



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:47 pm BST

PDB ID : 1RVE
Title : THE CRYSTAL STRUCTURE OF ECORV ENDONUCLEASE AND OF ITS COMPLEXES WITH COGNATE AND NON-COGNATE DNA FRAGMENTS
Authors : Winkler, F.K.
Deposited on : 1992-02-24
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

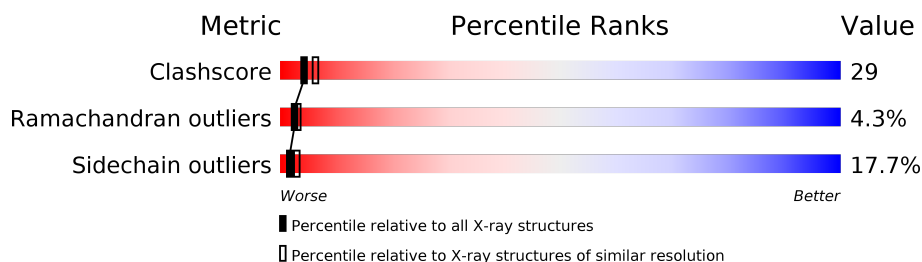
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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	245	
1	B	245	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4095 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 ENDONUCLEASE EcoR V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	195	0	0
			2023	1300	341	381	1			
1	B	244	Total	C	N	O	S	208	0	0
			2023	1300	341	381	1			

- Molecule 2 is water.

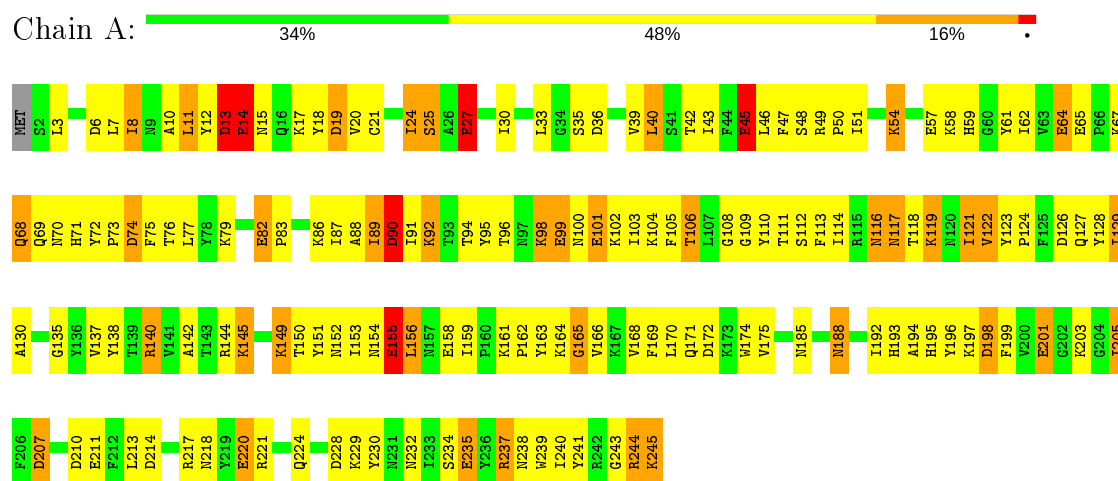
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	30	Total	O	0	0
			30	30		

3 Residue-property plots

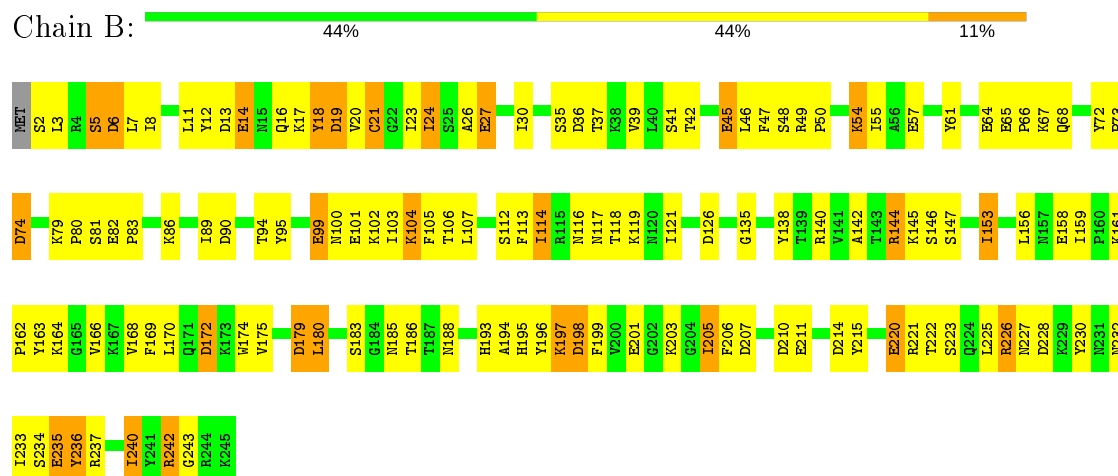
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: ENDONUCLEASE EcoR V



