



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:02 PM UTC

PDB ID : 1AZ0 / pdb_00001az0
Title : ECORV ENDONUCLEASE/DNA COMPLEX
Authors : Perona, J.J.; Martin, A.M.
Deposited on : 1997-11-24
Resolution : 2.00 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

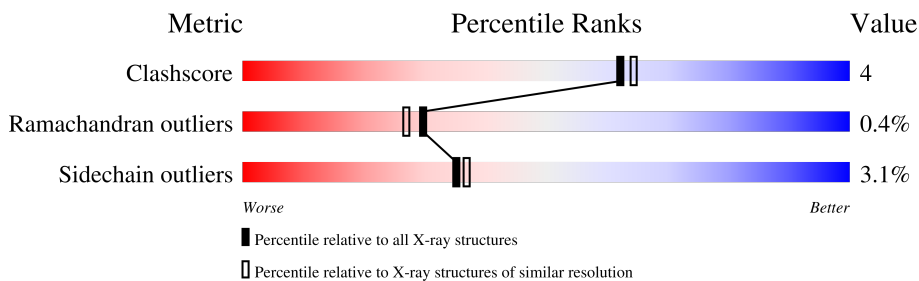
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	C	11	64% 27% 9%
1	D	11	55% 27% 9% 9%
2	A	244	76% 19% . .
2	B	244	73% 19% . 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4296 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 DNA chain called DNA (5'-D(*AP*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	11	Total	C	N	O	P	0	0	0
			223	109	41	63	10			
1	D	11	Total	C	N	O	P	0	0	0
			223	109	41	63	10			

- Molecule 2 is a protein called PROTEIN (TYPE II RESTRICTION ENZYME ECORV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	237	Total	C	N	O	S	0	0	0
			1838	1192	301	344	1			
2	B	229	Total	C	N	O	S	0	0	0
			1781	1158	295	327	1			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	15	Total	O	0	0
			15	15		
4	D	13	Total	O	0	0
			13	13		
4	A	108	Total	O	0	0
			108	108		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	93	Total	O	0	0
			93	93		

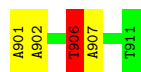
3 Residue-property plots [i](#)

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.

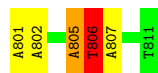
- Molecule 1: DNA (5'-D(*AP*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3')

Chain C: 



- Molecule 1: DNA (5'-D(*AP*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3')

Chain D: 



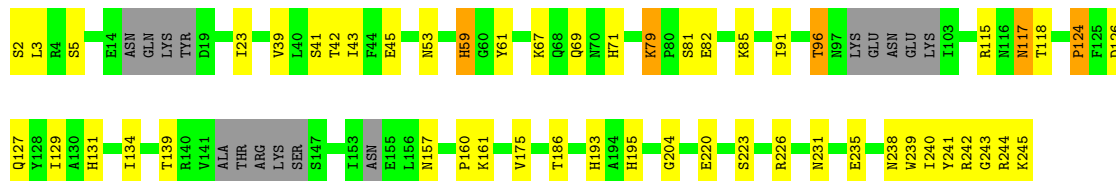
- Molecule 2: PROTEIN (TYPE II RESTRICTION ENZYME ECORV)

Chain A: 



- Molecule 2: PROTEIN (TYPE II RESTRICTION ENZYME ECORV)

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.00Å 50.20Å 64.10Å 109.00° 108.00° 96.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	88.0 (6.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4296	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	C	0.33	0/250	0.99	2/384 (0.5%)
1	D	0.34	0/250	1.01	2/384 (0.5%)
2	A	1.00	5/1888 (0.3%)	1.61	19/2580 (0.7%)
2	B	1.01	5/1826 (0.3%)	1.59	16/2487 (0.6%)
All	All	0.95	10/4214 (0.2%)	1.53	39/5835 (0.7%)

