



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:58 PM UTC

PDB ID : 1PQ4 / pdb_00001pq4
Title : Crystal structure of ZnuA
Authors : Banerjee, S.; Wei, B.; Bhattacharyya-Pakrasi, M.; Pakrasi, H.B.; Smith, T.J.
Deposited on : 2003-06-17
Resolution : 1.90 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

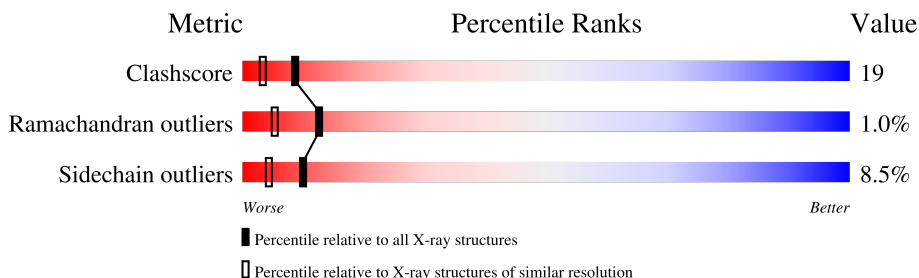
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	291	
1	B	291	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4203 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 periplasmic binding protein component of an ABC type zinc uptake transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1951	1244	324	379	4			
1	B	264	Total	C	N	O	S	0	1	0
			2010	1280	333	392	5			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	125	Total	O	0	0
			125	125		

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	64.99Å 78.30Å 68.40Å 90.00° 118.32° 90.00°	Depositor
Resolution (Å)	19.72 – 1.90	Depositor
% Data completeness (in resolution range)	89.9 (19.72-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.209	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4203	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: ZN

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	0.88	0/1991	1.14	12/2716 (0.4%)
1	B	0.92	1/2050 (0.0%)	1.55	21/2796 (0.8%)
All	All	0.90	1/4041 (0.0%)	1.36	33/5512 (0.6%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	MET	SD-CE	-7.92	1.59	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245[A]	SER	O-C-N	-35.87	77.51	122.34
1	B	245[B]	SER	O-C-N	-35.87	77.51	122.34
1	B	232	GLN	CA-C-N	-10.68	108.59	120.45
1	B	232	GLN	C-N-CA	-10.68	108.59	120.45
1	B	104	ILE	N-CA-C	-8.78	101.86	110.72
1	A	104	ILE	N-CA-C	-8.04	102.60	110.72
1	A	76	VAL	N-CA-C	8.02	115.86	107.76
1	B	319	TRP	N-CA-C	7.68	120.33	111.11
1	B	246	TRP	N-CA-C	7.57	121.35	112.72
1	A	319	TRP	N-CA-C	6.99	119.49	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ASP	CA-C-N	6.94	127.23	119.32
1	B	202	ASP	C-N-CA	6.94	127.23	119.32
1	B	177	ASP	N-CA-C	-6.76	99.85	109.24
1	B	72	VAL	N-CA-C	6.61	117.82	108.36
1	A	135	LEU	N-CA-C	-6.61	100.17	110.42
1	B	296	LYS	N-CA-C	6.46	118.32	111.28
1	A	202	ASP	CA-C-N	6.24	126.44	119.32
1	A	202	ASP	C-N-CA	6.24	126.44	119.32
1	A	289	GLY	N-CA-C	-6.03	102.85	111.42
1	A	72	VAL	N-CA-C	5.94	116.86	108.36
1	B	56	PRO	N-CA-C	5.94	117.95	110.70
1	A	318	ASP	N-CA-C	-5.87	100.82	109.62
1	A	312	LEU	N-CA-C	-5.80	99.95	109.40
1	B	135	LEU	N-CA-C	-5.79	101.95	110.52
1	B	289	GLY	N-CA-C	-5.74	103.27	111.42
1	A	56	PRO	N-CA-C	5.68	117.63	110.70
1	B	308	GLY	N-CA-C	-5.53	104.23	113.02
1	B	305	ILE	N-CA-C	5.47	117.44	112.29
1	A	98	ALA	N-CA-C	5.23	117.80	109.96
1	B	54	SER	N-CA-C	5.16	116.71	111.14
1	B	298	SER	N-CA-C	-5.14	105.76	111.36
1	B	140	HIS	N-CA-C	5.12	121.69	110.80
1	B	76	VAL	N-CA-C	5.03	113.40	107.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	245[A]	SER	Mainchain
1	B	245[B]	SER	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1951	0	1906	82	0
1	B	2010	0	1959	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	115	0	0	0	0
3	B	125	0	0	2	0
All	All	4203	0	3865	147	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 19.

