



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:21 AM BST

PDB ID : 1ALA  
Title : STRUCTURE OF CHICKEN ANNEXIN V AT 2.25-ANGSTROMS RESOLUTION  
Authors : Waller, D.A.; Bewley, M.C.; Huber, R.  
Deposited on : 1993-01-14  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

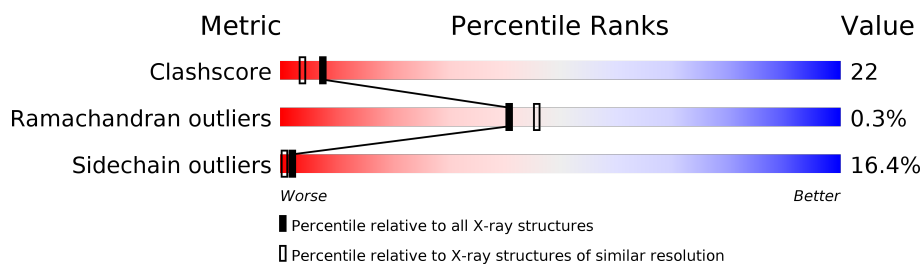
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	321	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2587 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	316	Total	C	N	O	S	0	0	0
			2503	1575	436	481	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLU	ASP	CONFLICT	UNP P17153

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

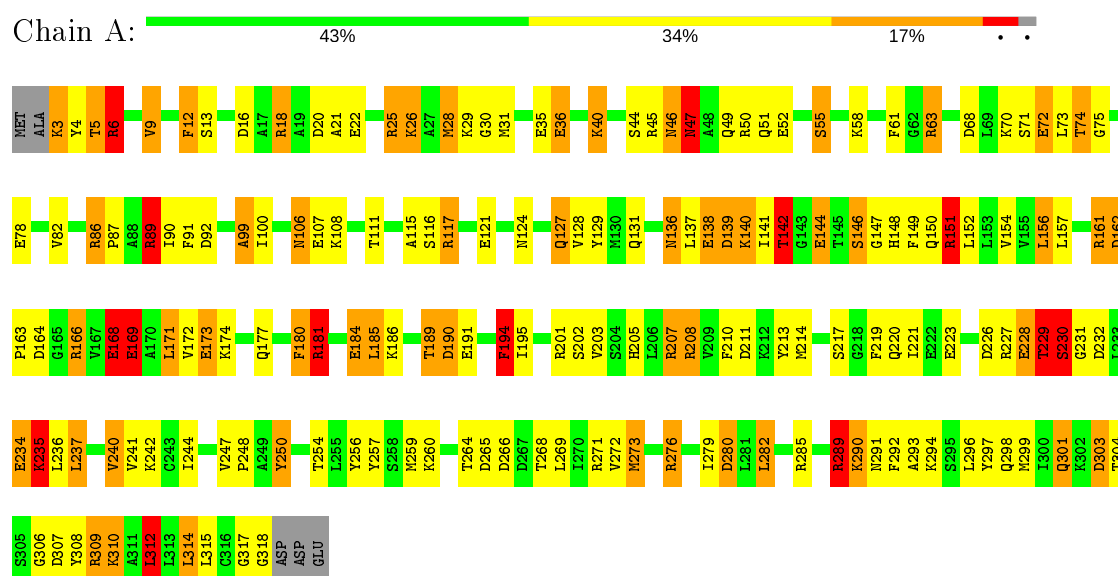
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		

### 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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.40 Å 99.40 Å 96.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.25)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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	0.98	1/2537 (0.0%)	2.66	171/3412 (5.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLU	CG-CD	-5.13	1.44	1.51