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	C	0	1
1	D	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	131	HIS	CD2-NE2	-6.73	1.30	1.37
2	A	59	HIS	CD2-NE2	-6.69	1.30	1.37
2	B	59	HIS	CD2-NE2	-6.68	1.30	1.37
2	B	193	HIS	CD2-NE2	-6.66	1.30	1.37
2	A	193	HIS	CD2-NE2	-6.34	1.30	1.37
2	A	71	HIS	CD2-NE2	-6.19	1.31	1.37
2	A	195	HIS	CD2-NE2	-6.10	1.31	1.37
2	B	131	HIS	CD2-NE2	-5.92	1.31	1.37
2	B	71	HIS	CD2-NE2	-5.49	1.31	1.37
2	B	195	HIS	CD2-NE2	-5.21	1.32	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	69	GLN	OE1-CD-NE2	-8.24	114.36	122.60
2	B	53	ASN	CA-CB-CG	-7.38	105.22	112.60
2	A	193	HIS	N-CA-C	-7.09	95.44	107.99
2	B	157	ASN	OD1-CG-ND2	-6.99	115.61	122.60
2	B	71	HIS	CB-CG-CD2	-6.81	122.34	131.20
2	A	195	HIS	CB-CG-CD2	-6.56	122.67	131.20
2	A	193	HIS	CB-CG-CD2	-6.49	122.77	131.20
2	A	69	GLN	CG-CD-NE2	6.47	126.10	116.40
2	A	106	THR	N-CA-C	-6.40	98.81	109.24
1	C	906	DT	N1-C1'-C2'	-6.23	104.16	113.50
2	A	71	HIS	CA-CB-CG	-6.20	107.60	113.80
2	A	53	ASN	CA-CB-CG	-6.15	106.45	112.60
2	A	71	HIS	CB-CG-CD2	-6.15	123.21	131.20
2	B	69	GLN	N-CA-C	6.14	120.38	113.01
2	B	69	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	A	205	ILE	CB-CG1-CD1	-6.05	101.10	113.80
1	D	806	DT	N1-C1'-C2'	-6.03	104.46	113.50
2	A	188	ASN	CB-CG-ND2	5.96	125.34	116.40
2	B	157	ASN	CB-CG-ND2	5.88	125.22	116.40
2	A	188	ASN	OD1-CG-ND2	-5.87	116.73	122.60
2	B	82	GLU	O-C-N	-5.79	116.15	121.42
2	A	79	LYS	N-CA-C	-5.79	102.49	109.72
2	B	193	HIS	CB-CG-CD2	-5.74	123.74	131.20
2	A	97	ASN	CA-CB-CG	-5.73	106.87	112.60
1	D	805	DA	N9-C1'-C2'	-5.72	104.92	113.50
1	C	906	DT	C4'-C3'-O3'	5.66	118.49	110.00
2	B	67	LYS	N-CA-C	-5.39	104.28	112.04
2	B	79	LYS	N-CA-C	-5.39	103.25	109.93
2	B	134	ILE	N-CA-C	-5.38	100.00	107.80
2	B	160	PRO	O-C-N	-5.38	116.83	123.01
2	B	195	HIS	CB-CG-CD2	-5.35	124.24	131.20
2	A	127	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	B	115	ARG	N-CA-C	-5.29	106.96	113.41
2	A	195	HIS	CA-CB-CG	-5.26	108.54	113.80
2	A	47	PHE	N-CA-CB	-5.24	102.42	110.12
2	B	117	ASN	N-CA-C	5.13	121.74	110.80
2	A	101	GLU	O-C-N	-5.11	116.66	122.68
2	B	231	ASN	CA-CB-CG	-5.05	107.55	112.60
2	A	13	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	906	DT	Sidechain
1	D	806	DT	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	C	223	0	127	7	0
1	D	223	0	127	4	0
2	A	1838	0	1669	14	142
2	B	1781	0	1652	13	172
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	108	0	0	1	39
4	B	93	0	0	1	9
4	C	15	0	0	0	0
4	D	13	0	0	0	0
All	All	4296	0	3575	30	181

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 4.

