



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 PM UTC

PDB ID : 1ANW / pdb_00001anw
Title : THE EFFECT OF METAL BINDING ON THE STRUCTURE OF AN-NEXIN V AND IMPLICATIONS FOR MEMBRANE BINDING
Authors : Lewit-Bentley, A.; Morera, S.; Huber, R.; Bodo, G.
Deposited on : 1993-10-26
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

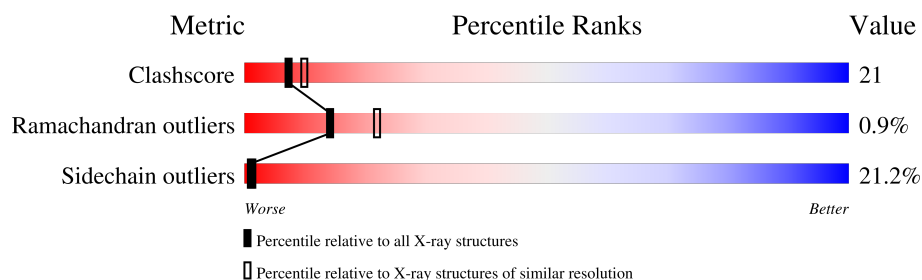
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5305 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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2518	1585	423	502	8			
1	B	319	Total	C	N	O	S	0	0	0
			2518	1585	423	502	8			

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

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

- Molecule 3 is water.

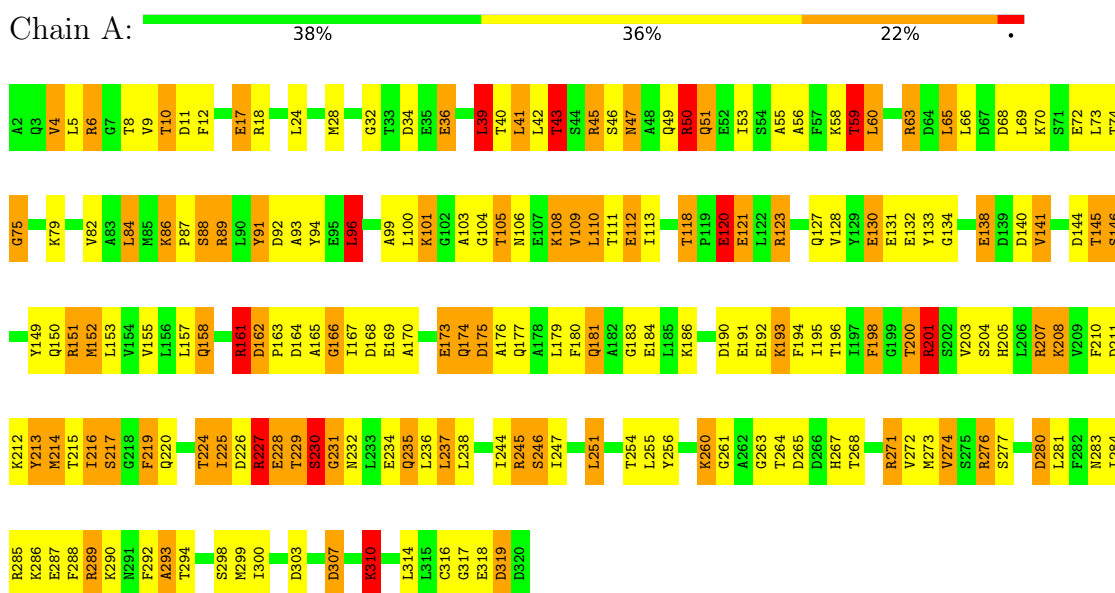
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		
3	B	130	Total	O	0	0
			130	130		

3 Residue-property plots

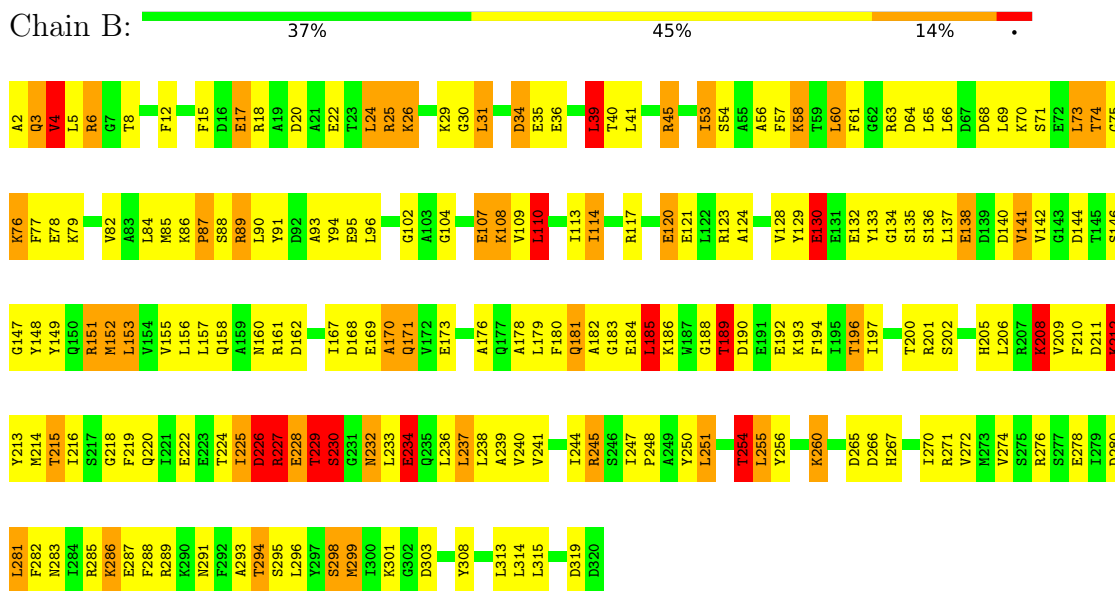
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ANNEXIN V



• Molecule 1: ANNEXIN V



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.90Å 80.90Å 71.40Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	12.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5305	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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	1.33	10/2552 (0.4%)	2.45	176/3434 (5.1%)
1	B	1.19	4/2552 (0.2%)	2.31	153/3434 (4.5%)
All	All	1.26	14/5104 (0.3%)	2.38	329/6868 (4.8%)