All (147) 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:272:LEU:HD11	1:A:301:ILE:HD11	1.25	1.13
1:B:240:ILE:HD12	1:B:258:ILE:HB	1.38	1.03
1:B:276:ILE:HG13	1:B:301:ILE:HD13	1.38	1.00
1:A:297:SER:O	1:A:301:ILE:HD13	1.64	0.97
1:B:286:MET:HE2	1:B:310:GLU:HG3	1.53	0.90
1:B:262:VAL:O	1:B:265:GLN:HG2	1.71	0.89
1:A:326:VAL:O	1:A:330:ILE:HD13	1.72	0.89
1:A:272:LEU:CD1	1:A:301:ILE:HD11	2.03	0.88
1:B:286:MET:HE2	1:B:310:GLU:CG	2.05	0.86
1:A:252:ASP:OD1	1:B:173:LEU:HD21	1.75	0.85
1:A:88:LYS:HB3	1:A:90:GLN:HE21	1.39	0.85
1:B:137:MET:HG2	1:B:177:ASP:HA	1.57	0.83
1:B:104:ILE:HD12	1:B:108:PHE:CE2	2.14	0.82
1:A:183:SER:OG	1:A:186:LEU:HD13	1.84	0.77
1:A:180:ILE:HD13	1:A:190:GLN:CD	2.10	0.76
1:A:240:ILE:HD11	1:A:284:LEU:HD12	1.67	0.75
1:B:260:ILE:HD13	1:B:275:LEU:HG	1.67	0.75
1:A:246:TRP:H	1:A:257:GLN:HE22	1.33	0.75
1:B:276:ILE:CG1	1:B:301:ILE:HD13	2.15	0.74
1:A:180:ILE:HD12	1:A:181:TRP:N	2.03	0.74
1:B:139:LYS:HA	1:B:259:PRO:HG3	1.70	0.74
1:A:237:ARG:HG2	1:A:254:ASN:O	1.89	0.72
1:A:188:LYS:NZ	1:A:221:GLU:HG2	2.07	0.69
1:A:189:ARG:NH2	1:B:172:ALA:HB2	2.07	0.69
1:B:240:ILE:HD12	1:B:258:ILE:CB	2.22	0.68
1:A:54:SER:HB2	1:A:104:ILE:CD1	2.24	0.67
1:B:236:GLN:HE21	1:B:238:LYS:H	1.41	0.67
1:A:251:ARG:HD3	1:B:173:LEU:HD12	1.75	0.67
1:A:236:GLN:HB3	1:A:334:ASN:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD11	1:A:301:ILE:CD1	2.16	0.65
1:B:197:GLU:O	1:B:201:LEU:HD13	1.95	0.65
1:B:292:GLN:H	1:B:292:GLN:NE2	1.95	0.65
1:A:90:GLN:H	1:A:90:GLN:CD	2.06	0.64
1:A:251:ARG:HD3	1:B:173:LEU:CD1	2.28	0.64
1:B:137:MET:O	1:B:138:GLU:HB2	1.98	0.64
1:A:334:ASN:HD22	1:A:334:ASN:N	1.96	0.62
1:B:286:MET:CE	1:B:310:GLU:HG2	2.29	0.62
1:A:188:LYS:HZ1	1:A:221:GLU:HG2	1.64	0.62
1:B:55:ILE:CD1	1:B:104:ILE:HD11	2.30	0.62
1:B:104:ILE:HD12	1:B:108:PHE:CD2	2.35	0.61
1:A:180:ILE:HD13	1:A:190:GLN:NE2	2.15	0.61
1:B:75:LEU:HD21	1:B:87:PRO:HB3	1.81	0.61
1:A:266:GLU:OE2	1:A:267:PRO:HD3	2.01	0.61
1:B:126:ILE:HD12	1:B:197:GLU:HB3	1.84	0.60
1:A:189:ARG:HH21	1:B:172:ALA:HB2	1.66	0.60
1:B:286:MET:CE	1:B:310:GLU:CG	2.80	0.59
1:B:169:ALA:O	1:B:170:LYS:CB	2.51	0.58
1:A:75:LEU:HD21	1:A:87:PRO:HB3	1.84	0.58
1:A:240:ILE:HG13	1:A:284:LEU:HD13	1.83	0.58
1:A:292:GLN:NE2	1:A:292:GLN:H	2.01	0.58
1:A:130:GLN:HG2	1:A:193:THR:HG21	1.85	0.57
1:A:260:ILE:HG22	1:A:267:PRO:HG3	1.86	0.57
1:B:286:MET:HE2	1:B:310:GLU:HG2	1.82	0.57
1:B:288:PHE:CZ	1:B:330:ILE:HD13	2.40	0.56
1:B:251:ARG:HH11	1:B:251:ARG:HB3	1.71	0.56
1:B:324:LYS:O	1:B:328:GLN:HG3	2.06	0.56
1:B:47:ASP:OD2	1:B:47:ASP:N	2.38	0.56
1:A:89:PRO:HG2	1:A:90:GLN:NE2	2.21	0.55
1:A:228:GLY:O	1:A:232:GLN:HG2	2.07	0.55
1:B:104:ILE:HD13	1:B:181:TRP:CZ3	2.42	0.54
1:B:251:ARG:NH1	3:B:1031:HOH:O	2.34	0.54
1:A:180:ILE:HD12	1:A:180:ILE:C	2.33	0.53
1:B:260:ILE:CD1	1:B:275:LEU:HG	2.35	0.53
1:A:180:ILE:HD13	1:A:190:GLN:OE1	2.08	0.53
1:B:138:GLU:HA	1:B:138:GLU:OE1	2.08	0.53
1:A:276:ILE:HG23	1:A:305:ILE:HG22	1.91	0.53
1:A:130:GLN:O	1:A:132:ILE:HD12	2.08	0.52
1:B:245[A]:SER:O	1:B:246:TRP:CG	2.63	0.52
1:B:104:ILE:HD13	1:B:181:TRP:CE3	2.45	0.52
1:B:334:ASN:HD22	1:B:334:ASN:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:CD1	1:B:241:VAL:HG13	2.45	0.52
1:A:89:PRO:HG2	1:A:90:GLN:HE22	1.76	0.51
1:A:237:ARG:CG	1:A:254:ASN:O	2.57	0.51
1:A:276:ILE:HG23	1:A:305:ILE:CG2	2.41	0.51
