



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1ANW
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

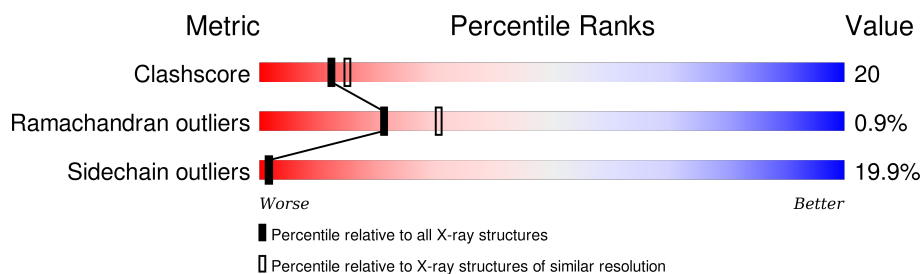
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

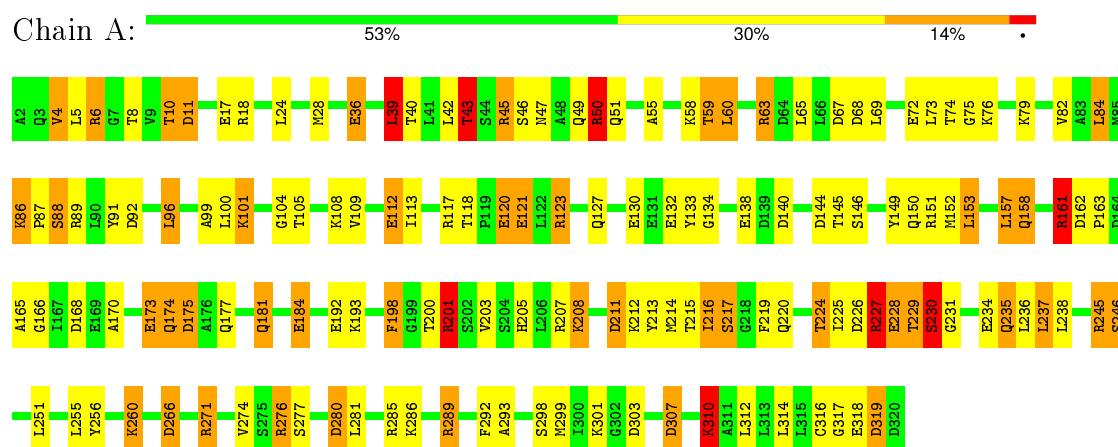
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		
3	B	130	Total	O	0	0
			130	130		

3 Residue-property plots

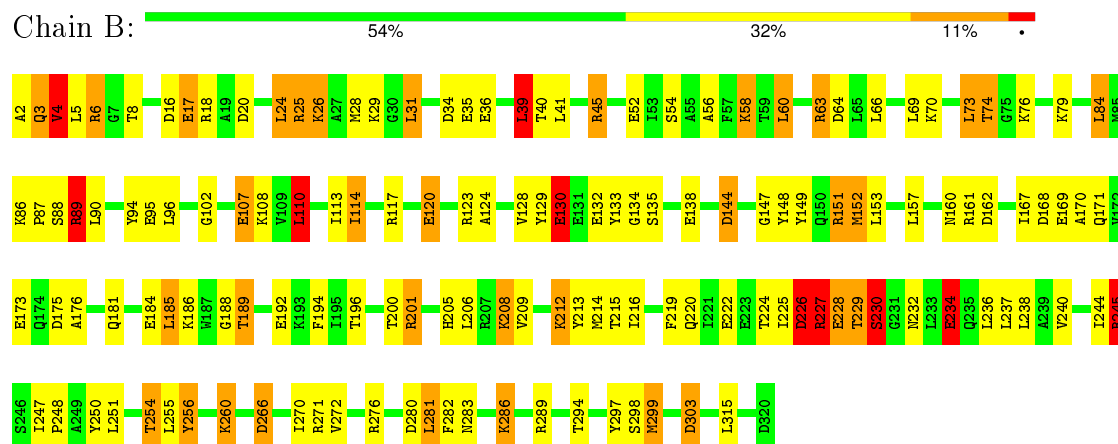
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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 will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.90 Å 80.90 Å 71.40 Å 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	1.04	5/2552 (0.2%)	1.92	66/3434 (1.9%)
1	B	0.94	0/2552	1.83	60/3434 (1.7%)
All	All	0.99	5/5104 (0.1%)	1.87	126/6868 (1.8%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	SER	C-N	9.38	1.50	1.33
1	A	158	GLN	C-N	8.30	1.53	1.34
1	A	161	ARG	C-N	6.89	1.50	1.34
1	A	4	VAL	C-N	-6.84	1.18	1.34
1	A	316	CYS	C-N	-5.29	1.23	1.33

