



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:19 PM UTC

PDB ID : 1CCT / pdb_00001cct
Title : STRUCTURE-ASSISTED REDESIGN OF A PROTEIN-ZINC BINDING SITE WITH FEMTOMOLAR AFFINITY
Authors : Ippolito, J.A.; Christianson, D.W.
Deposited on : 1994-12-09
Resolution : 2.20 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

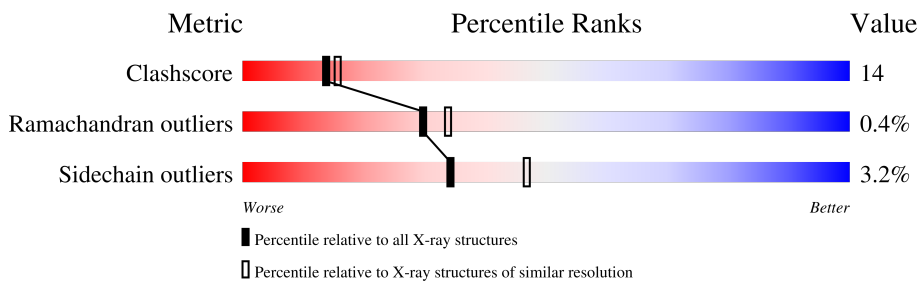
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	259	 46% 42% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2139 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 CARBONIC ANHYDRASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2031	1304	347	378	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLU	THR	conflict	UNP P00918

- 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		

- Molecule 3 is water.

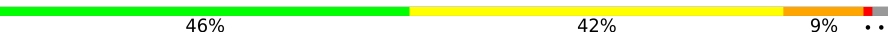
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		

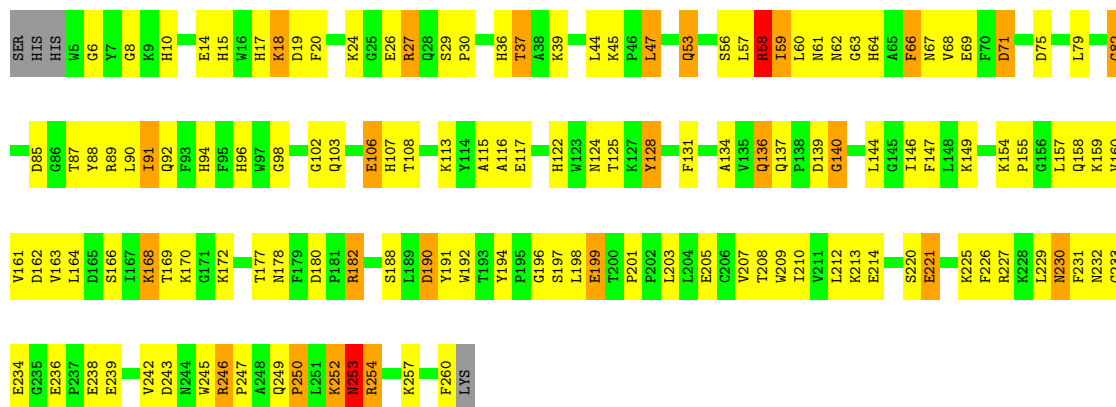
3 Residue-property plots

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: CARBONIC ANHYDRASE II

Chain A: 



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	42.70Å 41.70Å 73.00Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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	1.84	20/2091 (1.0%)	2.18	93/2838 (3.3%)