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	6
1	B	0	2
All	All	0	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	GLN	C-N	15.32	1.53	1.33
1	A	230	SER	C-N	12.65	1.50	1.33
1	A	4	VAL	C-N	-11.04	1.18	1.33
1	A	316	CYS	C-N	-8.10	1.23	1.33
1	A	161	ARG	C-N	7.90	1.50	1.33
1	B	61	PHE	C-N	-6.79	1.24	1.33
1	B	4	VAL	C-N	-6.75	1.23	1.33
1	A	70	LYS	C-N	5.71	1.42	1.33
1	B	170	ALA	C-N	-5.62	1.26	1.33
1	A	213	TYR	C-N	-5.57	1.25	1.33
1	A	276	ARG	CD-NE	-5.30	1.38	1.46
1	A	191	GLU	C-N	-5.24	1.27	1.34
1	B	202	SER	C-N	-5.20	1.27	1.33
1	A	111	THR	CA-CB	5.04	1.61	1.53

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	CYS	CA-C-N	18.01	153.12	120.87
1	A	316	CYS	C-N-CA	18.01	153.12	120.87
1	A	175	ASP	CA-CB-CG	13.11	125.71	112.60
1	A	230	SER	O-C-N	-12.92	105.41	122.59
1	B	194	PHE	CA-CB-CG	12.28	126.08	113.80
1	A	4	VAL	CA-C-N	11.80	139.57	121.99
1	A	4	VAL	C-N-CA	11.80	139.57	121.99
1	A	144	ASP	CA-CB-CG	10.16	122.76	112.60
1	B	197	ILE	N-CA-C	-10.05	100.97	110.42
1	B	314	LEU	CA-C-N	10.02	134.07	120.54
1	B	314	LEU	C-N-CA	10.02	134.07	120.54
1	B	245	ARG	CD-NE-CZ	-9.77	110.72	124.40
1	A	280	ASP	CA-CB-CG	9.69	122.29	112.60
1	A	198	PHE	CA-C-O	-9.31	110.68	120.55
1	B	64	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	319	ASP	O-C-N	-8.80	113.19	123.22
1	B	74	THR	CA-C-N	8.75	134.16	120.07
1	B	74	THR	C-N-CA	8.75	134.16	120.07
1	B	296	LEU	CA-C-N	8.62	132.18	120.54
1	B	296	LEU	C-N-CA	8.62	132.18	120.54
1	B	225	ILE	N-CA-C	8.61	122.81	113.43
1	A	261	GLY	CA-C-N	8.49	134.03	121.72
1	A	261	GLY	C-N-CA	8.49	134.03	121.72
1	A	198	PHE	CA-CB-CG	8.48	122.28	113.80
1	B	160	ASN	N-CA-CB	-8.47	98.89	111.43
1	B	68	ASP	CA-CB-CG	8.47	121.07	112.60
1	B	170	ALA	CA-C-N	8.39	131.88	120.38
1	B	170	ALA	C-N-CA	8.39	131.88	120.38
1	A	267	HIS	CA-CB-CG	-8.22	105.58	113.80
1	A	53	ILE	CA-C-O	8.12	129.46	120.85
1	A	68	ASP	CA-CB-CG	8.07	120.67	112.60
1	B	4	VAL	CA-C-N	7.91	132.72	121.02
1	B	4	VAL	C-N-CA	7.91	132.72	121.02
1	A	75	GLY	N-CA-C	7.76	125.00	111.50
1	A	130	GLU	CA-C-N	7.75	130.52	120.44
1	A	130	GLU	C-N-CA	7.75	130.52	120.44
1	A	274	VAL	CA-C-N	7.74	131.69	120.38
1	A	274	VAL	C-N-CA	7.74	131.69	120.38
1	B	149	TYR	N-CA-C	-7.72	102.56	110.97
1	A	10	THR	CB-CA-C	-7.67	93.57	110.67
1	A	287	GLU	CA-C-N	7.66	131.43	120.79
1	A	287	GLU	C-N-CA	7.66	131.43	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASP	CA-C-O	-7.65	112.67	121.54
1	A	245	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	A	110	LEU	CA-C-N	7.62	130.34	120.44
1	A	110	LEU	C-N-CA	7.62	130.34	120.44
1	A	186	LYS	N-CA-C	7.62	121.90	111.54
1	A	91	TYR	N-CA-C	7.60	120.23	111.11
1	B	129	TYR	CA-C-N	7.58	131.32	120.79
1	B	129	TYR	C-N-CA	7.58	131.32	120.79
1	A	307	ASP	N-CA-C	-7.57	103.04	111.82
1	A	51	GLN	CA-C-N	7.55	131.00	120.29
1	A	51	GLN	C-N-CA	7.55	131.00	120.29
1	A	271	ARG	CA-C-O	-7.53	112.50	120.63
1	B	274	VAL	N-CA-C	7.48	118.27	110.72
1	B	162	ASP	O-C-N	7.46	129.73	121.53
1	A	310	LYS	CA-C-N	7.43	130.24	120.28
1	A	310	LYS	C-N-CA	7.43	130.24	120.28
1	B	308	TYR	N-CA-C	-7.42	103.13	111.14
1	A	88	SER	CA-CB-OG	7.39	125.88	111.10
1	A	310	LYS	CB-CA-C	7.34	122.41	110.88
1	A	34	ASP	CA-CB-CG	-7.34	105.26	112.60
1	A	120	GLU	CB-CG-CD	7.34	125.08	112.60
1	B	93	ALA	CA-C-O	7.31	128.49	120.82
1	A	158	GLN	CB-CG-CD	7.27	124.95	112.60
1	A	60	LEU	CA-C-O	-7.26	110.30	119.31
1	B	110	LEU	CA-C-O	7.26	128.12	120.42
1	B	45	ARG	CA-C-O	-7.25	112.96	121.16
1	B	151	ARG	CD-NE-CZ	7.25	134.55	124.40
1	B	77	PHE	CA-CB-CG	-7.21	106.59	113.80
1	A	133	TYR	O-C-N	7.18	130.79	122.25
1	B	288	PHE	CA-C-N	7.17	129.76	120.44
1	B	288	PHE	C-N-CA	7.17	129.76	120.44
1	A	169	GLU	N-CA-C	7.16	121.46	112.87
1	A	268	THR	CA-CB-OG1	-7.11	98.93	109.60
1	B	210	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	45	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	B	146	SER	CA-C-N	7.09	131.57	120.65
1	B	146	SER	C-N-CA	7.09	131.57	120.65
1	B	232	ASN	CA-C-O	-7.04	112.14	120.10
1	B	278	GLU	CB-CG-CD	7.04	124.57	112.60
1	A	298	SER	CA-CB-OG	-7.02	97.06	111.10
1	B	132	GLU	N-CA-C	7.01	120.32	111.69
1	B	39	LEU	CB-CA-C	6.97	122.36	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ARG	CD-NE-CZ	6.95	134.13	124.40
1	B	57	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	43	THR	CA-CB-CG2	6.94	122.30	110.50
1	A	194	PHE	CA-CB-CG	6.90	120.70	113.80
1	B	285	ARG	CA-C-N	6.90	130.08	120.29
1	B	285	ARG	C-N-CA	6.90	130.08	120.29
1	A	127	GLN	CA-C-O	6.89	127.80	120.70
1	B	138	GLU	CB-CG-CD	6.84	124.22	112.60
1	B	123	ARG	CD-NE-CZ	-6.76	114.94	124.40
1	B	185	LEU	CA-C-N	6.75	132.19	122.40
1	B	185	LEU	C-N-CA	6.75	132.19	122.40
1	A	82	VAL	CB-CA-C	6.73	121.22	112.14
1	B	180	PHE	CA-CB-CG	-6.72	107.08	113.80
1	B	156	LEU	CA-C-N	6.69	130.48	120.31
1	B	156	LEU	C-N-CA	6.69	130.48	120.31
1	B	171	GLN	OE1-CD-NE2	6.67	129.27	122.60
1	B	12	PHE	CA-C-O	6.65	125.68	119.76