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH1	16.59	128.59	120.30
1	A	316	CYS	C-N-CA	14.67	153.12	122.30
1	B	289	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	A	201	ARG	NE-CZ-NH1	12.96	126.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	A	245	ARG	NE-CZ-NH2	11.56	126.08	120.30
1	A	276	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	B	280	ASP	CB-CG-OD2	11.44	128.59	118.30
1	A	230	SER	O-C-N	-10.47	105.41	123.20
1	A	271	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	B	289	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	11	ASP	CB-CG-OD2	9.64	126.98	118.30
1	A	201	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	271	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	B	245	ARG	CD-NE-CZ	-9.20	110.72	123.60
1	B	226	ASP	CB-CG-OD1	9.05	126.45	118.30
1	B	123	ARG	NE-CZ-NH1	-9.05	115.78	120.30
1	B	64	ASP	CB-CG-OD1	9.02	126.42	118.30
1	B	45	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	B	227	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	245	ARG	NE-CZ-NH2	8.63	124.62	120.30
1	B	245	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	A	67	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	121	GLU	OE1-CD-OE2	-7.91	113.81	123.30
1	B	271	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	A	211	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	151	ARG	CD-NE-CZ	7.82	134.55	123.60
1	B	148	TYR	CB-CG-CD1	-7.67	116.40	121.00
1	B	175	ASP	CB-CG-OD2	7.55	125.10	118.30
1	B	256	TYR	CB-CG-CD1	-7.54	116.48	121.00
1	B	276	ARG	CD-NE-CZ	7.52	134.13	123.60
1	A	63	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	A	11	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	A	157	LEU	CA-CB-CG	7.28	132.05	115.30
1	A	4	VAL	C-N-CA	7.15	139.57	121.70
1	A	43	THR	CA-CB-CG2	7.07	122.30	112.40
1	A	307	ASP	CB-CG-OD1	-6.98	112.01	118.30
1	A	266	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	299	MET	CA-CB-CG	-6.97	101.46	113.30
1	B	227	ARG	CD-NE-CZ	6.90	133.25	123.60
1	A	117	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	151	ARG	CG-CD-NE	6.70	125.86	111.80
1	A	10	THR	CB-CA-C	-6.68	93.57	111.60
1	A	211	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	280	ASP	OD1-CG-OD2	-6.54	110.86	123.30
1	A	280	ASP	CB-CG-OD2	6.51	124.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ASN	N-CA-CB	-6.51	98.89	110.60
1	B	289	ARG	CD-NE-CZ	6.50	132.70	123.60
1	A	92	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	50	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	227	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	B	16	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	138	GLU	CG-CD-OE1	6.40	131.11	118.30
1	B	39	LEU	CB-CA-C	6.40	122.36	110.20
1	A	36	GLU	CA-CB-CG	6.36	127.38	113.40
1	A	133	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	B	63	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	45	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
1	B	123	ARG	CD-NE-CZ	-6.19	114.94	123.60
1	B	20	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	133	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	A	138	GLU	CG-CD-OE2	-6.12	106.05	118.30
1	B	20	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	B	256	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	112	GLU	CG-CD-OE1	-6.06	106.18	118.30
1	B	89	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	310	LYS	CB-CA-C	6.01	122.41	110.40
1	A	271	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	266	ASP	CB-CG-OD1	6.00	123.69	118.30
1	A	312	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	149	TYR	CB-CG-CD2	5.97	124.58	121.00
1	B	84	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	319	ASP	O-C-N	-5.94	113.19	122.70
1	A	198	PHE	CA-C-N	5.93	128.06	116.20
1	B	28	MET	CG-SD-CE	5.91	109.65	100.20
1	A	123	ARG	CD-NE-CZ	-5.90	115.33	123.60
1	A	161	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	234	GLU	CG-CD-OE2	-5.78	106.75	118.30
1	B	95	GLU	CG-CD-OE1	5.75	129.79	118.30
1	A	161	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	144	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	74	THR	C-N-CA	5.65	134.16	122.30
1	B	132	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	B	234	GLU	OE1-CD-OE2	5.62	130.05	123.30
1	B	63	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	276	ARG	N-CA-CB	-5.61	100.51	110.60
1	A	184	GLU	CG-CD-OE1	-5.61	107.09	118.30
1	A	175	ASP	CA-CB-CG	5.59	125.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	153	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	289	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	A	168	ASP	CB-CA-C	5.48	121.37	110.40
1	A	120	GLU	CG-CD-OE1	5.47	129.24	118.30
1	A	149	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	88	SER	CA-CB-OG	5.43	125.88	111.20
1	B	266	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	129	TYR	CB-CG-CD1	5.41	124.25	121.00
1	B	162	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	227	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	39	LEU	CB-CA-C	5.33	120.33	110.20
1	A	132	GLU	CB-CA-C	-5.33	99.75	110.40
1	A	50	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	184	GLU	OE1-CD-OE2	5.28	129.63	123.30
1	A	235	GLN	CA-CB-CG	5.28	125.01	113.40
1	B	201	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	298	SER	CA-CB-OG	-5.24	97.06	111.20
1	A	310	LYS	CA-CB-CG	5.24	124.92	113.40
1	A	67	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	17	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	A	82	VAL	CB-CA-C	5.17	121.22	111.40
1	B	130	GLU	CG-CD-OE2	5.17	128.63	118.30
1	B	94	TYR	CA-CB-CG	-5.14	103.63	113.40
1	B	89	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	158	GLN	CB-CG-CD	5.13	124.95	111.60
1	B	110	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	31	LEU	CB-CA-C	5.10	119.89	110.20
1	A	285	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	A	127	GLN	CA-CB-CG	5.09	124.60	113.40
1	B	194	PHE	CA-CB-CG	5.08	126.08	113.90
1	A	60	LEU	CA-C-N	5.07	128.36	117.20
1	A	43	THR	N-CA-CB	-5.06	100.69	110.30
1	B	226	ASP	N-CA-C	5.05	124.62	111.00
1	B	52	GLU	CG-CD-OE2	5.03	128.36	118.30
1	B	130	GLU	CA-CB-CG	5.02	124.45	113.40
1	B	297	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	B	303	ASP	CB-CG-OD1	5.01	122.81	118.30