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	NE-CZ-NH1	28.24	134.42	120.30
1	A	285	ARG	NE-CZ-NH1	27.92	134.26	120.30
1	A	285	ARG	NE-CZ-NH2	-22.72	108.94	120.30
1	A	25	ARG	NE-CZ-NH1	21.07	130.83	120.30
1	A	6	ARG	CD-NE-CZ	19.39	150.75	123.60
1	A	207	ARG	NE-CZ-NH2	17.37	128.99	120.30
1	A	50	ARG	NE-CZ-NH2	16.83	128.72	120.30
1	A	6	ARG	NH1-CZ-NH2	-15.41	102.44	119.40
1	A	271	ARG	NE-CZ-NH2	-14.67	112.96	120.30
1	A	86	ARG	NE-CZ-NH1	13.95	127.27	120.30
1	A	18	ARG	NE-CZ-NH1	13.80	127.20	120.30
1	A	86	ARG	CD-NE-CZ	13.07	141.89	123.60
1	A	181	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	A	276	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	A	50	ARG	NE-CZ-NH1	-12.75	113.93	120.30
1	A	181	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	A	117	ARG	NE-CZ-NH2	-12.53	114.04	120.30
1	A	309	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	A	161	ARG	NE-CZ-NH1	-12.27	114.16	120.30
1	A	166	ARG	NE-CZ-NH1	11.29	125.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	PHE	CB-CG-CD1	11.16	128.62	120.80
1	A	144	GLU	OE1-CD-OE2	11.02	136.52	123.30
1	A	265	ASP	CB-CG-OD2	-10.95	108.45	118.30
1	A	207	ARG	NE-CZ-NH1	-10.68	114.96	120.30
1	A	166	ARG	CD-NE-CZ	10.30	138.02	123.60
1	A	161	ARG	CD-NE-CZ	10.17	137.84	123.60
1	A	6	ARG	CG-CD-NE	9.74	132.25	111.80
1	A	16	ASP	CB-CG-OD1	9.71	127.04	118.30
1	A	25	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	201	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	A	78	GLU	CB-CG-CD	9.39	139.54	114.20
1	A	297	TYR	CB-CG-CD1	9.39	126.63	121.00
1	A	3	LYS	CA-CB-CG	9.32	133.92	113.40
1	A	139	ASP	CB-CG-OD2	9.17	126.55	118.30
1	A	201	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	A	91	PHE	CB-CG-CD2	8.93	127.05	120.80
1	A	18	ARG	CD-NE-CZ	8.75	135.85	123.60
1	A	297	TYR	CB-CG-CD2	-8.53	115.89	121.00
1	A	289	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	A	18	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	144	GLU	CB-CA-C	-8.26	93.89	110.40
1	A	210	PHE	CB-CG-CD2	-8.22	115.05	120.80
1	A	213	TYR	CB-CG-CD1	8.10	125.86	121.00
1	A	166	ARG	CA-CB-CG	8.02	131.05	113.40
1	A	16	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	121	GLU	OE1-CD-OE2	-7.74	114.02	123.30
1	A	70	LYS	CA-CB-CG	-7.72	96.42	113.40
1	A	92	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	63	ARG	CD-NE-CZ	7.67	134.34	123.60
1	A	312	LEU	CB-CG-CD2	-7.67	97.96	111.00
1	A	208	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	A	271	ARG	NH1-CZ-NH2	7.61	127.77	119.40
1	A	211	ASP	CB-CG-OD2	7.53	125.08	118.30
1	A	213	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	A	28	MET	N-CA-CB	-7.40	97.28	110.60
1	A	190	ASP	CB-CG-OD1	-7.33	111.71	118.30
1	A	266	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	9	VAL	CA-CB-CG1	7.28	121.81	110.90
1	A	189	THR	O-C-N	7.23	134.26	122.70
1	A	230	SER	C-N-CA	7.20	137.43	122.30
1	A	208	ARG	C-N-CA	7.12	139.51	121.70
1	A	229	THR	CA-CB-CG2	7.10	122.33	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ARG	CD-NE-CZ	7.02	133.43	123.60
1	A	201	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	250	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	A	28	MET	CA-CB-CG	6.88	125.00	113.30
1	A	107	GLU	CG-CD-OE1	6.86	132.03	118.30
1	A	89	ARG	C-N-CA	6.85	138.82	121.70
1	A	234	GLU	OE1-CD-OE2	-6.83	115.11	123.30
1	A	194	PHE	CB-CA-C	6.73	123.86	110.40
1	A	161	ARG	CG-CD-NE	6.70	125.87	111.80
1	A	68	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	73	LEU	CA-C-O	6.49	133.74	120.10
1	A	290	LYS	CA-CB-CG	6.49	127.67	113.40
1	A	91	PHE	CB-CG-CD1	-6.47	116.27	120.80
1	A	40	LYS	N-CA-CB	6.44	122.19	110.60
1	A	151	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	303	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	280	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	280	ASP	O-C-N	6.36	132.88	122.70
1	A	307	ASP	O-C-N	6.36	132.88	122.70
1	A	129	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	257	TYR	CB-CG-CD1	6.32	124.79	121.00
1	A	184	GLU	OE1-CD-OE2	6.30	130.87	123.30