• Molecule 1: ENDONUCLEASE EcoR V



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.20 Å 71.70 Å 130.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4095	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	1.09	15/2074 (0.7%)	1.31	24/2804 (0.9%)
1	B	1.12	15/2074 (0.7%)	1.29	25/2804 (0.9%)
All	All	1.11	30/4148 (0.7%)	1.30	49/5608 (0.9%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CD-OE2	7.20	1.33	1.25
1	A	64	GLU	CD-OE2	6.92	1.33	1.25
1	A	158	GLU	CD-OE2	6.72	1.33	1.25
1	A	99	GLU	CD-OE1	6.65	1.32	1.25
1	B	64	GLU	CD-OE1	6.32	1.32	1.25
1	B	82	GLU	CD-OE2	6.32	1.32	1.25
1	A	220	GLU	CD-OE2	6.24	1.32	1.25
1	B	158	GLU	CD-OE1	6.03	1.32	1.25
1	A	27	GLU	CD-OE2	6.02	1.32	1.25
1	B	45	GLU	CD-OE1	5.96	1.32	1.25
1	B	211	GLU	CD-OE1	5.86	1.32	1.25
1	A	155	GLU	CD-OE2	5.83	1.32	1.25
1	B	201	GLU	CD-OE2	5.68	1.31	1.25
1	B	27	GLU	CD-OE1	5.57	1.31	1.25
1	B	235	GLU	CD-OE2	5.54	1.31	1.25
1	B	101	GLU	CD-OE1	5.51	1.31	1.25
1	B	99	GLU	CD-OE2	5.42	1.31	1.25
1	A	65	GLU	CD-OE2	5.35	1.31	1.25
1	A	211	GLU	CD-OE2	5.27	1.31	1.25
1	A	57	GLU	CD-OE2	5.26	1.31	1.25
1	B	14	GLU	CD-OE2	5.26	1.31	1.25
1	A	101	GLU	CD-OE2	5.23	1.31	1.25
1	A	45	GLU	CD-OE2	5.22	1.31	1.25
1	A	235	GLU	CD-OE2	5.22	1.31	1.25
1	A	235	GLU	CG-CD	-5.20	1.44	1.51
1	B	65	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	GLU	CD-OE2	5.10	1.31	1.25
1	A	14	GLU	CD-OE2	5.07	1.31	1.25
1	A	82	GLU	CD-OE2	5.04	1.31	1.25
1	B	61	TYR	CA-C	-5.01	1.40	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	A	198	ASP	CB-CG-OD2	8.48	125.94	118.30
1	A	244	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	B	90	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	172	ASP	CB-CG-OD1	-7.60	111.46	118.30
1	A	74	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	207	ASP	CB-CG-OD1	-7.24	111.78	118.30
1	B	198	ASP	CB-CG-OD1	7.18	124.77	118.30
1	A	126	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	74	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	172	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	126	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	19	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	198	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	242	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	210	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	B	172	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	36	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	210	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	13	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	228	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	90	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	B	228	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	13	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	6	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	172	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	126	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	B	19	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	207	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	B	179	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	A	19	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	6	ASP	CB-CG-OD1	-5.88	113.00	118.30
1	A	210	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	90	ASP	CB-CG-OD1	5.84	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	74	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	228	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	74	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	207	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	19	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	228	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	244	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	13	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	13	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	36	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	6	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	207	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	126	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	122	VAL	CB-CA-C	5.02	120.94	111.40

There are no chirality outliers.

There are no planarity outliers.

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	2023	0	1987	142	0
1	B	2023	0	1987	79	1
2	A	19	0	0	1	0
2	B	30	0	0	2	0
All	All	4095	0	3974	212	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 29.