All (30) 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:C:901:DA:H2'	1:C:902:DA:C8	2.06	0.90
2:A:112:SER:HA	2:A:119:LYS:HE2	1.60	0.83
2:A:62:ILE:HD11	2:A:80:PRO:HG3	1.65	0.79
1:C:901:DA:C2'	1:C:902:DA:C8	2.72	0.73
1:C:901:DA:H2''	1:C:902:DA:O4'	2.03	0.59
2:A:23:ILE:HG22	2:B:23:ILE:HG22	1.84	0.58
2:A:43:ILE:HD12	2:B:23:ILE:HG21	1.86	0.57
2:B:45:GLU:HA	2:B:91:ILE:HD13	1.87	0.57
2:A:42:THR:HG23	2:B:39:VAL:HG22	1.87	0.56
1:C:901:DA:H2'	1:C:902:DA:N7	2.22	0.54
2:B:220:GLU:HB2	2:B:226:ARG:HG2	1.90	0.53
1:C:906:DT:H71	2:A:186:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:THR:HG22	2:B:124:PRO:HG3	1.95	0.48
2:B:96:THR:O	2:B:139:THR:HA	2.14	0.48
1:D:805:DA:H2'	1:D:806:DT:C7	2.44	0.48
2:A:33:LEU:HB2	2:A:162:PRO:HG3	1.95	0.47
1:D:807:DA:H62	2:B:186:THR:HG21	1.80	0.47
2:B:161:LYS:NZ	4:B:348:HOH:O	2.47	0.47
1:D:801:DA:H2''	1:D:802:DA:C8	2.49	0.47
2:A:39:VAL:HG22	2:B:42:THR:HG23	1.97	0.46
1:C:902:DA:H3'	2:B:223:SER:OG	2.15	0.45
1:C:907:DA:H62	2:A:186:THR:HG21	1.83	0.44
2:A:117:ASN:OD1	2:A:125:PHE:HB3	2.17	0.44
2:A:49:ARG:HG2	2:A:75:PHE:HZ	1.83	0.44
1:D:805:DA:H2'	1:D:806:DT:H72	2.01	0.43
2:A:49:ARG:HG2	2:A:75:PHE:CZ	2.54	0.43
2:B:175:VAL:O	2:B:204:GLY:HA3	2.19	0.43
2:A:62:ILE:HD11	2:A:80:PRO:CG	2.42	0.43
2:B:85:LYS:HA	2:B:129:ILE:CG2	2.51	0.41
2:A:119:LYS:NZ	4:A:386:HOH:O	2.52	0.40

