



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 AM UTC

PDB ID : 1CVF / pdb_00001cvf
Title : STRUCTURAL CONSEQUENCES OF REDESIGNING A PROTEIN-ZINC BINDING SITE
Authors : Ippolito, J.A.; Christianson, D.W.
Deposited on : 1994-06-21
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

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

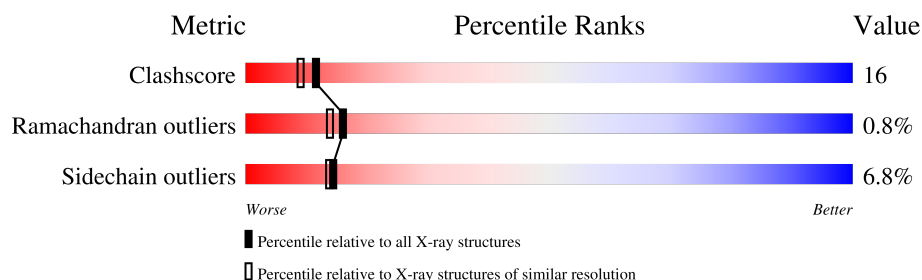
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (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 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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2127 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
			2024	1300	345	377	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	HIS	conflict	UNP P00918

- Molecule 2 is water.

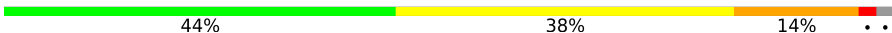
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total	O	0	0
			103	103		

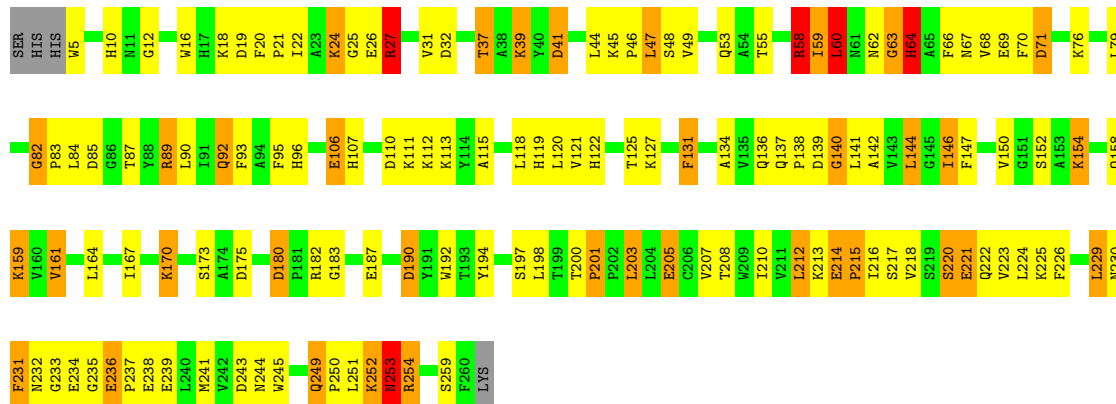
3 Residue-property plots

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 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2127	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	1.79	23/2083 (1.1%)	2.40	131/2828 (4.6%)

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	A	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ASP	N-CA	9.13	1.56	1.45
1	A	253	ASN	C-O	7.93	1.33	1.24
1	A	87	THR	CA-C	-7.60	1.43	1.52
1	A	222	GLN	C-O	7.39	1.32	1.24
1	A	216	ILE	N-CA	6.85	1.54	1.46
1	A	194	TYR	C-O	6.38	1.32	1.24
1	A	64	HIS	CE1-NE2	6.09	1.38	1.32
1	A	87	THR	CA-CB	6.04	1.62	1.53
1	A	167	ILE	CA-CB	5.89	1.62	1.54
1	A	95	PHE	C-O	5.54	1.30	1.23
1	A	140	GLY	C-O	5.50	1.30	1.23
1	A	10	HIS	CA-CB	5.47	1.62	1.53
1	A	37	THR	CB-OG1	5.38	1.52	1.43
1	A	71	ASP	C-O	5.35	1.30	1.24
1	A	251	LEU	N-CA	5.21	1.52	1.46
1	A	244	ASN	CA-C	5.20	1.59	1.52
1	A	217	SER	C-N	-5.18	1.26	1.33
1	A	170	LYS	C-O	5.14	1.30	1.23
1	A	118	LEU	C-O	5.12	1.30	1.24
1	A	107	HIS	CD2-NE2	-5.06	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	LYS	C-O	-5.04	1.19	1.24
1	A	173	SER	C-O	5.02	1.29	1.23
1	A	21	PRO	N-CA	-5.00	1.41	1.47

