.68
1:B:413[A]:ASN:ND2	3:B:2653:HOH:O	1.58	0.68
1:B:114[A]:THR:HG22	3:B:2191:HOH:O	1.85	0.68
1:B:419[B]:ASN:C	1:B:493[B]:PRO:CD	2.60	0.68
1:B:417[B]:TRP:NE1	1:B:490[B]:VAL:HG13	2.09	0.68
1:B:432[A]:ASN:OD1	3:B:2669:HOH:O	2.07	0.68
1:B:406[C]:ARG:HD2	3:B:2642:HOH:O	1.94	0.67
1:B:190[B]:GLN:HG3	1:B:211[B]:ARG:NH2	2.09	0.67
1:B:419[B]:ASN:H	1:B:491[B]:THR:C	1.97	0.66
1:B:85[A]:ARG:HH22	1:B:85[A]:ARG:NH1	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:A:372[A]:LYS:NZ	3:A:2582:HOH:O	2.29	0.65
1:B:190[B]:GLN:CG	1:B:211[B]:ARG:NE	2.59	0.65
1:B:406[B]:ARG:NE	1:B:406[B]:ARG:NH2	2.44	0.65
1:B:114[A]:THR:HG21	3:B:2191:HOH:O	1.86	0.64
1:B:339[C]:LYS:CB	1:B:339[C]:LYS:HD2	2.27	0.64
1:B:419[B]:ASN:C	1:B:493[B]:PRO:HD3	2.18	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:CB	1:B:85[B]:ARG:CD	2.76	0.63
1:B:420[B]:ALA:HB3	3:B:2663:HOH:O	1.99	0.63
1:B:367[B]:PHE:HE2	3:B:2203:HOH:O	1.69	0.63
1:B:422[B]:VAL:N	1:B:493[B]:PRO:O	2.31	0.63
1:A:114[C]:THR:HG22	3:A:2200:HOH:O	1.94	0.63
1:A:429[B]:SER:HB2	1:A:459[B]:THR:CG2	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365[B]:ARG:NH2	3:A:2614:HOH:O	2.32	0.62
1:B:240:GLN:HA	1:B:262[C]:GLN:HE22	1.65	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: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:B:420[B]:ALA:CB	3:B:2663:HOH:O	2.49	0.60
1:A:447[B]:ILE:CG2	1:A:451[B]:GLY:HA3	2.31	0.60
1:A:82[A]:GLN:HE21	1:A:82[A]:GLN:HG2	1.66	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:B:51[B]:THR:HG23	3:B:2045:HOH:O	1.99	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:383[C]:THR:HG21	3:B:2638:HOH:O	2.02	0.59
1:A:131[B]:GLN:CD	3:A:2236:HOH:O	2.40	0.59
1:B:299:GLU:OE1	3:B:2484:HOH:O	2.17	0.59
1:A:340[B]:ASN:HB2	3:A:2526:HOH:O	2.03	0.58
1:A:424[A]:TYR:O	1:A:425[A]:LYS:CG	2.51	0.58
1:B:420[B]:ALA:O	1:B:493[B]:PRO:HD2	2.03	0.58
1:B:85[A]:ARG:NE	1:B:85[A]:ARG:HH21	2.00	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:196[C]:GLN:CB	1:B:196[C]:GLN:CD	2.72	0.57
1:B:85[B]:ARG:HE	1:B:85[B]:ARG:CG	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:CG	1:A:82[B]:GLN:NE2	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:A:423[A]:ASN:O	1:A:424[A]:TYR:C	2.44	0.56
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:B:429[A]:SER:CB	1:B:459[A]:THR:HG22	2.30	0.56
1:A:423[B]:ASN:HB2	1:A:495[B]:LYS:HZ1	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447[B]:ILE:HG22	1:A:451[B]:GLY:HA3	1.85	0.56
1:B:460[B]:TRP:NE1	1:B:469[B]:VAL:HB	2.20	0.56
1:A:372[A]:LYS:NZ	3:A:2622:HOH:O	2.39	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:A:114[C]:THR:HG21	3:A:2200:HOH:O	1.95	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:465[B]:TYR:CG	1:B:466[B]:THR:N	2.68	0.55
1:B:460[B]:TRP:CE2	1:B:469[B]:VAL:HB	2.41	0.55
1:B:372[A]:LYS:NZ	3:B:2591:HOH:O	2.13	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:HA	1:B:196[C]:GLN:CG	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:A:423[A]:ASN:C	1:A:424[A]:TYR:O	2.44	0.53
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:B:51[B]:THR:HG22	3:B:2045:HOH:O	2.03	0.53
1:B:426[B]:ALA:O	1:B:462[B]:LEU:HA	2.08	0.53
1:A:406[B]:ARG:CZ	3:A:2683:HOH:O	0.83	0.52
1:A:455[B]:GLU:OE2	3:A:2750:HOH:O	2.19	0.52
1:B:190[B]:GLN:CD	1:B:211[B]:ARG:HH21	2.13	0.52
1:B:420[B]:ALA:N	3:B:2664:HOH:O	2.40	0.52
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:B:195[A]:ASN:C	1:B:196[A]:GLN:CA	2.72	0.51