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
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	104	0
1	B	2518	0	2518	96	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	5035	198	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 20.

All (198) 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:HG3	1:B:3:GLN:O	1.35	1.12
1:B:89:ARG:HG2	1:B:90:LEU:HD22	1.15	1.10
1:B:6:ARG:H	1:B:283:ASN:HD21	1.06	0.99
1:A:260:LYS:HZ3	1:A:260:LYS:HB2	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:CG	1:B:3:GLN:O	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:NZ	1:A:260:LYS:HA	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:CB	1:A:101:LYS:HZ2	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:NZ	1:A:260:LYS:HB2	2.03	0.74
1:B:214:MET:HG3	1:B:219:PHE:O	1.88	0.73
1:B:213:TYR:OH	1:B:224:THR:HG21	1.89	0.72
1:A:152:MET:CE	1:A:237:LEU:CD1	2.67	0.72
1:A:152:MET:HE3	1:A:237:LEU:CD1	2.19	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:HG13	1:A:216:ILE:O	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:229:THR:O	1:A:230:SER:C	2.29	0.68
1:A:58:LYS:HD2	1:A:63:ARG:O	1.93	0.68
1:A:39:LEU:HD23	1:A:39:LEU:C	2.14	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:231:GLY:O	1:A:235:GLN:HG2	1.94	0.66
1:A:118:THR:OG1	1:A:121:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG22	1:A:271:ARG:NH2	2.11	0.66
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: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:152:MET:HE3	1:A:237:LEU:HD12	1.80	0.63
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: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:214:MET:HG3	1:B:219:PHE:C	2.21	0.60
1:B:35:GLU:O	1:B:39:LEU:HB3	2.01	0.60
1:A:6:ARG:HG2	1:B:282:PHE:CZ	2.37	0.59
1:A:181:GLN:O	1:A:184:GLU:HB2	2.04	0.58
1:B:188:GLY:C	1:B:189:THR:HG22	2.24	0.57
1:A:211:ASP:O	1:A:215:THR:HG23	2.05	0.57
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:39:LEU:C	1:A:39:LEU:CD2	2.75	0.55
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:152:MET:HE1	1:A:237:LEU:CD1	2.37	0.53
1:A:213:TYR:OH	1:A:224:THR:HG21	2.08	0.53
1:A:175:ASP:CG	1:A:201:ARG:HH11	2.12	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:230:SER:HB2	1:B:234:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:THR:O	1:A:230:SER:O	2.28	0.51
1:A:170:ALA:HB3	3:A:958:HOH:O	2.10	0.51
1:B:70:LYS:HE3	3:B:872:HOH:O	2.10	0.51
1:A:145:THR:OG1	1:A:150:GLN:HB2	2.10	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:101:LYS:HG3	1:A:104:GLY:C	2.33	0.49
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:B:90:LEU:HB3	3:B:885:HOH:O	2.12	0.49
1:A:47:ASN:O	1:A:51:GLN:HG2	2.12	0.49
1:B:89:ARG:HB3	3:B:877:HOH:O	2.13	0.49
1:A:225:ILE:O	1:A:226:ASP:HB3	2.12	0.48
1:A:99:ALA:O	1:A:105:THR:HA	2.13	0.48