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	PRO	CB-CA-C	10.43	121.19	111.39
1	A	226	PHE	CA-CB-CG	10.01	123.81	113.80
1	A	122	HIS	CA-CB-CG	9.90	123.70	113.80
1	A	221	GLU	CA-CB-CG	9.71	133.53	114.10
1	A	95	PHE	CA-CB-CG	9.52	123.32	113.80
1	A	200	THR	O-C-N	9.48	129.96	121.80
1	A	92	GLN	OE1-CD-NE2	-9.39	113.21	122.60
1	A	10	HIS	CA-CB-CG	-9.23	104.57	113.80
1	A	85	ASP	CA-CB-CG	-9.12	103.47	112.60
1	A	230	ASN	CA-CB-CG	9.06	121.67	112.60
1	A	136	GLN	OE1-CD-NE2	-8.91	113.69	122.60
1	A	232	ASN	CA-C-O	8.89	132.18	121.87
1	A	158	GLN	CA-C-O	-8.71	111.68	120.82
1	A	96	HIS	CA-C-O	-8.46	111.25	120.30
1	A	89	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	A	84	LEU	CA-C-O	8.33	131.05	121.47
1	A	142	ALA	CA-C-N	-8.17	112.57	123.10
1	A	142	ALA	C-N-CA	-8.17	112.57	123.10
1	A	221	GLU	CA-C-O	-8.03	110.73	119.97
1	A	252	LYS	N-CA-C	7.90	122.14	111.24
1	A	238	GLU	CB-CG-CD	7.79	125.84	112.60
1	A	37	THR	CA-CB-OG1	-7.71	98.03	109.60
1	A	194	TYR	CA-C-N	7.63	129.38	119.84
1	A	194	TYR	C-N-CA	7.63	129.38	119.84
1	A	233	GLY	N-CA-C	-7.51	102.46	112.82
1	A	190	ASP	CA-CB-CG	7.49	120.08	112.60
1	A	41	ASP	CA-CB-CG	-7.38	105.22	112.60
1	A	207	VAL	N-CA-C	7.35	119.19	108.53
1	A	192	TRP	N-CA-CB	7.23	123.45	111.08
1	A	68	VAL	CA-C-O	-7.13	112.90	120.53
1	A	107	HIS	CA-C-O	-6.99	113.56	121.81
1	A	21	PRO	N-CA-C	6.92	122.83	113.84
1	A	158	GLN	O-C-N	6.84	129.12	122.07
1	A	20	PHE	CA-C-N	6.83	126.52	119.56
1	A	20	PHE	C-N-CA	6.83	126.52	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	THR	CA-CB-CG2	6.83	122.11	110.50
1	A	197	SER	N-CA-C	6.69	118.30	108.86
1	A	200	THR	CA-C-O	-6.63	112.97	120.46
1	A	175	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	192	TRP	N-CA-C	-6.50	99.32	109.72
1	A	207	VAL	CA-C-O	6.48	128.11	120.72
1	A	138	PRO	CB-CA-C	6.47	122.31	112.21
1	A	27	ARG	CA-CB-CG	6.47	127.04	114.10
1	A	239	GLU	CA-CB-CG	6.39	126.88	114.10
1	A	32	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	47	LEU	O-C-N	6.28	130.01	122.85
1	A	68	VAL	N-CA-C	-6.28	98.70	107.80
1	A	259	SER	N-CA-C	-6.27	105.50	113.02
1	A	59	ILE	CB-CA-C	6.27	119.96	110.62
1	A	115	ALA	CA-C-N	6.25	132.48	122.10
1	A	115	ALA	C-N-CA	6.25	132.48	122.10
1	A	251	LEU	CB-CA-C	6.24	121.45	110.85
1	A	49	VAL	CA-C-O	-6.22	113.52	120.74
1	A	208	THR	N-CA-CB	6.22	120.64	110.37
1	A	215	PRO	CA-C-O	-6.22	114.41	122.12
1	A	64	HIS	N-CA-CB	6.20	119.17	110.98
1	A	106	GLU	CG-CD-OE2	-6.17	104.20	118.40
1	A	235	GLY	N-CA-C	-6.13	106.62	115.27
1	A	12	GLY	N-CA-C	6.12	119.35	112.00
1	A	121	VAL	CB-CA-C	6.11	119.15	110.84
1	A	231	PHE	N-CA-C	-6.08	104.57	111.14
1	A	154	LYS	O-C-N	6.05	127.86	121.02
1	A	19	ASP	CA-CB-CG	-6.04	106.56	112.60
1	A	239	GLU	CA-C-O	-6.03	114.07	120.40
1	A	136	GLN	N-CA-C	-5.99	105.15	112.88
1	A	89	ARG	CA-C-O	-5.98	114.16	120.80