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:B:465[A]:TYR:C	1:B:466[A]:THR:CA	2.77	0.51
1:A:447[B]:ILE:HD11	1:A:453[B]:TYR:HB2	1.92	0.51
1:A:80[A]:THR:CG2	1:A:102[A]:GLN:HE21	2.22	0.51
1:A:71[B]:SER:OG	1:A:74[B]:ASP:OD2	2.28	0.51
1:B:450[B]:GLY:HA2	3:B:2692:HOH:O	2.10	0.51
1:B:88:ILE:H	1:B:108:ASN:HD22	1.59	0.51
1:B:109[B]:GLN:HG3	3:B:2174:HOH:O	2.11	0.50
1:B:339[B]:LYS:NZ	1:B:340[B]:ASN:HD21	2.09	0.50
1:A:121[B]:LYS:HB2	3:A:2166:HOH:O	2.11	0.50
1:B:465[B]:TYR:CE1	1:B:466[B]:THR:O	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372[A]:LYS:CE	3:B:2591:HOH:O	2.57	0.50
1:B:417[B]:TRP:CZ2	1:B:490[B]:VAL:CG2	2.85	0.50
1:B:337[A]:ASN:ND2	3:B:2545:HOH:O	2.45	0.49
1:B:406[A]:ARG:NH2	1:B:406[A]:ARG:CZ	2.74	0.49
1:B:189[A]:GLN:NE2	3:B:2336:HOH:O	2.46	0.49
1:A:56[B]:LYS:NZ	1:A:82[B]:GLN:C	2.57	0.49
1:B:339[B]:LYS:HZ3	1:B:340[B]:ASN:HD21	1.58	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:B:261:ASN:C	1:B:262[C]:GLN:HE21	2.15	0.48
1:A:131[B]:GLN:NE2	3:A:2236:HOH:O	2.45	0.48
1:B:383[C]:THR:CG2	3:B:2645:HOH:O	2.52	0.48
1:B:465[A]:TYR:CA	1:B:466[A]:THR:N	2.74	0.48
1:A:403[B]:ASN:ND2	3:A:2676:HOH:O	2.47	0.48
1:B:430[B]:ILE:HG12	1:B:460[B]:TRP:HZ3	1.78	0.48
1:B:339[C]:LYS:CA	1:B:339[C]:LYS:CG	2.92	0.48
1:B:429[B]:SER:HA	1:B:458[B]:ILE:O	2.14	0.47
1:A:189[C]:GLN:NE2	3:A:2352:HOH:O	2.47	0.47
1:B:262[C]:GLN:CD	3:B:2427:HOH:O	2.31	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:454[B]:THR:O	1:A:455[B]:GLU:C	2.54	0.46
1:B:422[B]:VAL:HG13	3:B:2666:HOH:O	2.04	0.46
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:425[A]:LYS:O	1:A:426[A]:ALA:C	2.54	0.46
1:A:88:ILE:H	1:A:108:ASN:ND2	2.14	0.46
1:B:454:THR:O	1:B:455[A]:GLU:C	2.54	0.45
1:B:85[A]:ARG:CD	1:B:85[A]:ARG:CG	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:A:195[A]:ASN:C	1:A:196[A]:GLN:CA	2.76	0.45
1:B:262[C]:GLN:N	1:B:262[C]:GLN:HE21	2.13	0.45
1:B:447[B]:ILE:O	1:B:448[B]:SER:O	2.35	0.45
1:B:418[B]:THR:CG2	1:B:491[B]:THR:HG21	2.37	0.45
1:B:419[B]:ASN:C	1:B:493[B]:PRO:HD2	2.36	0.45
1:B:450[B]:GLY:O	3:B:2690:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426[A]:ALA:HA	1:B:462[A]:LEU:O	2.17	0.45
1:B:420[B]:ALA:CA	3:B:2663:HOH:O	2.51	0.45
1:B:420[B]:ALA:C	1:B:493[B]:PRO:HD2	2.38	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:425[A]:LYS:CB	1:A:428[A]:VAL:HG13	2.40	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:A:454[A]:THR:O	1:A:455[A]:GLU:C	2.55	0.43
1:A:121[A]:LYS:HB2	3:A:2166:HOH:O	2.18	0.43
1:A:372[B]:LYS:CE	3:A:2622:HOH:O	2.55	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:A:416[A]:ALA:O	3:A:2696:HOH:O	2.19	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:451[B]:GLY:HA2	1:B:459[B]:THR:O	2.19	0.43
1:B:85[A]:ARG:HE	1:B:85[A]:ARG:HH21	1.67	0.43
1:A:195[A]:ASN:CA	1:A:196[A]:GLN:N	2.75	0.42
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:A:372[A]:LYS:CE	3:A:2622:HOH:O	2.66	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: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: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:419[B]:ASN:ND2	1:B:420[B]:ALA:N	2.47	0.41
1:A:383[C]:THR:CB	3:A:2647:HOH:O	1.97	0.41
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:B:448[B]:SER:O	1:B:449[B]:ASP:C	2.59	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%)	15	3
1	B	593/466 (127%)	542 (91%)	43 (7%)	8 (1%)	12	2
All	All	1203/932 (129%)	1104 (92%)	85 (7%)	14 (1%)	19	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