1	A	36	GLU	CA-CB-CG	6.64	127.38	114.10
1	A	45	ARG	N-CA-C	-6.62	99.04	109.50
1	B	158	GLN	CA-C-N	6.62	131.76	122.36
1	B	158	GLN	C-N-CA	6.62	131.76	122.36
1	A	231	GLY	CA-C-N	6.61	129.98	120.79
1	A	231	GLY	C-N-CA	6.61	129.98	120.79
1	B	294	THR	CA-C-O	-6.60	113.41	121.06
1	A	276	ARG	N-CA-CB	-6.59	100.51	110.73
1	B	301	LYS	CA-C-N	6.55	128.59	120.34
1	B	301	LYS	C-N-CA	6.55	128.59	120.34
1	B	226	ASP	N-CA-C	6.49	124.62	110.80
1	A	123	ARG	CD-NE-CZ	-6.47	115.33	124.40
1	A	272	VAL	N-CA-C	6.42	117.21	110.72
1	B	31	LEU	CB-CA-C	6.41	119.89	109.90
1	A	121	GLU	CB-CG-CD	6.38	123.45	112.60
1	A	284	ILE	N-CA-C	-6.38	104.11	110.62
1	B	271	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	A	310	LYS	O-C-N	-6.37	115.50	122.07
1	A	285	ARG	CA-C-N	6.37	128.72	120.44
1	A	285	ARG	C-N-CA	6.37	128.72	120.44
1	B	196	THR	CA-CB-OG1	-6.37	100.05	109.60
1	A	230	SER	CA-C-N	6.34	128.54	122.27
1	A	230	SER	C-N-CA	6.34	128.54	122.27
1	B	227	ARG	CD-NE-CZ	6.33	133.25	124.40
1	B	299	MET	CA-CB-CG	-6.32	101.46	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	O-C-N	6.32	128.58	121.32
1	B	229	THR	CB-CA-C	6.31	122.98	110.42
1	A	210	PHE	CA-C-N	6.31	129.02	120.44
1	A	210	PHE	C-N-CA	6.31	129.02	120.44
1	B	212	LYS	CA-C-N	6.31	128.73	120.28
1	B	212	LYS	C-N-CA	6.31	128.73	120.28
1	A	151	ARG	CG-CD-NE	6.30	125.86	112.00
1	B	289	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	B	160	ASN	CA-CB-CG	6.28	118.88	112.60
1	A	183	GLY	CA-C-N	6.27	128.68	120.28
1	A	183	GLY	C-N-CA	6.27	128.68	120.28
1	B	104	GLY	O-C-N	6.23	127.89	121.97
1	A	254	THR	CA-C-N	6.21	128.61	120.28
1	A	254	THR	C-N-CA	6.21	128.61	120.28
1	A	244	ILE	N-CA-C	-6.21	104.69	110.53
1	A	265	ASP	N-CA-C	-6.20	97.78	108.56
1	B	65	LEU	CA-C-O	-6.16	114.35	120.82
1	A	43	THR	CB-CA-C	6.15	123.17	110.31
1	A	66	LEU	N-CA-C	6.09	117.58	111.07
1	A	289	ARG	CD-NE-CZ	-6.07	115.90	124.40
1	A	12	PHE	N-CA-C	-6.07	102.00	109.65
1	A	138	GLU	CB-CG-CD	6.05	122.89	112.60
1	B	220	GLN	OE1-CD-NE2	-6.04	116.56	122.60
1	B	245	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	A	132	GLU	CB-CA-C	-5.99	99.75	110.70
1	A	168	ASP	CB-CA-C	5.99	121.37	111.31
1	B	215	THR	N-CA-C	-5.96	104.70	111.14
1	A	105	THR	CA-CB-OG1	-5.94	100.69	109.60
1	B	289	ARG	CD-NE-CZ	5.93	132.70	124.40
1	B	121	GLU	CA-C-O	-5.92	114.60	120.70
1	B	137	LEU	CA-C-N	5.91	128.51	120.54
1	B	137	LEU	C-N-CA	5.91	128.51	120.54
1	A	294	THR	CB-CA-C	5.88	121.33	109.68
1	A	43	THR	N-CA-CB	-5.84	100.69	110.39
1	A	108	LYS	CB-CA-C	5.84	120.16	110.81
1	B	12	PHE	CB-CA-C	5.84	118.87	109.41
1	A	176	ALA	CA-C-O	5.84	126.68	119.97
1	A	128	VAL	CA-C-N	5.83	128.03	120.44
1	A	128	VAL	C-N-CA	5.83	128.03	120.44
1	A	131	GLU	CB-CA-C	-5.82	101.74	110.88
1	B	20	ASP	CA-C-N	5.82	128.35	120.38
1	B	20	ASP	C-N-CA	5.82	128.35	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASN	CA-C-N	5.79	128.04	120.28
1	A	47	ASN	C-N-CA	5.79	128.04	120.28
1	A	149	TYR	N-CA-C	-5.79	104.60	111.03
1	B	225	ILE	CA-C-O	-5.79	113.46	118.96
1	A	288	PHE	O-C-N	5.78	128.27	122.08
1	A	225	ILE	N-CA-C	5.75	116.56	111.90
1	B	76	LYS	O-C-N	5.75	129.34	122.27
1	B	30	GLY	CA-C-O	5.74	126.94	122.29
1	A	145	THR	CA-CB-OG1	-5.73	101.00	109.60
1	B	123	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	A	201	ARG	CA-C-O	-5.72	115.58	121.87
1	B	241	VAL	CB-CA-C	5.72	119.29	111.97
1	B	291	ASN	N-CA-C	5.72	118.45	111.82
1	A	200	THR	CB-CA-C	5.71	119.31	109.15
1	B	94	TYR	CA-CB-CG	-5.71	103.63	113.90
1	B	75	GLY	N-CA-C	5.71	121.72	111.34
1	A	264	THR	O-C-N	5.70	129.78	123.33
1	B	155	VAL	N-CA-C	-5.69	105.18	110.53
1	B	108	LYS	CB-CG-CD	5.69	124.38	111.30
1	A	300	ILE	CB-CA-C	-5.68	104.69	111.97
1	B	265	ASP	N-CA-C	-5.67	97.97	108.24
1	A	161	ARG	O-C-N	-5.66	116.57	123.19
1	A	94	TYR	CA-C-N	5.62	127.81	120.28
1	A	94	TYR	C-N-CA	5.62	127.81	120.28
1	A	91	TYR	O-C-N	-5.61	116.25	122.09
1	B	267	HIS	CB-CA-C	5.61	119.69	110.88
1	B	237	LEU	CA-C-N	5.61	128.05	120.65
1	B	237	LEU	C-N-CA	5.61	128.05	120.65
1	A	92	ASP	CA-C-O	-5.60	114.48	120.42
1	B	130	GLU	CA-C-N	5.58	128.08	120.54
1	B	130	GLU	C-N-CA	5.58	128.08	120.54
1	A	290	LYS	CB-CA-C	-5.58	102.11	110.88
1	A	39	LEU	CB-CA-C	5.58	120.33	110.85
1	A	263	GLY	O-C-N	5.57	128.20	122.91
1	A	293	ALA	N-CA-CB	-5.57	103.77	112.41
1	A	219	PHE	CA-CB-CG	-5.57	108.23	113.80
1	B	229	THR	N-CA-C	-5.57	98.94	110.80
1	A	146	SER	N-CA-C	5.55	117.85	109.41
1	A	59	THR	CA-C-O	-5.55	114.99	120.70
1	B	85	MET	CA-C-N	5.55	130.15	121.17
1	B	85	MET	C-N-CA	5.55	130.15	121.17
1	A	207	ARG	CA-C-N	5.54	127.64	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	C-N-CA	5.54	127.64	120.44
1	A	82	VAL	CA-C-N	5.54	127.70	120.28
1	A	82	VAL	C-N-CA	5.54	127.70	120.28
1	A	56	ALA	N-CA-C	-5.53	105.33	111.36
1	A	141	VAL	CA-C-O	5.53	127.21	121.29
1	A	138	GLU	CG-CD-OE1	5.52	131.11	118.40
1	B	170	ALA	O-C-N	5.51	127.98	122.03