1	A	90	LEU	CA-C-N	-5.97	116.86	122.66
1	A	90	LEU	C-N-CA	-5.97	116.86	122.66
1	A	208	THR	O-C-N	5.95	130.13	123.05
1	A	253	ASN	CB-CG-ND2	5.90	125.25	116.40
1	A	31	VAL	CA-CB-CG1	5.85	120.35	110.40
1	A	47	LEU	CA-C-O	-5.84	114.92	121.81
1	A	201	PRO	N-CA-C	-5.80	104.90	110.47
1	A	221	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	142	ALA	CA-C-O	-5.75	113.01	120.25
1	A	58	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	A	26	GLU	N-CA-C	5.68	119.93	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	131	PHE	CA-C-N	5.66	126.26	119.98
1	A	131	PHE	C-N-CA	5.66	126.26	119.98
1	A	92	GLN	CB-CG-CD	5.64	122.18	112.60
1	A	60	LEU	CA-C-O	5.62	127.58	121.06
1	A	231	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	220	SER	O-C-N	5.46	127.91	122.12
1	A	234	GLU	CA-C-O	-5.46	114.69	120.92
1	A	142	ALA	O-C-N	5.46	130.24	123.14
1	A	205	GLU	CA-C-N	5.45	130.74	122.08
1	A	205	GLU	C-N-CA	5.45	130.74	122.08
1	A	112	LYS	O-C-N	5.43	129.40	123.04
1	A	63	GLY	O-C-N	5.42	129.52	122.42
1	A	48	SER	CA-C-N	5.41	130.02	122.93
1	A	48	SER	C-N-CA	5.41	130.02	122.93
1	A	175	ASP	N-CA-C	-5.41	102.61	110.24
1	A	187	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	203	LEU	CA-C-N	5.38	128.41	120.82
1	A	203	LEU	C-N-CA	5.38	128.41	120.82
1	A	222	GLN	CB-CG-CD	5.37	121.72	112.60
1	A	121	VAL	O-C-N	5.36	128.98	123.03
1	A	120	LEU	CA-C-O	-5.36	114.63	120.36
1	A	146	ILE	CB-CG1-CD1	5.36	125.05	113.80
1	A	192	TRP	O-C-N	5.36	130.15	123.19
1	A	212	LEU	CA-C-N	5.35	127.39	120.44
1	A	212	LEU	C-N-CA	5.35	127.39	120.44
1	A	39	LYS	N-CA-C	5.34	117.44	108.73
1	A	236	GLU	CG-CD-OE1	5.34	130.69	118.40
1	A	82	GLY	CA-C-N	5.33	126.17	120.47
1	A	82	GLY	C-N-CA	5.33	126.17	120.47
1	A	127	LYS	N-CA-C	-5.30	105.61	111.71
1	A	46	PRO	CB-CA-C	5.29	118.00	111.23
1	A	139	ASP	CA-C-N	5.28	125.85	119.98
1	A	139	ASP	C-N-CA	5.28	125.85	119.98
1	A	92	GLN	O-C-N	5.28	128.80	123.26
1	A	137	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	24	LYS	CA-CB-CG	5.26	124.62	114.10
1	A	159	LYS	N-CA-CB	5.25	117.94	110.06
1	A	147	PHE	CA-C-O	-5.21	115.11	121.05
1	A	147	PHE	O-C-N	5.19	129.13	123.01
1	A	249	GLN	O-C-N	5.18	127.48	121.21
1	A	198	LEU	N-CA-C	-5.16	103.23	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASP	N-CA-C	-5.13	102.79	110.23
1	A	234	GLU	CA-CB-CG	-5.13	103.84	114.10
1	A	16	TRP	CA-C-O	-5.09	114.34	120.10
1	A	120	LEU	O-C-N	5.08	129.00	123.22
1	A	70	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	216	ILE	N-CA-C	-5.07	101.11	108.97
1	A	93	PHE	N-CA-C	-5.05	101.39	109.23
1	A	161	VAL	O-C-N	5.05	126.86	121.91
1	A	19	ASP	O-C-N	5.04	129.37	122.46
1	A	214	GLU	CA-C-N	5.03	125.24	120.31
1	A	214	GLU	C-N-CA	5.03	125.24	120.31
1	A	152	SER	CA-CB-OG	-5.02	101.06	111.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ARG	Sidechain
1	A	58	ARG	Sidechain