1:B:55:ILE:HG12	1:B:104:ILE:HD11	1.91	0.50
1:A:90:GLN:H	1:A:90:GLN:NE2	2.09	0.50
1:A:180:ILE:C	1:A:180:ILE:CD1	2.85	0.50
1:A:75:LEU:HD22	1:A:85:TYR:HE2	1.76	0.50
1:A:260:ILE:HA	1:A:275:LEU:HD21	1.95	0.49
1:A:186:LEU:HD12	1:A:186:LEU:N	2.27	0.49
1:B:126:ILE:HD12	1:B:197:GLU:CB	2.43	0.49
1:B:140:HIS:CB	1:B:257:GLN:O	2.61	0.49
1:A:75:LEU:HD22	1:A:85:TYR:CE2	2.48	0.48
1:A:266:GLU:HG3	1:A:267:PRO:HD2	1.94	0.48
1:B:140:HIS:O	1:B:247:ALA:CB	2.61	0.48
1:A:268:SER:HB2	1:A:271:GLU:HG3	1.95	0.48
1:B:139:LYS:O	1:B:141:ASP:N	2.40	0.48
1:B:285:THR:HG23	1:B:286:MET:HG2	1.94	0.48
1:A:189:ARG:CZ	1:B:172:ALA:HB2	2.44	0.48
1:B:244:PRO:HB3	1:B:259:PRO:HB3	1.96	0.47
1:B:240:ILE:N	1:B:240:ILE:HD13	2.29	0.47
1:B:241:VAL:HG12	1:B:288:PHE:HB2	1.95	0.47
1:A:246:TRP:H	1:A:257:GLN:NE2	2.07	0.47
1:B:141:ASP:HA	3:B:1019:HOH:O	2.15	0.47
1:A:75:LEU:CD2	1:A:85:TYR:HE2	2.29	0.47
1:B:75:LEU:HD23	1:B:75:LEU:O	2.16	0.46
1:A:88:LYS:HB3	1:A:90:GLN:NE2	2.19	0.46
1:A:318:ASP:OD2	1:A:321:SER:OG	2.34	0.46
1:A:59:GLN:HE21	1:A:59:GLN:HB3	1.61	0.46
1:A:186:LEU:HD11	1:B:173:LEU:HG	1.98	0.46
1:A:240:ILE:HD11	1:A:284:LEU:CD1	2.41	0.45
1:A:95:LEU:HD11	1:A:116:LEU:HD22	1.98	0.45
1:A:49:MET:HE3	1:A:49:MET:HB2	1.83	0.45
1:A:286:MET:HE2	1:A:286:MET:HB2	1.69	0.45
1:A:110:GLN:N	1:A:111:PRO:CD	2.80	0.45
1:A:226:GLU:OE2	1:A:324:LYS:HD3	2.17	0.45
1:A:285:THR:HB	1:A:333:ALA:O	2.16	0.45
1:B:201:LEU:CD1	1:B:201:LEU:N	2.80	0.45
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.81	0.44
1:A:244:PRO:HD3	1:A:261:GLU:HG2	1.99	0.44
1:B:114:GLU:HA	1:B:114:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HG12	1:A:104:ILE:HD11	2.00	0.44
1:B:288:PHE:CE1	1:B:330:ILE:HD13	2.52	0.44
1:A:139:LYS:C	1:A:174:MET:HA	2.43	0.44
1:A:301:ILE:CD1	1:A:301:ILE:N	2.81	0.44
1:A:266:GLU:OE2	1:A:267:PRO:CD	2.66	0.43
1:B:240:ILE:N	1:B:240:ILE:CD1	2.81	0.43
1:B:243:HIS:HA	1:B:261:GLU:HG2	2.00	0.43
1:A:188:LYS:HZ1	1:A:221:GLU:CG	2.29	0.42
1:B:55:ILE:CG1	1:B:104:ILE:HD11	2.48	0.42
1:A:334:ASN:N	1:A:334:ASN:ND2	2.67	0.42
1:A:244:PRO:HA	1:A:257:GLN:NE2	2.34	0.42
1:A:53:VAL:HG12	1:A:102:VAL:HB	2.02	0.42
1:B:75:LEU:HD23	1:B:75:LEU:C	2.45	0.42
1:A:244:PRO:HB3	1:A:259:PRO:HB3	2.02	0.41
1:A:189:ARG:HH21	1:B:172:ALA:CB	2.31	0.41
1:A:296:LYS:HB2	1:A:296:LYS:HE3	1.94	0.41
1:B:55:ILE:HD11	1:B:104:ILE:HD11	2.02	0.41
1:B:240:ILE:HG21	1:B:260:ILE:HD11	2.02	0.41
1:B:251:ARG:HH11	1:B:251:ARG:CB	2.33	0.41
1:A:49:MET:HE1	1:A:202:ASP:HB2	2.03	0.41
1:A:279:ALA:HB1	1:A:305:ILE:HD13	2.03	0.41
1:A:260:ILE:HG12	1:A:275:LEU:HD21	2.03	0.41
1:B:112:TRP:CD1	1:B:112:TRP:N	2.89	0.41
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.91	0.41
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.34	0.41
1:A:132:ILE:HD12	1:A:132:ILE:N	2.36	0.41
1:B:126:ILE:CD1	1:B:197:GLU:HB3	2.49	0.41
1:B:262:VAL:O	1:B:263:GLU:C	2.64	0.40
1:A:75:LEU:HD23	1:A:91:GLN:NE2	2.36	0.40
1:A:79:ASN:OD1	1:A:80:ASN:ND2	2.54	0.40
1:A:129:ALA:C	1:A:132:ILE:HD13	2.47	0.40
1:A:266:GLU:OE2	1:A:297:SER:OG	2.34	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	251/291 (86%)	247 (98%)	3 (1%)	1 (0%)	30	22
1	B	261/291 (90%)	250 (96%)	7 (3%)	4 (2%)	8	2
All	All	512/582 (88%)	497 (97%)	10 (2%)	5 (1%)	12	5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	B	138	GLU
1	B	140	HIS
1	B	170	LYS
1	B	169	ALA