1	B	183	GLY	O-C-N	5.51	127.53	122.19
1	A	162	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	96	LEU	CA-C-N	5.50	127.97	120.54
1	A	96	LEU	C-N-CA	5.50	127.97	120.54
1	B	287	GLU	CA-C-N	5.50	127.96	120.54
1	B	287	GLU	C-N-CA	5.50	127.96	120.54
1	A	32	GLY	CA-C-N	5.48	131.55	121.85
1	A	32	GLY	C-N-CA	5.48	131.55	121.85
1	B	133	TYR	N-CA-CB	-5.48	102.59	110.65
1	A	251	LEU	O-C-N	-5.48	115.53	122.27
1	B	17	GLU	N-CA-C	5.48	118.01	111.71
1	B	153	LEU	CB-CA-C	5.48	119.48	110.88
1	A	141	VAL	CB-CA-C	5.47	118.65	111.81
1	A	227	ARG	O-C-N	-5.47	115.39	122.56
1	A	195	ILE	O-C-N	-5.46	116.20	121.83
1	A	235	GLN	CA-CB-CG	5.45	125.01	114.10
1	B	34	ASP	O-C-N	-5.44	116.40	122.55
1	A	271	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	140	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	310	LYS	CA-CB-CG	5.41	124.92	114.10
1	B	148	TYR	CA-CB-CG	-5.40	104.18	113.90
1	A	300	ILE	N-CA-CB	5.39	116.86	110.55
1	A	106	ASN	CA-C-N	5.39	128.50	120.31
1	A	106	ASN	C-N-CA	5.39	128.50	120.31
1	A	196	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	68	ASP	N-CA-C	-5.38	105.31	111.07
1	A	128	VAL	N-CA-C	5.38	116.11	110.62
1	A	4	VAL	N-CA-C	-5.38	102.13	109.55
1	B	298	SER	CA-CB-OG	-5.38	100.35	111.10
1	A	138	GLU	CG-CD-OE2	-5.37	106.05	118.40
1	B	227	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
1	A	65	LEU	O-C-N	5.34	127.79	122.12
1	A	63	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	232	ASN	N-CA-C	-5.33	104.51	111.02
1	B	4	VAL	O-C-N	-5.33	115.90	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	THR	CA-C-O	-5.31	115.17	120.96
1	A	112	GLU	CG-CD-OE1	-5.31	106.18	118.40
1	B	136	SER	CA-C-O	-5.30	114.82	120.92
1	A	18	ARG	N-CA-C	-5.30	105.08	112.45
1	A	195	ILE	CA-C-N	5.30	127.92	120.28
1	A	195	ILE	C-N-CA	5.30	127.92	120.28
1	B	245	ARG	NE-CZ-NH1	-5.29	116.22	121.50
1	A	201	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	53	ILE	CA-C-O	5.26	126.89	121.05
1	A	103	ALA	O-C-N	5.26	129.88	122.41
1	A	193	LYS	CB-CA-C	5.26	119.62	110.79
1	B	91	TYR	N-CA-C	5.26	116.69	111.07
1	B	121	GLU	CA-C-N	5.26	127.32	120.28
1	B	121	GLU	C-N-CA	5.26	127.32	120.28
1	A	127	GLN	CA-CB-CG	5.25	124.60	114.10
1	A	300	ILE	N-CA-C	-5.24	105.39	110.42
1	B	276	ARG	CA-C-O	-5.24	113.22	119.35
1	B	293	ALA	N-CA-CB	-5.24	104.29	112.41
1	A	43	THR	CA-C-O	5.24	125.82	119.38
1	A	45	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
1	B	182	ALA	CA-C-N	5.24	125.76	120.00
1	B	182	ALA	C-N-CA	5.24	125.76	120.00
1	A	89	ARG	N-CA-CB	5.23	117.81	110.12
1	A	190	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	59	THR	N-CA-CB	5.23	117.65	110.07
1	B	190	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	178	ALA	CA-C-O	5.21	126.30	120.82
1	B	211	ASP	CA-C-O	-5.21	115.33	120.80
1	A	166	GLY	CA-C-N	-5.21	113.01	122.43
1	A	166	GLY	C-N-CA	-5.21	113.01	122.43
1	A	41	LEU	CA-C-N	5.20	127.51	120.38
1	A	41	LEU	C-N-CA	5.20	127.51	120.38
1	A	53	ILE	O-C-N	-5.20	116.48	121.83
1	A	267	HIS	N-CA-CB	5.18	117.52	110.01
1	B	87	PRO	CA-C-N	5.18	127.48	120.38
1	B	87	PRO	C-N-CA	5.18	127.48	120.38
1	B	130	GLU	CA-CB-CG	5.17	124.45	114.10
1	A	9	VAL	CB-CA-C	5.17	118.67	110.81
1	B	22	GLU	CB-CA-C	-5.16	102.08	110.85
1	A	276	ARG	CA-C-N	5.16	127.71	120.28
1	A	276	ARG	C-N-CA	5.16	127.71	120.28
1	B	179	LEU	N-CA-CB	-5.16	102.28	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LEU	N-CA-CB	-5.15	102.54	110.12
1	B	82	VAL	CA-C-N	5.14	127.13	120.44
1	B	82	VAL	C-N-CA	5.14	127.13	120.44
1	B	271	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	B	15	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	276	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	A	93	ALA	CA-C-O	5.13	125.88	119.97
1	B	233	LEU	N-CA-CB	5.12	117.83	110.20
1	A	144	ASP	CA-C-O	-5.12	113.55	119.59
1	A	283	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	109	VAL	O-C-N	-5.12	116.56	121.83
1	A	247	ILE	CB-CA-C	5.11	120.66	111.36
1	B	271	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	B	31	LEU	CA-C-N	-5.10	113.97	122.43
1	B	31	LEU	C-N-CA	-5.10	113.97	122.43
1	B	189	THR	CB-CA-C	5.08	120.75	109.94
1	B	148	TYR	N-CA-C	-5.07	106.61	112.89
1	B	234	GLU	CG-CD-OE2	-5.07	106.75	118.40
1	B	254	THR	CA-C-N	5.07	127.48	120.29
1	B	254	THR	C-N-CA	5.07	127.48	120.29
1	B	208	LYS	CB-CA-C	-5.06	103.17	110.96
1	B	313	LEU	CB-CA-C	5.05	119.44	110.85
1	A	180	PHE	CA-C-O	5.05	125.90	120.70
1	A	109	VAL	CA-C-N	5.04	127.35	120.54
1	A	109	VAL	C-N-CA	5.04	127.35	120.54
1	B	132	GLU	CB-CA-C	-5.04	101.47	110.70
1	B	251	LEU	CB-CA-C	5.04	119.15	110.79
1	A	118	THR	CA-CB-OG1	-5.03	102.06	109.60
1	B	239	ALA	O-C-N	5.03	127.32	122.09
1	B	78	GLU	CB-CG-CD	5.03	121.14	112.60
1	B	181	GLN	N-CA-C	-5.01	105.70	111.07
1	B	280	ASP	OD1-CG-OD2	-5.01	110.86	122.90
1	B	95	GLU	CA-C-N	5.00	127.25	120.44
1	B	95	GLU	C-N-CA	5.00	127.25	120.44
1	A	265	ASP	CA-C-O	-5.00	116.62	122.37