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	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLY	N-CA	12.05	1.55	1.44
1	A	6	GLY	C-O	8.05	1.29	1.23
1	A	198	LEU	N-CA	6.17	1.53	1.46
1	A	91	ILE	C-O	6.03	1.29	1.23
1	A	66	PHE	N-CA	5.86	1.53	1.46
1	A	20	PHE	CA-C	5.71	1.58	1.52
1	A	87	THR	CA-CB	5.69	1.61	1.53
1	A	149	LYS	CA-C	5.68	1.59	1.52
1	A	122	HIS	ND1-CE1	5.63	1.38	1.32
1	A	18	LYS	N-CA	5.63	1.53	1.46
1	A	177	THR	CB-OG1	5.59	1.52	1.43
1	A	17	HIS	C-N	-5.40	1.26	1.33
1	A	36	HIS	N-CA	5.37	1.53	1.46
1	A	253	ASN	C-O	5.33	1.30	1.24
1	A	64	HIS	CE1-NE2	5.27	1.37	1.32
1	A	234	GLU	N-CA	-5.26	1.39	1.46
1	A	220	SER	CA-C	5.23	1.59	1.52
1	A	8	GLY	C-O	5.14	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	TRP	C-N	-5.13	1.27	1.33
1	A	227	ARG	CD-NE	5.01	1.53	1.46

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	PHE	CA-CB-CG	10.04	123.84	113.80
1	A	94	HIS	CA-CB-CG	-9.86	103.94	113.80
1	A	24	LYS	CA-CB-CG	9.13	132.36	114.10
1	A	58	ARG	CD-NE-CZ	8.68	136.55	124.40
1	A	253	ASN	CA-CB-CG	8.59	121.19	112.60
1	A	236	GLU	O-C-N	8.11	128.24	121.35
1	A	14	GLU	CA-CB-CG	7.83	129.76	114.10
1	A	226	PHE	CA-CB-CG	7.83	121.63	113.80
1	A	239	GLU	CA-CB-CG	7.66	129.42	114.10
1	A	116	ALA	O-C-N	7.60	131.24	123.26
1	A	68	VAL	CA-C-O	-7.58	112.33	120.59
1	A	39	LYS	N-CA-C	7.51	120.90	108.96
1	A	20	PHE	O-C-N	7.42	128.07	121.32
1	A	158	GLN	CA-C-N	7.36	130.14	120.28
1	A	158	GLN	C-N-CA	7.36	130.14	120.28
1	A	96	HIS	CA-C-O	-7.35	112.16	120.32
1	A	128	TYR	N-CA-C	7.33	121.82	113.02
1	A	10	HIS	CA-CB-CG	-7.00	106.80	113.80
1	A	159	LYS	N-CA-CB	6.92	120.29	110.12
1	A	246	ARG	CA-C-N	6.88	126.80	119.85
1	A	246	ARG	C-N-CA	6.88	126.80	119.85
1	A	82	GLY	O-C-N	6.80	128.57	121.77
1	A	230	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	190	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	221	GLU	CA-CB-CG	6.59	127.28	114.10
1	A	117	GLU	CA-C-N	6.57	131.17	122.30
1	A	117	GLU	C-N-CA	6.57	131.17	122.30
1	A	250	PRO	CA-C-O	-6.55	114.22	121.23
1	A	147	PHE	O-C-N	6.52	130.32	122.96
1	A	122	HIS	CA-CB-CG	6.42	120.22	113.80
1	A	68	VAL	N-CA-C	-6.27	98.84	107.99
1	A	122	HIS	CA-C-O	-6.27	113.78	121.11
1	A	14	GLU	CB-CG-CD	6.22	123.17	112.60
1	A	231	PHE	N-CA-C	-6.19	104.46	111.14
1	A	136	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	A	115	ALA	N-CA-C	6.11	118.73	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TYR	CA-C-O	-6.08	113.79	120.36