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	203/241 (84%)	184 (91%)	19 (9%)	8	3
1	B	208/241 (86%)	192 (92%)	16 (8%)	12	5
All	All	411/482 (85%)	376 (92%)	35 (8%)	10	4

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	75	LEU
1	A	80	ASN
1	A	90	GLN
1	A	113	LEU
1	A	180	ILE
1	A	201	LEU

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Mol	Chain	Res	Type
1	A	206	ARG
1	A	210	GLU
1	A	213	LEU
1	A	225	GLN
1	A	231	LEU
1	A	237	ARG
1	A	270	GLN
1	A	285	THR
1	A	291	THR
1	A	292	GLN
1	A	301	ILE
1	A	334	ASN
1	B	47	ASP
1	B	75	LEU
1	B	112	TRP
1	B	137	MET
1	B	173	LEU
1	B	178	PRO
1	B	186	LEU
1	B	213	LEU
1	B	231	LEU
1	B	232	GLN
1	B	240	ILE
1	B	251	ARG
1	B	262	VAL
1	B	275	LEU
1	B	285	THR
1	B	292	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	80	ASN
1	A	90	GLN
1	A	208	GLN
1	A	229	GLN
1	A	257	GLN
1	A	292	GLN
1	A	334	ASN
1	B	59	GLN
1	B	80	ASN

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Mol	Chain	Res	Type
1	B	225	GLN
1	B	232	GLN
1	B	236	GLN
1	B	292	GLN
1	B	334	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 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](#)

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.