1	A	289	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	A	237	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	240	VAL	CG1-CB-CG2	-6.21	100.96	110.90
1	A	318	GLY	CA-C-O	-6.21	109.42	120.60
1	A	273	MET	CA-CB-CG	6.21	123.85	113.30
1	A	55	SER	O-C-N	6.20	132.62	122.70
1	A	230	SER	N-CA-C	6.19	127.71	111.00
1	A	4	TYR	N-CA-C	-6.15	94.40	111.00
1	A	6	ARG	CA-CB-CG	6.14	126.92	113.40
1	A	236	LEU	CB-CA-C	6.14	121.87	110.20
1	A	25	ARG	CD-NE-CZ	6.12	132.17	123.60
1	A	168	GLU	OE1-CD-OE2	6.06	130.57	123.30
1	A	289	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	309	ARG	CD-NE-CZ	6.03	132.04	123.60
1	A	211	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	A	45	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	144	GLU	CG-CD-OE2	-5.98	106.35	118.30
1	A	3	LYS	N-CA-CB	5.97	121.35	110.60
1	A	219	PHE	N-CA-CB	5.96	121.34	110.60
1	A	254	THR	CA-CB-CG2	5.94	120.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LEU	CB-CA-C	5.94	121.49	110.20
1	A	162	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	314	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	A	169	GLU	OE1-CD-OE2	5.86	130.34	123.30
1	A	63	ARG	CB-CG-CD	5.85	126.82	111.60
1	A	146	SER	CB-CA-C	5.85	121.22	110.10
1	A	180	PHE	CB-CG-CD1	-5.84	116.72	120.80
1	A	172	VAL	CA-C-O	5.83	132.35	120.10
1	A	4	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	308	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	82	VAL	CB-CA-C	5.81	122.43	111.40
1	A	140	LYS	CB-CA-C	-5.79	98.82	110.40
1	A	99	ALA	CA-C-O	5.75	132.17	120.10
1	A	149	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	A	229	THR	N-CA-CB	5.72	121.17	110.30
1	A	166	ARG	CG-CD-NE	5.63	123.63	111.80
1	A	230	SER	N-CA-CB	-5.60	102.10	110.50
1	A	36	GLU	CA-C-N	5.59	129.50	117.20
1	A	6	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	121	GLU	CG-CD-OE2	5.58	129.45	118.30
1	A	61	PHE	CG-CD1-CE1	5.56	126.91	120.80
1	A	310	LYS	CB-CA-C	-5.55	99.29	110.40
1	A	47	ASN	CB-CA-C	5.54	121.49	110.40
1	A	20	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	296	LEU	CB-CA-C	5.50	120.65	110.20
1	A	232	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	75	GLY	O-C-N	5.48	131.47	122.70
1	A	72	GLU	CB-CA-C	-5.48	99.44	110.40
1	A	161	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	A	74	THR	N-CA-CB	-5.46	99.93	110.30
1	A	309	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
1	A	265	ASP	N-CA-C	-5.46	96.27	111.00
1	A	276	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	A	195	ILE	C-N-CA	5.34	135.06	121.70
1	A	30	GLY	C-N-CA	5.33	135.03	121.70
1	A	242	LYS	O-C-N	5.32	131.22	122.70
1	A	171	LEU	O-C-N	5.31	131.20	122.70
1	A	61	PHE	CD1-CE1-CZ	-5.29	113.75	120.10
1	A	36	GLU	O-C-N	-5.28	114.25	122.70
1	A	211	ASP	CA-CB-CG	5.28	125.02	113.40
1	A	21	ALA	O-C-N	-5.28	114.26	122.70
1	A	35	GLU	N-CA-CB	5.28	120.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLU	CA-CB-CG	-5.27	101.81	113.40
1	A	26	LYS	CB-CA-C	-5.26	99.87	110.40
1	A	86	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	90	ILE	N-CA-CB	-5.26	98.71	110.80
1	A	172	VAL	CA-C-N	-5.25	105.66	117.20
1	A	25	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
1	A	303	ASP	CB-CG-OD1	-5.22	113.61	118.30
1	A	151	ARG	CD-NE-CZ	-5.21	116.30	123.60
1	A	12	PHE	CA-C-O	5.21	131.03	120.10
1	A	219	PHE	CA-C-N	-5.20	105.76	117.20
1	A	205	HIS	O-C-N	-5.18	114.40	122.70
1	A	303	ASP	CA-CB-CG	-5.18	101.99	113.40
1	A	301	GLN	OE1-CD-NE2	5.17	133.79	121.90
1	A	282	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	235	LYS	CB-CA-C	-5.16	100.08	110.40
1	A	256	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	185	LEU	CB-CA-C	5.12	119.92	110.20
1	A	52	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	A	142	THR	O-C-N	-5.07	114.58	123.20
1	A	21	ALA	CA-C-O	5.05	130.71	120.10
1	A	151	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	317	GLY	CA-C-N	5.04	126.28	116.20
1	A	161	ARG	N-CA-CB	-5.03	101.55	110.60
1	A	138	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	A	156	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2503	0	2535	111	0
2	A	3	0	0	0	0
3	A	81	0	0	5	3
All	All	2587	0	2535	111	3