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Mainchain
1	A	201	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	227	ARG	Mainchain
1	A	230	SER	Mainchain
1	A	319	ASP	Mainchain
1	A	50	ARG	Sidechain
1	B	34	ASP	Mainchain
1	B	4	VAL	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	2518	0	2517	110	0
1	B	2518	0	2519	100	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	135	0	0	3	0
3	B	130	0	0	11	0
All	All	5305	0	5036	208	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 (208) 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:89:ARG:HD3	3:B:986:HOH:O	1.27	1.30
1:A:101:LYS:HB3	1:A:101:LYS:NZ	1.54	1.22
1:B:3:GLN:O	1:B:3:GLN:HG3	1.35	1.12
1:B:89:ARG:HG2	1:B:90:LEU:HD22	1.15	1.10
1:A:152:MET:HE1	1:A:237:LEU:CD1	1.92	1.00
1:B:6:ARG:H	1:B:283:ASN:HD21	1.06	0.99
1:A:260:LYS:HB2	1:A:260:LYS:HZ3	1.28	0.99
1:B:89:ARG:HG2	1:B:90:LEU:CD2	1.93	0.97
1:A:101:LYS:HB3	1:A:101:LYS:HZ2	1.12	0.94
1:B:3:GLN:O	1:B:3:GLN:CG	2.15	0.94
1:A:260:LYS:HZ2	1:A:260:LYS:HA	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HA	1:A:260:LYS:NZ	1.87	0.88
1:B:6:ARG:H	1:B:283:ASN:ND2	1.73	0.85
1:A:260:LYS:HZ3	1:A:260:LYS:CB	1.89	0.85
1:B:176:ALA:HB1	1:B:216:ILE:HD12	1.56	0.85
1:A:260:LYS:NZ	1:A:260:LYS:CB	2.40	0.85
1:B:87:PRO:HB2	1:B:90:LEU:HD23	1.59	0.84
1:B:240:VAL:O	1:B:244:ILE:HG12	1.77	0.84
1:A:101:LYS:HB3	1:A:101:LYS:HZ3	1.41	0.83
1:B:196:THR:O	1:B:200:THR:HB	1.79	0.82
1:A:101:LYS:HZ2	1:A:101:LYS:CB	1.90	0.79
1:A:220:GLN:OE1	3:A:946:HOH:O	1.99	0.79
1:B:113:ILE:O	1:B:117:ARG:HG2	1.83	0.77
1:B:4:VAL:HG23	1:B:6:ARG:NH1	1.99	0.77
1:A:39:LEU:O	1:A:43:THR:HB	1.84	0.76
1:A:161:ARG:NH2	1:A:198:PHE:O	2.20	0.75
1:A:260:LYS:HB2	1:A:260:LYS:NZ	2.03	0.74
1:B:214:MET:HG3	1:B:219:PHE:O	1.88	0.73
1:A:229:THR:O	1:A:230:SER:C	2.29	0.73
1:A:39:LEU:C	1:A:39:LEU:HD23	2.14	0.73
1:A:152:MET:CE	1:A:237:LEU:CD1	2.67	0.72
1:B:213:TYR:OH	1:B:224:THR:HG21	1.89	0.72
1:A:46:SER:OG	1:A:49:GLN:HG3	1.89	0.72
1:A:100:LEU:HD13	1:A:140:ASP:HB3	1.72	0.72
1:A:260:LYS:NZ	1:A:260:LYS:CA	2.53	0.71
1:B:89:ARG:CG	1:B:90:LEU:HD22	2.08	0.71
1:A:260:LYS:HZ2	1:A:260:LYS:CA	2.03	0.70
1:A:216:ILE:O	1:A:216:ILE:HG13	1.91	0.69
1:B:176:ALA:CB	1:B:216:ILE:HD12	2.23	0.69
1:B:152:MET:HG2	1:B:236:LEU:HD21	1.73	0.69
1:B:250:TYR:O	1:B:254:THR:HG23	1.92	0.69
1:B:152:MET:HG2	1:B:236:LEU:CD2	2.22	0.69
1:A:58:LYS:HD2	1:A:63:ARG:O	1.93	0.68
1:B:135:SER:HB3	3:B:753:HOH:O	1.94	0.68
1:A:317:GLY:O	1:A:318:GLU:HB2	1.92	0.68
1:A:96:LEU:HD13	1:A:113:ILE:HD12	1.76	0.67
1:B:229:THR:O	1:B:230:SER:O	2.14	0.66
1:B:135:SER:CB	3:B:753:HOH:O	2.44	0.66
1:B:170:ALA:O	1:B:173:GLU:HB3	1.95	0.66
1:A:118:THR:OG1	1:A:121:GLU:HG3	1.95	0.66
1:A:231:GLY:O	1:A:235:GLN:HG2	1.94	0.66
1:A:109:VAL:HG22	1:A:271:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:N	1:B:283:ASN:HD21	1.87	0.66
1:B:107:GLU:OE1	1:B:232:ASN:ND2	2.29	0.66
1:B:227:ARG:HB2	1:B:238:LEU:CD1	2.26	0.65
1:A:175:ASP:OD2	1:A:201:ARG:HD2	1.95	0.65
1:B:214:MET:HG3	1:B:219:PHE:C	2.21	0.65
1:A:225:ILE:HG23	1:A:234:GLU:HB3	1.78	0.65
1:B:102:GLY:HA2	1:B:144:ASP:OD1	1.97	0.64
1:A:152:MET:HG2	1:A:236:LEU:CD2	2.27	0.64
1:B:58:LYS:HG3	1:B:63:ARG:O	1.98	0.64
1:A:230:SER:HB2	1:A:234:GLU:HB2	1.81	0.63
1:A:152:MET:HG2	1:A:236:LEU:HD21	1.81	0.63