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	2024	0	1980	64	0
2	A	103	0	0	9	1
All	All	2127	0	1980	64	1

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 16.

All (64) 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	1.68	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.51	0.92
1:A:253:ASN:HD22	1:A:254:ARG:N	1.71	0.89
1:A:164:LEU:HD22	1:A:229:LEU:HD21	1.60	0.82
1:A:253:ASN:ND2	1:A:254:ARG:N	2.32	0.78
1:A:250:PRO:HG2	1:A:252:LYS:HE3	1.68	0.75
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.16	0.71
1:A:66:PHE:C	1:A:67:ASN:HD22	1.99	0.71
1:A:253:ASN:HD22	1:A:253:ASN:C	1.99	0.69
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.23	0.69
1:A:64:HIS:ND1	2:A:358:HOH:O	2.26	0.67
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.10	0.66
1:A:47:LEU:HD21	1:A:210:ILE:HG21	1.78	0.65
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.80	0.63
1:A:250:PRO:HB2	1:A:252:LYS:HG3	1.80	0.62
1:A:63:GLY:HA3	1:A:170:LYS:HZ3	1.64	0.61
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.81	0.61
1:A:55:THR:HG23	2:A:291:HOH:O	2.00	0.61
1:A:22:ILE:HD11	1:A:205:GLU:OE1	2.03	0.59
1:A:25:GLY:O	1:A:252:LYS:NZ	2.33	0.58
1:A:60:LEU:HB2	2:A:365:HOH:O	2.04	0.57
1:A:58:ARG:CD	1:A:69:GLU:OE1	2.48	0.57
1:A:62:ASN:O	1:A:170:LYS:NZ	2.40	0.55
1:A:59:ILE:HA	1:A:67:ASN:O	2.06	0.55
1:A:253:ASN:ND2	1:A:253:ASN:C	2.62	0.54
1:A:134:ALA:O	1:A:140:GLY:HA3	2.08	0.54
1:A:60:LEU:HD12	2:A:365:HOH:O	2.09	0.53
1:A:5:TRP:HA	2:A:325:HOH:O	2.08	0.53
1:A:144:LEU:CD2	1:A:212:LEU:HD11	2.38	0.53
1:A:159:LYS:HB2	2:A:316:HOH:O	2.08	0.53
1:A:89:ARG:HG3	1:A:125:THR:CG2	2.40	0.52
1:A:45:LYS:O	1:A:82:GLY:HA2	2.10	0.52
1:A:180:ASP:OD2	1:A:182:ARG:NH2	2.34	0.52
1:A:67:ASN:HD22	1:A:67:ASN:N	2.01	0.51
1:A:190:ASP:CB	1:A:213:LYS:HE2	2.41	0.51
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.40	0.51
1:A:106:GLU:OE1	1:A:119:HIS:HE1	1.94	0.51
1:A:154:LYS:HE3	1:A:183:GLY:O	2.12	0.49
1:A:190:ASP:HB2	1:A:213:LYS:HE2	1.95	0.48