1	A	169	THR	CA-CB-OG1	-6.04	100.54	109.60
1	A	208	THR	N-CA-C	-6.02	97.34	107.99
1	A	252	LYS	N-CA-C	6.01	119.54	111.24
1	A	208	THR	N-CA-CB	6.00	120.43	110.47
1	A	168	LYS	N-CA-C	5.92	117.73	111.28
1	A	124	ASN	OD1-CG-ND2	5.92	128.52	122.60
1	A	197	SER	N-CA-C	5.92	117.20	108.86
1	A	190	ASP	O-C-N	5.87	130.09	122.87
1	A	199	GLU	CB-CG-CD	5.86	122.56	112.60
1	A	158	GLN	CA-C-O	-5.82	114.38	120.55
1	A	131	PHE	CA-C-N	5.70	126.42	120.03
1	A	131	PHE	C-N-CA	5.70	126.42	120.03
1	A	37	THR	CA-CB-CG2	5.69	120.17	110.50
1	A	182	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	194	TYR	O-C-N	5.65	126.85	121.71
1	A	207	VAL	N-CA-C	5.60	116.65	108.53
1	A	85	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	71	ASP	CA-C-O	-5.57	114.31	120.60
1	A	56	SER	N-CA-C	-5.54	102.31	110.52
1	A	249	GLN	O-C-N	5.52	126.23	120.99
1	A	221	GLU	O-C-N	5.51	129.04	122.27
1	A	242	VAL	CA-C-O	-5.45	116.00	121.45
1	A	168	LYS	O-C-N	5.45	127.89	122.12
1	A	221	GLU	CG-CD-OE2	5.43	130.90	118.40
1	A	155	PRO	CB-CA-C	5.41	120.49	111.56
1	A	59	ILE	CB-CA-C	5.39	118.80	110.50
1	A	106	GLU	CG-CD-OE2	-5.37	106.05	118.40
1	A	154	LYS	O-C-N	5.37	127.09	121.02
1	A	26	GLU	CA-C-O	-5.34	113.03	119.27
1	A	27	ARG	CA-CB-CG	5.33	124.77	114.10
1	A	233	GLY	N-CA-C	-5.33	104.55	113.02
1	A	178	ASN	N-CA-CB	-5.33	104.09	112.13
1	A	257	LYS	CA-C-N	5.28	130.86	122.94
1	A	257	LYS	C-N-CA	5.28	130.86	122.94
1	A	220	SER	O-C-N	5.28	127.71	122.12
1	A	172	LYS	N-CA-CB	5.25	117.73	110.17
1	A	102	GLY	N-CA-C	5.25	120.44	114.67
1	A	196	GLY	O-C-N	5.22	129.49	122.70
1	A	108	THR	CA-C-O	-5.20	115.02	121.11
1	A	90	LEU	O-C-N	5.20	129.51	122.96
1	A	140	GLY	CA-C-O	-5.17	114.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	TRP	N-CA-C	-5.17	101.44	109.72
1	A	19	ASP	O-C-N	5.17	129.70	122.36
1	A	36	HIS	CA-C-N	5.17	130.86	121.92
1	A	36	HIS	C-N-CA	5.17	130.86	121.92
1	A	68	VAL	O-C-N	5.16	129.78	122.97
1	A	226	PHE	CA-C-N	5.16	131.39	121.18
1	A	226	PHE	C-N-CA	5.16	131.39	121.18
1	A	166	SER	N-CA-C	5.14	119.40	113.18
1	A	61	ASN	CB-CA-C	5.10	119.10	110.79
1	A	107	HIS	O-C-N	5.04	128.66	122.96
1	A	47	LEU	CA-C-O	-5.04	115.67	121.47
1	A	162	ASP	CA-C-O	-5.04	113.39	119.49
1	A	53	GLN	N-CA-CB	-5.02	103.24	110.56
1	A	87	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	221	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Sidechain
1	A	58	ARG	Sidechain