1:B:188:GLY:C	1:B:189:THR:HG22	2.24	0.62
1:A:152:MET:CE	1:A:237:LEU:HD13	2.30	0.61
1:B:25:ARG:O	1:B:25:ARG:HG3	2.00	0.61
1:A:203:VAL:O	1:A:207:ARG:HG3	2.01	0.60
1:A:55:ALA:O	1:A:59:THR:HG23	2.01	0.60
1:B:35:GLU:O	1:B:39:LEU:HB3	2.01	0.60
1:A:39:LEU:C	1:A:39:LEU:CD2	2.75	0.59
1:A:6:ARG:HG2	1:B:282:PHE:CZ	2.37	0.59
1:A:152:MET:HE1	1:A:237:LEU:HD11	1.85	0.58
1:A:181:GLN:O	1:A:184:GLU:HB2	2.04	0.58
1:A:175:ASP:CG	1:A:201:ARG:HH11	2.12	0.57
1:A:211:ASP:O	1:A:215:THR:HG23	2.05	0.57
1:A:152:MET:HE1	1:A:237:LEU:HD12	1.80	0.56
1:B:226:ASP:O	1:B:227:ARG:HB3	2.06	0.56
1:A:212:LYS:O	1:A:216:ILE:HG23	2.05	0.56
1:A:175:ASP:OD1	1:A:201:ARG:NH1	2.39	0.55
1:B:69:LEU:O	1:B:73:LEU:HB2	2.07	0.55
1:A:75:GLY:O	1:A:79:LYS:HG2	2.07	0.55
1:B:90:LEU:HD22	1:B:90:LEU:N	2.22	0.55
1:B:266:ASP:O	1:B:270:ILE:HD12	2.06	0.55
1:A:101:LYS:HG3	1:A:104:GLY:C	2.33	0.54
1:A:101:LYS:HG3	1:A:101:LYS:O	2.07	0.54
1:A:213:TYR:O	1:A:217:SER:HB3	2.07	0.54
1:B:90:LEU:HD13	1:B:128:VAL:HG11	1.90	0.54
1:A:109:VAL:HG22	1:A:271:ARG:CZ	2.38	0.54
1:A:112:GLU:OE2	1:A:271:ARG:HD2	2.08	0.54
1:A:213:TYR:OH	1:A:224:THR:HG21	2.08	0.53
1:A:11:ASP:OD1	1:B:2:ALA:HA	2.09	0.53
1:A:162:ASP:HB3	1:A:163:PRO:HD2	1.90	0.53
1:B:120:GLU:H	1:B:120:GLU:CD	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:SER:HB2	1:B:234:GLU:HB2	1.90	0.52
1:B:201:ARG:HB2	1:B:206:LEU:HG	1.91	0.52
1:B:90:LEU:HD13	1:B:128:VAL:CG1	2.39	0.52
1:A:201:ARG:HD3	1:A:205:HIS:CD2	2.45	0.52
1:B:90:LEU:HD21	3:B:986:HOH:O	2.10	0.51
1:A:292:PHE:O	1:A:293:ALA:HB3	2.09	0.51
1:A:84:LEU:HD13	1:A:274:VAL:HG22	1.91	0.51
1:A:170:ALA:HB3	3:A:958:HOH:O	2.10	0.51
1:A:192:GLU:CD	1:A:192:GLU:H	2.18	0.51
1:A:229:THR:O	1:A:230:SER:O	2.28	0.51
1:B:70:LYS:HE3	3:B:872:HOH:O	2.10	0.51
1:B:214:MET:HE2	1:B:218:GLY:O	2.10	0.51
1:A:145:THR:OG1	1:A:150:GLN:HB2	2.10	0.51
1:B:39:LEU:C	1:B:39:LEU:HD23	2.35	0.51
1:B:54:SER:O	1:B:58:LYS:HD3	2.11	0.51
1:B:76:LYS:HE2	1:B:266:ASP:OD2	2.10	0.50
1:A:256:TYR:CE2	1:A:260:LYS:HD2	2.46	0.50
1:A:173:GLU:O	1:A:177:GLN:HG2	2.13	0.49
1:A:28:MET:SD	1:A:72:GLU:HG3	2.52	0.49
1:A:47:ASN:O	1:A:51:GLN:HG2	2.12	0.49
1:B:90:LEU:HB3	3:B:885:HOH:O	2.12	0.49
1:B:89:ARG:HB3	3:B:877:HOH:O	2.13	0.49
1:A:99:ALA:O	1:A:105:THR:HA	2.13	0.48
1:A:225:ILE:O	1:A:226:ASP:HB3	2.12	0.48
1:A:69:LEU:O	1:A:73:LEU:HB2	2.13	0.48
1:A:164:ASP:OD2	1:A:204:SER:OG	2.27	0.48
1:B:286:LYS:HD2	1:B:286:LYS:N	2.26	0.48
1:A:39:LEU:CD2	1:A:40:THR:N	2.77	0.48
1:B:58:LYS:HD3	1:B:58:LYS:N	2.29	0.47
1:B:185:LEU:HB3	1:B:189:THR:HG23	1.96	0.47
1:B:147:GLY:O	1:B:151:ARG:HG3	2.14	0.47
1:A:43:THR:HG21	1:A:314:LEU:HD12	1.95	0.47
1:A:173:GLU:HG3	1:A:174:GLN:N	2.28	0.47
1:A:165:ALA:O	1:A:166:GLY:C	2.57	0.47
1:B:135:SER:HB2	3:B:753:HOH:O	2.12	0.47
1:B:188:GLY:C	1:B:189:THR:CG2	2.88	0.47
1:B:41:LEU:C	1:B:41:LEU:HD23	2.40	0.47
1:A:39:LEU:HD11	1:A:310:LYS:HG2	1.97	0.46
1:A:50:ARG:HG3	1:A:50:ARG:NH1	2.29	0.46
1:B:124:ALA:O	1:B:128:VAL:HG23	2.16	0.46
1:B:205:HIS:CD2	1:B:205:HIS:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLN:O	1:B:184:GLU:HB2	2.15	0.46
1:B:110:LEU:O	1:B:114:ILE:HG13	2.15	0.46
1:A:101:LYS:HZ3	1:A:101:LYS:CB	2.11	0.46
1:A:39:LEU:HD12	1:A:307:ASP:HB3	1.96	0.46
1:A:174:GLN:O	1:A:177:GLN:HB2	2.15	0.46