1:A:249:GLN:HB3	1:A:250:PRO:HD2	1.95	0.48
1:A:18:LYS:HE3	2:A:269:HOH:O	2.14	0.48
1:A:60:LEU:HD22	1:A:69:GLU:OE2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLY:HA3	2:A:355:HOH:O	2.14	0.46
1:A:252:LYS:O	1:A:253:ASN:CB	2.63	0.46
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.87	0.45
1:A:220:SER:O	1:A:223:VAL:HG12	2.17	0.45
1:A:110:ASP:O	1:A:111:LYS:HB2	2.18	0.44
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.74	0.44
1:A:41:ASP:C	1:A:41:ASP:OD1	2.59	0.44
1:A:201:PRO:HA	1:A:203:LEU:HG	2.00	0.44
1:A:252:LYS:O	1:A:253:ASN:CG	2.61	0.44
1:A:231:PHE:CE1	1:A:241:MET:HG3	2.52	0.44
1:A:150:VAL:HA	1:A:218:VAL:O	2.17	0.44
1:A:253:ASN:C	1:A:254:ARG:O	2.62	0.42
1:A:60:LEU:O	1:A:66:PHE:HA	2.19	0.42
1:A:253:ASN:HD22	1:A:254:ARG:CA	2.29	0.42
1:A:164:LEU:HB3	1:A:229:LEU:HD11	2.01	0.42
1:A:146:ILE:HG12	1:A:212:LEU:HD22	2.00	0.42
1:A:113:LYS:NZ	2:A:345:HOH:O	2.52	0.41
1:A:243:ASP:HA	1:A:245:TRP:CD1	2.55	0.41
1:A:131:PHE:CE1	1:A:141:LEU:HD21	2.55	0.41
1:A:201:PRO:HA	1:A:203:LEU:N	2.36	0.41
1:A:67:ASN:N	1:A:67:ASN:ND2	2.66	0.41
1:A:71:ASP:OD2	1:A:76:LYS:NZ	2.55	0.40

All (1) 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)
2:A:282:HOH:O	2:A:346:HOH:O[2_545]	1.63	0.57

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%)	235 (93%)	16 (6%)	2 (1%)	16 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	254	ARG

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	219/223 (98%)	204 (93%)	15 (7%)	14 14

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	37	THR
1	A	39	LYS
1	A	44	LEU
1	A	53	GLN
1	A	58	ARG
1	A	60	LEU
1	A	64	HIS
1	A	79	LEU
1	A	83	PRO
1	A	92	GLN
1	A	144	LEU
1	A	221	GLU
1	A	229	LEU
1	A	253	ASN

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	67	ASN
1	A	92	GLN
1	A	137	GLN
1	A	178	ASN
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 [i](#)

There are no ligands in this entry.

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.