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 22.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:HD21	1:A:108:LYS:HB3	1.08	1.17
1:A:5:THR:HG23	1:A:279:ILE:O	1.45	1.16
1:A:28:MET:HG3	1:A:72:GLU:HG3	1.28	1.10
1:A:106:ASN:ND2	1:A:108:LYS:HB3	1.65	1.10
1:A:226:ASP:OD2	1:A:229:THR:CG2	2.05	1.05
1:A:89:ARG:NH1	3:A:448:HOH:O	1.89	1.03
1:A:136:ASN:HD21	1:A:138:GLU:HB3	1.28	0.97
1:A:226:ASP:OD2	1:A:229:THR:HG22	1.64	0.96
1:A:36:GLU:HG2	1:A:40:LYS:HE2	1.49	0.95
1:A:227:ARG:HG3	1:A:228:GLU:H	1.35	0.91
1:A:139:ASP:O	1:A:142:THR:HG22	1.70	0.90
1:A:5:THR:CG2	1:A:279:ILE:O	2.21	0.89
1:A:28:MET:CG	1:A:72:GLU:HG3	2.03	0.88
1:A:226:ASP:OD2	1:A:229:THR:HG23	1.73	0.86
1:A:25:ARG:O	1:A:29:LYS:HB2	1.76	0.84
1:A:36:GLU:CG	1:A:40:LYS:HE2	2.07	0.84
1:A:139:ASP:C	1:A:142:THR:HG22	2.01	0.81
1:A:28:MET:HG3	1:A:72:GLU:CG	2.08	0.81
1:A:18:ARG:O	1:A:22:GLU:HG3	1.79	0.81
1:A:127:GLN:O	1:A:131:GLN:HG3	1.81	0.81
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.49	0.78
1:A:89:ARG:NH2	1:A:128:VAL:HG22	1.99	0.78
1:A:229:THR:OG1	1:A:230:SER:N	2.16	0.78
1:A:100:ILE:HG12	1:A:144:GLU:HG3	1.66	0.77
1:A:148:HIS:CD2	3:A:482:HOH:O	2.38	0.77
1:A:148:HIS:HD2	3:A:482:HOH:O	1.69	0.75
1:A:177:GLN:OE1	1:A:181:ARG:NE	2.21	0.73
1:A:268:THR:O	1:A:272:VAL:HG23	1.90	0.72
1:A:180:PHE:CD2	1:A:181:ARG:HD2	2.27	0.70
1:A:164:ASP:OD1	1:A:202:SER:HB2	1.90	0.70
1:A:191:GLU:HA	1:A:194:PHE:CE2	2.26	0.70
1:A:162:ASP:HB3	1:A:163:PRO:HD2	1.73	0.69
1:A:240:VAL:O	1:A:244:ILE:HD12	1.93	0.69
1:A:136:ASN:ND2	1:A:138:GLU:HB3	2.05	0.69
1:A:177:GLN:O	1:A:181:ARG:HD3	1.94	0.68
1:A:181:ARG:HG2	1:A:181:ARG:NH1	2.07	0.68
1:A:47:ASN:O	1:A:51:GLN:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:O	1:A:140:LYS:HB2	1.95	0.67
1:A:147:GLY:O	1:A:151:ARG:HD2	1.97	0.64
1:A:231:GLY:HA3	1:A:234:GLU:OE1	1.99	0.63
1:A:276:ARG:HB3	1:A:280:ASP:OD1	1.99	0.62
1:A:150:GLN:O	1:A:154:VAL:HG23	2.00	0.62
1:A:151:ARG:HD3	3:A:482:HOH:O	2.02	0.60
1:A:180:PHE:HD2	1:A:181:ARG:HD2	1.67	0.59
1:A:6:ARG:HD3	1:A:282:LEU:HD23	1.85	0.58
1:A:227:ARG:HG3	1:A:228:GLU:N	2.15	0.56
1:A:228:GLU:HG3	1:A:229:THR:N	2.21	0.56
1:A:220:GLN:HB2	1:A:223:GLU:HG3	1.88	0.55
1:A:304:THR:O	1:A:309:ARG:HD3	2.07	0.55
1:A:247:VAL:O	1:A:250:TYR:HB3	2.07	0.54
1:A:292:PHE:O	1:A:293:ALA:HB3	2.06	0.54
1:A:229:THR:HG1	1:A:230:SER:H	1.47	0.54
1:A:46:ASN:HD21	1:A:49:GLN:HG3	1.73	0.54
1:A:89:ARG:NH2	1:A:128:VAL:CG2	2.70	0.53
1:A:138:GLU:O	1:A:142:THR:HB	2.08	0.53
1:A:148:HIS:HA	1:A:151:ARG:HD2	1.91	0.53
1:A:221:ILE:HG23	1:A:241:VAL:HG11	1.91	0.52