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	2031	0	1981	58	0
2	A	1	0	0	0	0
3	A	107	0	0	3	0
All	All	2139	0	1981	58	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 14.

All (58) 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:58:ARG:HD2	1:A:69:GLU:OE1	1.72	0.89
1:A:161:VAL:HG13	1:A:225:LYS:HD3	1.66	0.78
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.10	0.76
1:A:60:LEU:HD23	1:A:60:LEU:N	2.03	0.73
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.76	0.68
1:A:106:GLU:OE1	1:A:199:GLU:HG3	1.95	0.67
1:A:161:VAL:CG1	1:A:225:LYS:HD3	2.26	0.65
1:A:136:GLN:NE2	1:A:136:GLN:HA	2.13	0.64
1:A:44:LEU:HG	1:A:191:TYR:OH	1.97	0.64
1:A:253:ASN:HD22	1:A:254:ARG:N	1.96	0.64
1:A:60:LEU:HD23	1:A:60:LEU:H	1.61	0.63
1:A:59:ILE:HA	1:A:67:ASN:O	1.99	0.63
1:A:164:LEU:HD22	1:A:229:LEU:HD11	1.80	0.63
1:A:136:GLN:HA	1:A:136:GLN:HE21	1.64	0.62
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.46	0.61
1:A:213:LYS:HD3	1:A:260:PHE:CE2	2.36	0.61
1:A:60:LEU:HD21	1:A:67:ASN:HB2	1.83	0.60
1:A:62:ASN:O	1:A:170:LYS:NZ	2.37	0.58
1:A:45:LYS:O	1:A:82:GLY:HA2	2.02	0.58
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.87	0.57
1:A:157:LEU:O	1:A:157:LEU:HG	2.06	0.56
1:A:63:GLY:HA3	1:A:170:LYS:HZ2	1.71	0.55
1:A:201:PRO:HA	1:A:203:LEU:HG	1.88	0.54
1:A:253:ASN:HD22	1:A:253:ASN:C	2.15	0.54
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.38	0.54
1:A:252:LYS:O	1:A:253:ASN:CG	2.51	0.54
1:A:253:ASN:ND2	1:A:254:ARG:N	2.56	0.53
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.44	0.53
1:A:168:LYS:NZ	3:A:332:HOH:O	2.42	0.52
1:A:30:PRO:HG3	1:A:106:GLU:HB3	1.90	0.52
1:A:139:ASP:HA	3:A:349:HOH:O	2.10	0.52
1:A:60:LEU:O	1:A:66:PHE:HA	2.10	0.52
1:A:113:LYS:NZ	3:A:345:HOH:O	2.42	0.52
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.46	0.50
1:A:75:ASP:OD1	1:A:89:ARG:NE	2.38	0.49
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.48	0.48
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.96	0.48
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.29	0.47
1:A:60:LEU:HD23	1:A:67:ASN:O	2.15	0.46
1:A:146:ILE:HG12	1:A:212:LEU:HD12	1.97	0.46
1:A:252:LYS:O	1:A:253:ASN:CB	2.65	0.45
1:A:103:GLN:NE2	1:A:243:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:HIS:ND1	1:A:18:LYS:NZ	2.44	0.45
1:A:190:ASP:CB	1:A:213:LYS:HE2	2.46	0.45
1:A:164:LEU:HD22	1:A:229:LEU:HD21	1.99	0.45
1:A:128:TYR:CZ	1:A:137:GLN:HG3	2.52	0.44
1:A:190:ASP:HB2	1:A:213:LYS:HE2	2.00	0.44
1:A:91:ILE:HG23	1:A:92:GLN:HG3	1.99	0.44
1:A:250:PRO:HB2	1:A:252:LYS:HG3	2.00	0.43
1:A:180:ASP:OD2	1:A:182:ARG:NH2	2.51	0.42
1:A:230:ASN:HB3	1:A:232:ASN:OD1	2.19	0.42
1:A:188:SER:HB3	1:A:214:GLU:OE1	2.20	0.42
1:A:47:LEU:HD23	1:A:47:LEU:HA	1.84	0.41
1:A:246:ARG:HA	1:A:247:PRO:HD3	1.87	0.41
1:A:230:ASN:CG	1:A:238:GLU:HG3	2.46	0.40
1:A:160:VAL:O	1:A:163:VAL:HG12	2.20	0.40
1:A:134:ALA:O	1:A:140:GLY:HA3	2.21	0.40
1:A:29:SER:O	1:A:246:ARG:NH1	2.53	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	253/259 (98%)	241 (95%)	11 (4%)	1 (0%)	30 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN

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	220/224 (98%)	213 (97%)	7 (3%)	34 47

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	53	GLN
1	A	58	ARG
1	A	79	LEU
1	A	144	LEU
1	A	221	GLU
1	A	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	136	GLN
1	A	253	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

Of 1 ligands modelled in this entry, 1 is 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 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.