All (212) 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:117:ASN:HD21	1:A:124:PRO:HB3	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HG2	1:A:229:LYS:HE3	1.50	0.93
1:A:117:ASN:ND2	1:A:124:PRO:HB3	1.90	0.86
1:A:24:ILE:HD12	1:A:30:ILE:HG12	1.57	0.84
1:B:21:CYS:HB3	1:B:161:LYS:CE	2.08	0.84
1:A:67:LYS:HG2	1:A:68:GLN:HE21	1.42	0.83
1:B:21:CYS:HB3	1:B:161:LYS:HE3	1.60	0.83
1:A:67:LYS:HG3	1:A:68:GLN:HG3	1.60	0.82
1:A:218:ASN:HD21	1:A:244:ARG:HH22	1.28	0.82
1:B:162:PRO:HG2	1:B:163:TYR:HD2	1.45	0.82
1:A:67:LYS:HG3	1:A:68:GLN:N	1.97	0.80
1:B:162:PRO:HG2	1:B:163:TYR:CD2	2.18	0.79
1:A:108:GLY:O	1:A:188:ASN:HB2	1.82	0.78
1:A:213:LEU:O	1:A:217:ARG:HG3	1.85	0.77
1:B:21:CYS:HB3	1:B:161:LYS:NZ	1.99	0.77
1:B:95:TYR:HB3	1:B:138:TYR:CZ	2.18	0.77
1:A:72:TYR:CE1	1:A:73:PRO:HB3	2.20	0.76
1:B:179:ASP:O	1:B:180:LEU:HD23	1.87	0.74
1:A:72:TYR:CD1	1:A:73:PRO:HB3	2.22	0.74
1:A:19:ASP:OD2	1:B:26:ALA:HB3	1.88	0.74
1:A:201:GLU:HB3	1:A:203:LYS:HE3	1.70	0.73
1:A:94:THR:HG22	1:A:105:PHE:CE1	2.23	0.72
1:A:67:LYS:CE	1:A:68:GLN:HG3	2.20	0.71
1:A:104:LYS:HB3	1:A:193:HIS:CD2	2.26	0.71
1:A:152:ASN:H	1:A:155:GLU:HG3	1.57	0.70
1:A:108:GLY:C	1:A:188:ASN:HB2	2.13	0.69
1:A:201:GLU:HG2	1:A:203:LYS:HE2	1.73	0.69
1:A:39:VAL:HG22	1:B:42:THR:HG22	1.74	0.69
1:B:94:THR:HG22	1:B:105:PHE:CE2	2.27	0.69
1:A:152:ASN:OD1	1:A:154:ASN:N	2.26	0.69
1:A:68:GLN:OE1	1:A:71:HIS:ND1	2.26	0.68
1:B:116:ASN:O	1:B:118:THR:N	2.27	0.67
1:A:201:GLU:CB	1:A:203:LYS:HE3	2.24	0.66
1:A:198:ASP:CG	1:A:203:LYS:HZ2	1.98	0.66
1:A:92:LYS:HE3	1:A:106:THR:O	1.96	0.66
1:A:67:LYS:NZ	1:A:68:GLN:HG3	2.11	0.65
1:A:3:LEU:HD22	1:A:61:TYR:CE2	2.31	0.65
1:A:232:ASN:OD1	1:A:234:SER:N	2.30	0.65
1:A:73:PRO:HG3	1:A:88:ALA:HB1	1.78	0.65
1:A:39:VAL:HG22	1:B:42:THR:CG2	2.27	0.65
1:A:195:HIS:HD2	1:A:197:LYS:H	1.45	0.64
1:B:35:SER:HA	1:B:162:PRO:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:CYS:CB	1:B:161:LYS:HE3	2.27	0.64
1:A:197:LYS:HD3	1:A:201:GLU:OE2	1.98	0.64
1:A:58:LYS:HD3	1:A:59:HIS:CE1	2.31	0.64
1:A:74:ASP:HB2	1:A:90:ASP:HA	1.80	0.64
1:B:179:ASP:C	1:B:180:LEU:HD23	2.18	0.63
1:A:104:LYS:HB3	1:A:193:HIS:HD2	1.64	0.63
1:A:201:GLU:HG2	1:A:203:LYS:CE	2.28	0.62
1:A:135:GLY:O	1:A:168:VAL:HA	1.99	0.62
1:A:67:LYS:HG2	1:A:68:GLN:NE2	2.14	0.61
1:A:86:LYS:O	1:A:129:ILE:HG13	2.00	0.61
1:A:149:LYS:HD3	1:A:151:TYR:CZ	2.35	0.60