1:A:106:ASN:HD21	1:A:108:LYS:CB	2.00	0.52
1:A:106:ASN:C	1:A:106:ASN:HD22	2.12	0.52
1:A:259:MET:HG2	1:A:264:THR:HG23	1.91	0.52
1:A:180:PHE:O	1:A:184:GLU:HG2	2.10	0.52
1:A:136:ASN:HD22	1:A:139:ASP:H	1.58	0.51
1:A:89:ARG:CZ	1:A:128:VAL:HG22	2.40	0.51
1:A:231:GLY:O	1:A:235:LYS:HD3	2.11	0.51
1:A:310:LYS:O	1:A:314:LEU:HG	2.10	0.51
1:A:108:LYS:NZ	3:A:439:HOH:O	2.34	0.50
1:A:99:ALA:O	1:A:106:ASN:N	2.30	0.50
1:A:168:GLU:HG2	1:A:171:LEU:H	1.76	0.50
1:A:185:LEU:O	1:A:186:LYS:HB2	2.11	0.49
1:A:36:GLU:OE2	1:A:40:LYS:CE	2.61	0.49
1:A:169:GLU:O	1:A:173:GLU:HB2	2.13	0.49
1:A:58:LYS:HB2	1:A:58:LYS:HE3	1.64	0.49
1:A:240:VAL:HG13	1:A:244:ILE:CD1	2.43	0.48
1:A:152:LEU:O	1:A:156:LEU:HG	2.13	0.48
1:A:247:VAL:N	1:A:248:PRO:CD	2.75	0.48
1:A:191:GLU:HA	1:A:194:PHE:CZ	2.48	0.47
1:A:139:ASP:CA	1:A:142:THR:HG22	2.44	0.47
1:A:306:GLY:O	1:A:309:ARG:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:HA	1:A:142:THR:CG2	2.45	0.47
1:A:273:MET:HG3	1:A:312:LEU:HD12	1.97	0.47
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.96	0.47
1:A:227:ARG:NH1	1:A:228:GLU:HB3	2.30	0.46
1:A:124:ASN:ND2	1:A:128:VAL:HG23	2.29	0.46
1:A:124:ASN:HD21	1:A:128:VAL:HG23	1.81	0.46
1:A:203:VAL:O	1:A:207:ARG:HG3	2.16	0.46
1:A:294:LYS:HE2	1:A:294:LYS:HB3	1.79	0.46
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.46
1:A:289:ARG:HA	1:A:294:LYS:O	2.15	0.46
1:A:6:ARG:O	1:A:280:ASP:HA	2.18	0.44
1:A:290:LYS:HG3	1:A:291:ASN:ND2	2.33	0.44
1:A:46:ASN:ND2	1:A:49:GLN:HG3	2.32	0.44
1:A:6:ARG:HH11	1:A:282:LEU:HD21	1.84	0.43
1:A:86:ARG:HA	1:A:87:PRO:HD3	1.88	0.43
1:A:106:ASN:ND2	1:A:108:LYS:CB	2.58	0.43
1:A:5:THR:HG23	1:A:279:ILE:C	2.32	0.43
1:A:189:THR:HA	1:A:191:GLU:OE1	2.17	0.43
1:A:124:ASN:HD21	1:A:128:VAL:CG2	2.32	0.43
1:A:298:GLN:HE21	1:A:298:GLN:HB3	1.49	0.42
1:A:139:ASP:O	1:A:142:THR:CG2	2.55	0.42
1:A:240:VAL:CG1	1:A:244:ILE:CD1	2.98	0.42
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.87	0.42
1:A:162:ASP:HB3	1:A:163:PRO:CD	2.46	0.42
1:A:89:ARG:HB2	1:A:89:ARG:HE	1.49	0.42
1:A:289:ARG:HA	1:A:289:ARG:HD2	1.78	0.42
1:A:116:SER:OG	1:A:117:ARG:NH1	2.48	0.41
1:A:12:PHE:HB2	1:A:44:SER:O	2.20	0.41
1:A:139:ASP:HA	1:A:142:THR:HG21	2.03	0.41
1:A:168:GLU:OE2	1:A:171:LEU:HB2	2.21	0.41
1:A:28:MET:HG3	1:A:72:GLU:CD	2.41	0.40
1:A:111:THR:O	1:A:115:ALA:HB3	2.20	0.40
1:A:28:MET:SD	1:A:72:GLU:HG3	2.62	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:484:HOH:O	3:A:484:HOH:O[3_555]	1.96	0.24
3:A:432:HOH:O	3:A:483:HOH:O[2_555]	2.05	0.15
3:A:464:HOH:O	3:A:471:HOH:O[6_455]	2.17	0.03