1:A:69:LEU:O	1:A:73:LEU:HB2	2.13	0.48
1:B:120:GLU:CD	1:B:120:GLU:H	2.16	0.48
1:B:286:LYS:N	1:B:286:LYS:HD2	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:216:ILE:O	1:A:216:ILE:CG1	2.60	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:B:135:SER:HB2	3:B:753:HOH:O	2.12	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:A:192:GLU:H	1:A:192:GLU:CD	2.18	0.46
1:B:124:ALA:O	1:B:128:VAL:HG23	2.16	0.46
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:CB	1:A:101:LYS:HZ3	2.11	0.46
1:B:39:LEU:C	1:B:39:LEU:HD23	2.35	0.46
1:A:39:LEU:HD12	1:A:307:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:A:228:GLU:OE1	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:283:ASN:ND2	1:B:283:ASN:H	2.14	0.45
1:B:230:SER:HB2	1:B:234:GLU:CB	2.47	0.45
1:A:175:ASP:OD2	1:A:205:HIS:NE2	2.47	0.45
1:B:214:MET:HE3	1:B:219:PHE:HA	1.99	0.44
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:B:2:ALA:N	3:B:787:HOH:O	2.50	0.44
1:A:208:LYS:HE2	1:A:208:LYS:HA	1.99	0.44
1:A:42:LEU:O	1:A:50:ARG:NH2	2.51	0.44
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:B:66:LEU:O	1:B:70:LYS:HG3	2.18	0.43
1:A:227:ARG:HB3	1:A:238:LEU:CD2	2.48	0.43
1:A:65:LEU:HD12	1:A:65:LEU:O	2.17	0.43
1:B:205:HIS:O	1:B:208:LYS:HB2	2.18	0.43
1:B:153:LEU:O	1:B:157:LEU:HB2	2.18	0.43
1:B:208:LYS:HA	1:B:208:LYS:HD2	1.48	0.43
1:A:245:ARG:O	1:A:246:SER:HB2	2.19	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: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: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:165:ALA:O	1:A:166:GLY:C	2.57	0.42
1:B:130:GLU:HA	1:B:135:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ALA:N	3:B:791:HOH:O	2.52	0.42
1:B:41:LEU:C	1:B:41:LEU:HD23	2.40	0.42
1:B:283:ASN:HD22	1:B:283:ASN:H	1.68	0.42
1:A:256:TYR:O	1:A:260:LYS:HB3	2.20	0.42
1:B:120:GLU:HB3	3:B:779:HOH:O	2.20	0.41
1:B:205:HIS:C	1:B:205:HIS:CD2	2.93	0.41
1:B:168:ASP:O	1:B:171:GLN:HB3	2.20	0.41
1:A:123:ARG:HD2	1:A:123:ARG:HH11	1.57	0.41
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.94	0.41
1:A:76:LYS:NZ	1:A:266:ASP:OD2	2.47	0.41
1:B:26:LYS:HB3	1:B:26:LYS:HE3	1.84	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:B:8:THR:HG23	1:B:281:LEU:HB3	2.01	0.41
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.72	0.41
1:A:96:LEU:HA	1:A:96:LEU:HD12	1.84	0.41
1:B:24:LEU:HD13	1:B:41:LEU:HD13	2.02	0.41
1:B:176:ALA:HB2	1:B:212:LYS:HB3	2.03	0.40
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.77	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 [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	317/319 (99%)	301 (95%)	14 (4%)	2 (1%)	30 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	317/319 (99%)	298 (94%)	15 (5%)	4 (1%)	15	21
All	All	634/638 (99%)	599 (94%)	29 (5%)	6 (1%)	21	30