1:A:276:ARG:HD3	1:A:280:ASP:OD1	2.15	0.46
1:A:86:LYS:HG2	1:A:91:TYR:HD1	1.81	0.46
1:A:152:MET:HG2	1:A:236:LEU:HD23	1.98	0.45
1:B:205:HIS:CD2	1:B:209:VAL:HG23	2.50	0.45
1:B:295:SER:OG	1:B:319:ASP:OD1	2.28	0.45
1:B:222:GLU:OE2	1:B:245:ARG:NH1	2.49	0.45
1:A:152:MET:O	1:A:152:MET:HG3	2.16	0.45
1:A:228:GLU:OE1	1:A:228:GLU:HA	2.17	0.45
1:A:130:GLU:O	1:A:134:GLY:HA2	2.16	0.45
1:B:58:LYS:HD3	1:B:58:LYS:H	1.82	0.45
1:B:110:LEU:O	1:B:114:ILE:CG1	2.64	0.45
1:B:230:SER:HB2	1:B:234:GLU:CB	2.47	0.45
1:B:283:ASN:ND2	1:B:283:ASN:H	2.14	0.45
1:A:175:ASP:OD2	1:A:205:HIS:NE2	2.47	0.45
1:A:289:ARG:O	1:A:289:ARG:HD3	2.17	0.44
1:B:102:GLY:CA	1:B:144:ASP:OD1	2.64	0.44
1:A:208:LYS:HA	1:A:208:LYS:HE2	1.99	0.44
1:B:2:ALA:N	3:B:787:HOH:O	2.50	0.44
1:A:42:LEU:O	1:A:50:ARG:NH2	2.51	0.44
1:A:65:LEU:O	1:A:65:LEU:HD12	2.17	0.43
1:A:227:ARG:HB3	1:A:238:LEU:CD2	2.48	0.43
1:B:66:LEU:O	1:B:70:LYS:HG3	2.18	0.43
1:B:152:MET:HG2	1:B:236:LEU:HD23	1.98	0.43
1:B:227:ARG:O	1:B:228:GLU:CB	2.66	0.43
1:A:41:LEU:C	1:A:41:LEU:HD23	2.43	0.43
1:B:205:HIS:O	1:B:208:LYS:HB2	2.18	0.43
1:A:101:LYS:CG	1:A:104:GLY:C	2.92	0.43
1:B:153:LEU:O	1:B:157:LEU:HB2	2.18	0.43
1:A:245:ARG:O	1:A:246:SER:HB2	2.19	0.43
1:B:208:LYS:HD2	1:B:208:LYS:HA	1.48	0.43
1:B:247:ILE:HB	1:B:248:PRO:HD3	1.99	0.43
1:A:181:GLN:HB2	3:A:843:HOH:O	2.18	0.43
1:B:66:LEU:HG	1:B:70:LYS:HE2	2.00	0.43
1:A:109:VAL:CG2	1:A:271:ARG:NH2	2.80	0.42
1:A:219:PHE:CE1	1:A:224:THR:HG22	2.54	0.42
1:A:273:MET:HE3	1:A:273:MET:HB3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLU:H	1:A:17:GLU:CD	2.27	0.42
1:A:43:THR:HG21	1:A:314:LEU:CD1	2.50	0.42
1:A:177:GLN:NE2	1:A:216:ILE:HD12	2.35	0.42
1:A:214:MET:HE3	1:A:214:MET:HB2	1.62	0.42
1:B:130:GLU:O	1:B:134:GLY:N	2.46	0.42
1:B:255:LEU:HD13	1:B:272:VAL:HB	2.00	0.42
1:A:86:LYS:HA	1:A:87:PRO:HD3	1.94	0.42
1:A:289:ARG:HD3	1:A:289:ARG:C	2.43	0.42
1:B:53:ILE:O	1:B:54:SER:C	2.62	0.42
1:B:130:GLU:HA	1:B:135:SER:O	2.20	0.42
1:B:2:ALA:N	3:B:791:HOH:O	2.52	0.42
1:A:256:TYR:O	1:A:260:LYS:HB3	2.20	0.42
1:B:283:ASN:H	1:B:283:ASN:HD22	1.68	0.42
1:B:120:GLU:HB3	3:B:779:HOH:O	2.20	0.41
1:A:123:ARG:HH11	1:A:123:ARG:HD2	1.57	0.41
1:B:168:ASP:O	1:B:171:GLN:HB3	2.20	0.41
1:B:206:LEU:HD23	1:B:206:LEU:HA	1.94	0.41
1:B:26:LYS:HB3	1:B:26:LYS:HE3	1.84	0.41
1:B:141:VAL:O	1:B:142:VAL:C	2.63	0.41
1:B:161:ARG:CG	1:B:201:ARG:O	2.68	0.41
1:A:39:LEU:HD23	1:A:40:THR:N	2.34	0.41
1:A:8:THR:N	1:A:277:SER:O	2.52	0.41
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.72	0.41
1:B:8:THR:HG23	1:B:281:LEU:HB3	2.01	0.41
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.84	0.41
1:A:120:GLU:H	1:A:120:GLU:CD	2.28	0.41
1:B:24:LEU:HD13	1:B:41:LEU:HD13	2.02	0.41
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.77	0.40
1:B:176:ALA:HB2	1:B:212:LYS:HB3	2.03	0.40
1:B:120:GLU:N	1:B:120:GLU:OE1	2.54	0.40
1:B:256:TYR:CE2	1:B:260:LYS:HD2	2.56	0.40
1:B:39:LEU:HD23	1:B:40:THR:N	2.36	0.40
1:B:56:ALA:O	1:B:60:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/319 (99%)	301 (95%)	14 (4%)	2 (1%)	21	32
1	B	317/319 (99%)	298 (94%)	15 (5%)	4 (1%)	9	14
All	All	634/638 (99%)	599 (94%)	29 (5%)	6 (1%)	14	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	B	230	SER
1	B	228	GLU
1	B	226	ASP
1	B	227	ARG
1	A	246	SER