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

5.3.2　Protein sidechains (i)

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%)	50	20
1	B	542/418 (130%)	525 (97%)	17 (3%)	40	11
All	All	1100/836 (132%)	1070 (97%)	30 (3%)	62	15

All (30) 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	428[A]	VAL
1	A	428[B]	VAL
1	A	461[A]	ASN
1	A	461[B]	ASN
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	189[A]	GLN

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Mol	Chain	Res	Type
1	B	189[B]	GLN
1	B	189[C]	GLN
1	B	195[A]	ASN
1	B	195[B]	ASN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	394	GLN
1	B	40	GLN
1	B	108	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)

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 (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	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 (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, 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%)	0.20	26 (5%)	24	26	9, 13, 26, 41	1 (0%)
1	B	461/466 (98%)	0.22	36 (7%)	13	13	9, 14, 26, 36	0
All	All	925/932 (99%)	0.21	62 (6%)	17	19	9, 13, 26, 41	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423[A]	ASN	9.4
1	B	423[A]	ASN	8.9
1	B	420[A]	ALA	8.5
1	B	464[A]	SER	7.9
1	A	465	TYR	7.7
1	A	463[A]	PRO	7.7
1	B	463[A]	PRO	7.7
1	A	406[A]	ARG	7.1
1	A	34	GLY	6.9
1	B	421[A]	PRO	6.8
1	A	420[A]	ALA	6.8
1	A	494[A]	LEU	6.7
1	A	422[A]	VAL	6.4
1	A	464[A]	SER	6.3
1	B	462[A]	LEU	6.2
1	B	424[A]	TYR	6.1
1	A	33	LEU	6.1
1	B	466[A]	THR	6.0
1	B	426[A]	ALA	5.8
1	A	496	ALA	5.7
1	A	466[A]	THR	5.6
1	B	465[A]	TYR	5.6
1	A	495[A]	LYS	5.5
1	B	422[A]	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	469[A]	VAL	5.0
1	A	424[A]	TYR	5.0
1	B	496	ALA	4.8
1	B	494[A]	LEU	4.6
1	B	461[A]	ASN	4.6
1	A	462[A]	LEU	4.3
1	A	426[A]	ALA	4.3
1	A	450[A]	GLY	4.2
1	A	427[A]	ASN	4.1
1	B	460[A]	TRP	4.1
1	A	467[A]	ASN	4.1
1	B	450[A]	GLY	4.0
1	B	427[A]	ASN	4.0
1	B	467[A]	ASN	3.8
1	B	419[A]	ASN	3.7
1	B	495[A]	LYS	3.7
1	B	428[A]	VAL	3.7
1	A	35	SER	3.7
1	B	36	ALA	3.5
1	B	430[A]	ILE	3.4
1	A	428[A]	VAL	3.4
1	B	418[A]	THR	3.0
1	A	461[A]	ASN	2.8
1	B	449[A]	ASP	2.7
1	B	425[A]	LYS	2.6
1	B	39	THR	2.5
1	A	421[A]	PRO	2.5
1	B	447[A]	ILE	2.5
1	B	468[A]	GLU	2.3
1	A	449[A]	ASP	2.3
1	B	458[A]	ILE	2.3
1	B	431[A]	PRO	2.2
1	B	493[A]	PRO	2.2
1	B	448[A]	SER	2.1
1	B	490[A]	VAL	2.1
1	A	460[A]	TRP	2.1
1	B	417[A]	TRP	2.1
1	A	459[A]	THR	2.0

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

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. 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(Å^2)	Q<0.9
2	CA	B	1497	1/1	1.00	0.09	7,7,7,7	1
2	CA	A	1497	1/1	1.00	0.08	7,7,7,7	1

6.5 Other polymers (i)

There are no such residues in this entry.