All (181) 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:B:85:LYS:CA	4:A:391:HOH:O[1_554]	0.27	1.93
2:A:7:LEU:N	2:B:242:ARG:CA[1_666]	0.39	1.81
2:A:9:ASN:N	2:B:243:GLY:CA[1_666]	0.48	1.72
2:A:9:ASN:ND2	2:B:244:ARG:CB[1_666]	0.53	1.67
2:A:5:SER:CB	2:B:245:LYS:C[1_666]	0.55	1.65
2:A:55:ILE:CG1	2:B:241:TYR:CB[1_666]	0.69	1.51
2:B:240:ILE:CA	4:A:311:HOH:O[1_444]	0.79	1.41
2:B:240:ILE:CG2	4:A:371:HOH:O[1_444]	0.83	1.37
2:B:127:GLN:CA	4:A:323:HOH:O[1_554]	0.88	1.32
2:B:127:GLN:CG	4:A:351:HOH:O[1_554]	0.88	1.32
2:A:208:SER:CB	2:B:2:SER:C[1_556]	0.94	1.26
2:B:59:HIS:O	4:A:304:HOH:O[1_554]	0.96	1.24
2:A:208:SER:CB	2:B:2:SER:CA[1_556]	0.97	1.23
2:A:5:SER:OG	2:B:245:LYS:C[1_666]	0.98	1.22
2:A:55:ILE:CG1	2:B:241:TYR:CG[1_666]	0.98	1.22
2:A:208:SER:OG	2:B:2:SER:CB[1_556]	0.99	1.21
2:A:5:SER:OG	2:B:245:LYS:OXT[1_666]	1.00	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:ILE:CB	2:B:241:TYR:CD2[1_666]	1.00	1.20
2:A:207:ASP:O	2:B:59:HIS:ND1[1_556]	1.00	1.20
2:A:6:ASP:C	2:B:242:ARG:CA[1_666]	1.01	1.19
2:B:85:LYS:CB	4:A:392:HOH:O[1_554]	1.01	1.19
2:B:59:HIS:C	4:A:304:HOH:O[1_554]	1.03	1.17
2:A:58:LYS:NZ	2:B:235:GLU:O[1_666]	1.04	1.16
2:A:208:SER:OG	2:B:2:SER:CA[1_556]	1.06	1.14
2:B:240:ILE:N	4:A:311:HOH:O[1_444]	1.07	1.13
2:A:6:ASP:OD1	2:B:239:TRP:CA[1_666]	1.08	1.12
2:A:6:ASP:C	2:B:242:ARG:N[1_666]	1.09	1.11
2:A:55:ILE:CD1	2:B:241:TYR:CB[1_666]	1.11	1.09
2:A:59:HIS:NE2	2:B:238:ASN:OD1[1_666]	1.15	1.05
2:A:2:SER:O	2:B:242:ARG:NE[1_666]	1.16	1.04
2:A:9:ASN:CG	2:B:244:ARG:CB[1_666]	1.20	1.00
2:A:5:SER:OG	2:B:245:LYS:O[1_666]	1.28	0.92
2:A:10:ALA:N	2:B:240:ILE:O[1_666]	1.29	0.91
2:A:6:ASP:O	2:B:242:ARG:N[1_666]	1.30	0.90
2:A:59:HIS:CD2	2:B:238:ASN:OD1[1_666]	1.31	0.89
2:A:55:ILE:CG2	2:B:241:TYR:CD2[1_666]	1.33	0.87
2:A:241:TYR:OH	2:B:126:ASP:O[1_556]	1.34	0.86
2:A:55:ILE:CB	2:B:241:TYR:CG[1_666]	1.35	0.85
2:A:5:SER:CB	2:B:245:LYS:CA[1_666]	1.36	0.84
2:A:9:ASN:CG	2:B:244:ARG:CA[1_666]	1.37	0.83
2:A:9:ASN:ND2	2:B:244:ARG:CA[1_666]	1.38	0.82
2:B:240:ILE:C	4:A:311:HOH:O[1_444]	1.38	0.82
2:B:85:LYS:N	4:A:391:HOH:O[1_554]	1.39	0.81
2:A:208:SER:N	4:B:323:HOH:O[1_556]	1.40	0.80
2:A:8:ILE:C	2:B:243:GLY:CA[1_666]	1.41	0.79
2:A:9:ASN:OD1	2:B:243:GLY:O[1_666]	1.42	0.78
2:A:58:LYS:CD	2:B:238:ASN:CB[1_666]	1.43	0.77
2:A:8:ILE:N	2:B:242:ARG:O[1_666]	1.44	0.76
2:A:9:ASN:ND2	2:B:244:ARG:CG[1_666]	1.44	0.76