## 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	314/321 (98%)	305 (97%)	8 (2%)	1 (0%)	41	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	THR

### 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	269/273 (98%)	225 (84%)	44 (16%)	2	1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	THR
1	A	6	ARG
1	A	9	VAL
1	A	13	SER
1	A	31	MET
1	A	46	ASN
1	A	47	ASN
1	A	55	SER
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	71	SER
1	A	74	THR
1	A	89	ARG
1	A	106	ASN
1	A	127	GLN
1	A	136	ASN
1	A	141	ILE
1	A	142	THR
1	A	146	SER
1	A	151	ARG
1	A	157	LEU
1	A	161	ARG
1	A	166	ARG
1	A	168	GLU
1	A	169	GLU
1	A	174	LYS
1	A	181	ARG
1	A	190	ASP
1	A	194	PHE
1	A	208	ARG
1	A	214	MET
1	A	217	SER
1	A	228	GLU
1	A	229	THR
1	A	230	SER
1	A	235	LYS
1	A	237	LEU
1	A	260	LYS
1	A	289	ARG
1	A	299	MET
1	A	301	GLN
1	A	303	ASP
1	A	312	LEU
1	A	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	ASN
1	A	106	ASN
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	148	HIS
1	A	291	ASN
1	A	298	GLN
1	A	301	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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](#)

There are no chain breaks in this entry.

## 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.