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	271/271 (100%)	215 (79%)	56 (21%)	1	1
1	B	271/271 (100%)	212 (78%)	59 (22%)	1	1
All	All	542/542 (100%)	427 (79%)	115 (21%)	1	1

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	5	LEU
1	A	6	ARG
1	A	10	THR
1	A	17	GLU
1	A	24	LEU
1	A	36	GLU
1	A	39	LEU
1	A	43	THR
1	A	45	ARG
1	A	50	ARG
1	A	59	THR
1	A	60	LEU
1	A	74	THR
1	A	84	LEU
1	A	86	LYS
1	A	88	SER
1	A	89	ARG
1	A	96	LEU
1	A	101	LYS
1	A	108	LYS
1	A	110	LEU
1	A	120	GLU
1	A	138	GLU
1	A	141	VAL
1	A	146	SER
1	A	151	ARG
1	A	152	MET
1	A	153	LEU
1	A	155	VAL
1	A	157	LEU
1	A	158	GLN
1	A	167	ILE
1	A	173	GLU
1	A	174	GLN
1	A	179	LEU
1	A	181	GLN
1	A	193	LYS
1	A	200	THR
1	A	201	ARG
1	A	208	LYS
1	A	214	MET
1	A	216	ILE

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Mol	Chain	Res	Type
1	A	217	SER
1	A	224	THR
1	A	228	GLU
1	A	229	THR
1	A	230	SER
1	A	237	LEU
1	A	251	LEU
1	A	255	LEU
1	A	260	LYS
1	A	281	LEU
1	A	299	MET
1	A	303	ASP
1	A	310	LYS
1	B	3	GLN
1	B	4	VAL
1	B	5	LEU
1	B	6	ARG
1	B	17	GLU
1	B	18	ARG
1	B	24	LEU
1	B	25	ARG
1	B	26	LYS
1	B	29	LYS
1	B	31	LEU
1	B	36	GLU
1	B	39	LEU
1	B	45	ARG
1	B	58	LYS
1	B	60	LEU
1	B	71	SER
1	B	73	LEU
1	B	74	THR
1	B	84	LEU
1	B	86	LYS
1	B	88	SER
1	B	89	ARG
1	B	96	LEU
1	B	107	GLU
1	B	108	LYS
1	B	110	LEU
1	B	114	ILE
1	B	120	GLU

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Mol	Chain	Res	Type
1	B	130	GLU
1	B	138	GLU
1	B	141	VAL
1	B	152	MET
1	B	167	ILE
1	B	169	GLU
1	B	185	LEU
1	B	186	LYS
1	B	189	THR
1	B	192	GLU
1	B	193	LYS
1	B	208	LYS
1	B	212	LYS
1	B	215	THR
1	B	225	ILE
1	B	229	THR
1	B	230	SER
1	B	234	GLU
1	B	237	LEU
1	B	251	LEU
1	B	254	THR
1	B	255	LEU
1	B	260	LYS
1	B	281	LEU
1	B	286	LYS
1	B	294	THR
1	B	298	SER
1	B	299	MET
1	B	303	ASP
1	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	174	GLN
1	B	232	ASN
1	B	235	GLN
1	B	283	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4:VAL	C	5:LEU	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.