2:A:9:ASN:CG	2:B:244:ARG:N[1_666]	1.45	0.75
2:A:241:TYR:CD1	2:B:129:ILE:CG2[1_556]	1.46	0.74
2:A:9:ASN:CB	2:B:244:ARG:N[1_666]	1.48	0.72
2:A:6:ASP:CA	2:B:242:ARG:CB[1_666]	1.49	0.71
2:A:5:SER:CB	2:B:245:LYS:O[1_666]	1.51	0.69
2:A:5:SER:CB	2:B:245:LYS:OXT[1_666]	1.51	0.69
2:B:126:ASP:OD1	4:A:346:HOH:O[1_554]	1.51	0.69
2:B:85:LYS:C	4:A:391:HOH:O[1_554]	1.51	0.69
2:A:6:ASP:N	2:B:242:ARG:CB[1_666]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ASP:OD2	2:B:242:ARG:NH1[1_666]	1.53	0.67
2:A:7:LEU:N	2:B:242:ARG:N[1_666]	1.54	0.66
2:A:9:ASN:N	2:B:243:GLY:N[1_666]	1.54	0.66
2:B:127:GLN:N	4:A:346:HOH:O[1_554]	1.56	0.64
2:A:210:ASP:OD1	2:B:5:SER:OG[1_556]	1.57	0.63
2:A:207:ASP:O	2:B:59:HIS:CE1[1_556]	1.58	0.62
2:A:55:ILE:O	2:B:238:ASN:ND2[1_666]	1.60	0.60
2:A:7:LEU:N	2:B:242:ARG:CB[1_666]	1.61	0.59
2:A:2:SER:O	2:B:242:ARG:CD[1_666]	1.62	0.58
2:B:59:HIS:CA	4:A:304:HOH:O[1_554]	1.63	0.57
2:B:127:GLN:C	4:A:323:HOH:O[1_554]	1.63	0.57
2:A:209:GLU:N	2:B:2:SER:N[1_556]	1.64	0.56
2:A:6:ASP:CG	2:B:239:TRP:CA[1_666]	1.67	0.53
2:A:7:LEU:O	2:B:241:TYR:O[1_666]	1.67	0.53
2:A:7:LEU:CA	2:B:242:ARG:CA[1_666]	1.67	0.53
2:A:210:ASP:OD2	2:B:5:SER:CB[1_556]	1.67	0.53
2:A:8:ILE:N	2:B:242:ARG:C[1_666]	1.68	0.52
2:A:6:ASP:C	2:B:242:ARG:CB[1_666]	1.69	0.51
2:A:6:ASP:OD1	2:B:239:TRP:CB[1_666]	1.70	0.50
2:B:127:GLN:CB	4:A:351:HOH:O[1_554]	1.70	0.50
2:B:239:TRP:O	4:A:352:HOH:O[1_444]	1.70	0.50
2:A:9:ASN:N	2:B:243:GLY:C[1_666]	1.71	0.49
2:A:58:LYS:CG	2:B:238:ASN:CB[1_666]	1.71	0.49
2:B:127:GLN:N	4:A:323:HOH:O[1_554]	1.71	0.49
2:A:9:ASN:CG	2:B:244:ARG:CG[1_666]	1.72	0.48
2:A:7:LEU:CA	2:B:241:TYR:O[1_666]	1.74	0.46
2:A:208:SER:CB	2:B:3:LEU:N[1_556]	1.74	0.46
2:B:239:TRP:C	4:A:352:HOH:O[1_444]	1.74	0.46
2:A:9:ASN:OD1	2:B:243:GLY:C[1_666]	1.75	0.45
2:A:208:SER:OG	2:B:2:SER:C[1_556]	1.75	0.45
2:A:210:ASP:OD1	2:B:2:SER:OG[1_556]	1.75	0.45
2:B:240:ILE:CB	4:A:378:HOH:O[1_444]	1.76	0.44
2:A:7:LEU:N	2:B:242:ARG:C[1_666]	1.78	0.42
2:B:85:LYS:CB	4:A:391:HOH:O[1_554]	1.78	0.42
2:A:6:ASP:O	2:B:241:TYR:C[1_666]	1.79	0.41
2:A:208:SER:CA	2:B:2:SER:CA[1_556]	1.79	0.41
2:A:210:ASP:CB	2:B:2:SER:OG[1_556]	1.79	0.41
2:A:59:HIS:CE1	2:B:242:ARG:NH1[1_666]	1.80	0.40
2:A:6:ASP:C	2:B:242:ARG:C[1_666]	1.81	0.39
2:A:3:LEU:O	2:B:242:ARG:CG[1_666]	1.82	0.38