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%)	221 (82%)	50 (18%)	2	2
1	B	271/271 (100%)	213 (79%)	58 (21%)	1	1
All	All	542/542 (100%)	434 (80%)	108 (20%)	1	2

All (108) 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	18	ARG
1	A	24	LEU
1	A	36	GLU
1	A	39	LEU
1	A	43	THR

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Mol	Chain	Res	Type
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	120	GLU
1	A	144	ASP
1	A	146	SER
1	A	153	LEU
1	A	157	LEU
1	A	158	GLN
1	A	173	GLU
1	A	174	GLN
1	A	181	GLN
1	A	193	LYS
1	A	200	THR
1	A	208	LYS
1	A	214	MET
1	A	216	ILE
1	A	217	SER
1	A	224	THR
1	A	227	ARG
1	A	228	GLU
1	A	229	THR
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	301	LYS
1	A	303	ASP
1	A	310	LYS
1	B	3	GLN
1	B	4	VAL

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Mol	Chain	Res	Type
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	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
1	B	130	GLU
1	B	138	GLU
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	208	LYS
1	B	212	LYS
1	B	215	THR
1	B	220	GLN
1	B	225	ILE
1	B	227	ARG
1	B	229	THR

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Mol	Chain	Res	Type
1	B	230	SER
1	B	234	GLU
1	B	237	LEU
1	B	245	ARG
1	B	251	LEU
1	B	254	THR
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	174	GLN
1	A	291	ASN
1	B	174	GLN
1	B	235	GLN
1	B	283	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.