2:A:7:LEU:C	2:B:241:TYR:O[1_666]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:ASN:OD1	2:B:244:ARG:CB[1_666]	1.82	0.38
2:A:6:ASP:O	2:B:243:GLY:N[1_666]	1.83	0.37
2:A:6:ASP:CB	2:B:242:ARG:CG[1_666]	1.83	0.37
2:A:9:ASN:CA	2:B:243:GLY:CA[1_666]	1.83	0.37
2:A:58:LYS:CE	2:B:235:GLU:O[1_666]	1.83	0.37
2:B:59:HIS:CB	4:A:304:HOH:O[1_554]	1.83	0.37
2:B:79:LYS:CD	4:A:372:HOH:O[1_554]	1.83	0.37
2:A:6:ASP:OD2	2:B:242:ARG:CZ[1_666]	1.86	0.34
2:B:239:TRP:C	4:A:311:HOH:O[1_444]	1.90	0.30
2:A:9:ASN:OD1	2:B:244:ARG:N[1_666]	1.94	0.26
2:A:6:ASP:O	2:B:242:ARG:CA[1_666]	1.95	0.25
2:A:9:ASN:OD1	2:B:244:ARG:CA[1_666]	1.95	0.25
2:A:10:ALA:CA	2:B:240:ILE:O[1_666]	1.95	0.25
2:B:244:ARG:CG	4:A:373:HOH:O[1_444]	1.95	0.25
2:A:10:ALA:CB	2:B:241:TYR:CA[1_666]	1.96	0.24
2:A:59:HIS:NE2	2:B:242:ARG:NH1[1_666]	1.96	0.24
2:A:207:ASP:C	4:B:323:HOH:O[1_556]	1.97	0.23
2:A:5:SER:CA	2:B:245:LYS:C[1_666]	1.98	0.22
2:A:8:ILE:CA	4:B:361:HOH:O[1_666]	1.98	0.22
2:B:240:ILE:CB	4:A:371:HOH:O[1_444]	1.98	0.22
2:A:59:HIS:CD2	2:B:238:ASN:CG[1_666]	1.99	0.21
2:A:208:SER:CB	2:B:2:SER:O[1_556]	1.99	0.21
2:A:208:SER:OG	2:B:2:SER:OG[1_556]	1.99	0.21
2:A:4:ARG:O	2:B:242:ARG:O[1_666]	2.00	0.20
2:A:210:ASP:CG	2:B:2:SER:OG[1_556]	2.00	0.20
2:A:55:ILE:CG1	2:B:241:TYR:CD2[1_666]	2.01	0.19
2:A:6:ASP:CB	2:B:242:ARG:CB[1_666]	2.02	0.18
2:A:7:LEU:O	4:B:342:HOH:O[1_666]	2.02	0.18
2:A:6:ASP:CB	2:B:238:ASN:O[1_666]	2.03	0.17
2:A:7:LEU:C	2:B:242:ARG:C[1_666]	2.03	0.17
2:A:11:LEU:N	4:B:304:HOH:O[1_666]	2.03	0.17
2:A:58:LYS:CE	2:B:235:GLU:CA[1_666]	2.03	0.17
2:B:129:ILE:CD1	4:A:312:HOH:O[1_554]	2.03	0.17
2:A:8:ILE:N	4:B:361:HOH:O[1_666]	2.04	0.16
2:A:9:ASN:CG	2:B:243:GLY:C[1_666]	2.04	0.16
2:A:207:ASP:OD1	2:B:79:LYS:NZ[1_556]	2.04	0.16
2:A:7:LEU:O	4:B:304:HOH:O[1_666]	2.05	0.15
2:A:9:ASN:CA	2:B:243:GLY:C[1_666]	2.05	0.15
2:A:58:LYS:NZ	2:B:235:GLU:C[1_666]	2.05	0.15
2:B:240:ILE:CG2	4:A:378:HOH:O[1_444]	2.05	0.15
2:A:5:SER:CB	2:B:245:LYS:CB[1_666]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:8:ILE:CG1	4:B:361:HOH:O[1_666]	2.06	0.14
2:A:55:ILE:CD1	2:B:241:TYR:CA[1_666]	2.06	0.14
2:A:210:ASP:CG	2:B:5:SER:OG[1_556]	2.07	0.13
2:B:61:TYR:CZ	4:A:372:HOH:O[1_554]	2.07	0.13
2:A:6:ASP:CG	2:B:242:ARG:CZ[1_666]	2.08	0.12
2:A:9:ASN:CB	2:B:243:GLY:C[1_666]	2.08	0.12
2:B:241:TYR:N	4:A:311:HOH:O[1_444]	2.08	0.12
2:B:127:GLN:CD	4:A:351:HOH:O[1_554]	2.08	0.12
2:B:244:ARG:NH1	4:A:373:HOH:O[1_444]	2.08	0.12
2:B:126:ASP:O	4:A:323:HOH:O[1_554]	2.09	0.11
2:A:55:ILE:CG1	2:B:241:TYR:CD1[1_666]	2.10	0.10
2:A:58:LYS:CB	2:B:238:ASN:ND2[1_666]	2.10	0.10
2:A:58:LYS:CE	2:B:235:GLU:C[1_666]	2.10	0.10
2:A:208:SER:CB	2:B:2:SER:N[1_556]	2.10	0.10
2:A:208:SER:C	2:B:2:SER:CA[1_556]	2.10	0.10
2:A:5:SER:O	2:B:244:ARG:N[1_666]	2.11	0.09
2:A:51:ILE:O	2:B:241:TYR:CD1[1_666]	2.11	0.09
2:B:239:TRP:CD2	4:A:352:HOH:O[1_444]	2.11	0.09
2:B:79:LYS:CG	4:A:372:HOH:O[1_554]	2.11	0.09
2:A:5:SER:CA	2:B:245:LYS:OXT[1_666]	2.12	0.08
2:A:5:SER:O	2:B:243:GLY:C[1_666]	2.12	0.08
2:A:6:ASP:CG	2:B:239:TRP:N[1_666]	2.12	0.08
2:A:7:LEU:CA	2:B:242:ARG:N[1_666]	2.12	0.08
2:A:9:ASN:CB	2:B:244:ARG:CG[1_666]	2.12	0.08
2:A:55:ILE:CG1	2:B:241:TYR:CA[1_666]	2.12	0.08
2:A:7:LEU:CA	2:B:241:TYR:C[1_666]	2.13	0.07
2:A:8:ILE:CA	2:B:243:GLY:CA[1_666]	2.13	0.07
2:A:207:ASP:C	2:B:59:HIS:ND1[1_556]	2.13	0.07
2:A:208:SER:C	2:B:2:SER:N[1_556]	2.13	0.07
2:B:126:ASP:C	4:A:346:HOH:O[1_554]	2.13	0.07
2:A:6:ASP:O	2:B:242:ARG:C[1_666]	2.14	0.06
2:A:55:ILE:CB	2:B:241:TYR:CB[1_666]	2.14	0.06
2:A:8:ILE:N	2:B:243:GLY:N[1_666]	2.15	0.05
2:A:55:ILE:CB	2:B:241:TYR:CE2[1_666]	2.16	0.04
2:B:126:ASP:C	4:A:323:HOH:O[1_554]	2.16	0.04
2:A:6:ASP:CA	2:B:242:ARG:CA[1_666]	2.17	0.03
2:A:210:ASP:CG	2:B:5:SER:CB[1_556]	2.17	0.03
2:B:240:ILE:CB	4:A:311:HOH:O[1_444]	2.17	0.03
2:A:2:SER:O	2:B:242:ARG:CZ[1_666]	2.18	0.02
2:A:5:SER:O	2:B:242:ARG:C[1_666]	2.18	0.02
2:A:207:ASP:N	4:B:323:HOH:O[1_556]	2.19	0.01

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	
2	A	233/244 (96%)	224 (96%)	8 (3%)	1 (0%)	30	27
2	B	219/244 (90%)	213 (97%)	5 (2%)	1 (0%)	24	21
All	All	452/488 (93%)	437 (97%)	13 (3%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	117	ASN
2	B	117	ASN

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	
2	A	179/220 (81%)	173 (97%)	6 (3%)	32	33
2	B	176/220 (80%)	171 (97%)	5 (3%)	38	41
All	All	355/440 (81%)	344 (97%)	11 (3%)	35	37

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	58	LYS
2	A	82	GLU
2	A	96	THR
2	A	129	ILE

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Mol	Chain	Res	Type
2	A	188	ASN
2	A	210	ASP
2	B	41	SER
2	B	43	ILE
2	B	81	SER
2	B	96	THR
2	B	124	PRO

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

Mol	Chain	Res	Type
2	A	15	ASN
2	B	71	HIS
2	B	116	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.