1:A:67:LYS:CG	1:A:68:GLN:HE21	2.14	0.60
1:A:135:GLY:O	1:A:168:VAL:HG23	2.02	0.60
1:A:67:LYS:HE3	1:A:68:GLN:HG3	1.83	0.60
1:B:72:TYR:O	1:B:121:ILE:HG13	2.02	0.59
1:A:151:TYR:HB3	1:A:155:GLU:HB2	1.83	0.59
1:B:24:ILE:HG13	1:B:30:ILE:HG12	1.84	0.59
1:B:237:ARG:O	1:B:240:ILE:HG12	2.02	0.59
1:A:195:HIS:CD2	1:A:197:LYS:H	2.21	0.59
1:B:195:HIS:N	2:B:256:HOH:O	2.30	0.58
1:B:174:TRP:CE2	1:B:175:VAL:HG23	2.40	0.57
1:A:94:THR:HG22	1:A:105:PHE:CZ	2.38	0.57
1:A:109:GLY:HA2	1:A:188:ASN:HB3	1.87	0.57
1:B:206:PHE:CE1	1:B:233:ILE:HD13	2.39	0.57
1:B:41:SER:O	1:B:45:GLU:HG3	2.05	0.57
1:B:230:TYR:CD1	1:B:236:TYR:HB2	2.39	0.56
1:A:169:PHE:CZ	1:A:199:PHE:CD2	2.93	0.56
1:A:218:ASN:ND2	1:A:244:ARG:HH22	1.99	0.56
1:A:96:THR:CG2	1:A:103:ILE:HG22	2.35	0.56
1:A:214:ASP:OD2	1:A:244:ARG:NH1	2.38	0.56
1:A:72:TYR:HD2	1:A:121:ILE:HD12	1.69	0.56
1:B:47:PHE:O	1:B:50:PRO:HD2	2.06	0.56
1:A:121:ILE:HG13	1:A:122:VAL:N	2.20	0.56
1:A:116:ASN:HB2	1:A:119:LYS:HB2	1.88	0.55
1:A:47:PHE:O	1:A:50:PRO:HD2	2.07	0.55
1:B:135:GLY:O	1:B:168:VAL:HA	2.06	0.55
1:A:99:GLU:O	1:A:100:ASN:HB2	2.07	0.54
1:B:170:LEU:HD23	1:B:170:LEU:C	2.27	0.54
1:A:7:LEU:O	1:A:10:ALA:HB3	2.08	0.54
1:B:94:THR:HG22	1:B:105:PHE:CZ	2.43	0.54
1:A:39:VAL:HA	1:B:42:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:NZ	2:A:261:HOH:O	2.38	0.53
1:B:196:TYR:O	1:B:199:PHE:HB2	2.08	0.53
1:B:232:ASN:OD1	1:B:235:GLU:HG3	2.08	0.53
1:B:116:ASN:OD1	1:B:119:LYS:HB2	2.07	0.53
1:B:168:VAL:HG22	1:B:169:PHE:N	2.23	0.53
1:A:95:TYR:CD1	1:A:140:ARG:HG3	2.44	0.53
1:A:198:ASP:OD1	1:A:203:LYS:NZ	2.27	0.52
1:B:162:PRO:CD	1:B:163:TYR:H	2.23	0.52
1:A:112:SER:OG	1:A:113:PHE:N	2.43	0.52
1:A:121:ILE:HG12	1:A:123:TYR:O	2.09	0.52
1:A:239:TRP:CZ3	1:A:244:ARG:NH1	2.78	0.52
1:A:153:ILE:HD13	1:B:153:ILE:HD13	1.92	0.52
1:B:243:GLY:N	2:B:273:HOH:O	2.43	0.52
1:B:102:LYS:NZ	1:B:102:LYS:HB2	2.25	0.51
1:A:42:THR:CG2	1:B:39:VAL:HG22	2.40	0.51
1:B:8:ILE:O	1:B:8:ILE:HG13	2.10	0.51
1:A:73:PRO:HG3	1:A:88:ALA:CB	2.39	0.51
1:A:239:TRP:HZ3	1:A:244:ARG:NH1	2.09	0.51
1:A:117:ASN:HD22	1:A:118:THR:HG23	1.76	0.51
1:A:218:ASN:HD21	1:A:244:ARG:NH2	2.05	0.51
1:B:80:PRO:O	1:B:83:PRO:HD3	2.10	0.51
1:A:46:LEU:C	1:A:46:LEU:HD23	2.31	0.51
1:A:67:LYS:CG	1:A:68:GLN:HG3	2.36	0.51
1:B:113:PHE:CD1	1:B:114:ILE:N	2.79	0.51
1:A:124:PRO:HD2	1:A:127:GLN:NE2	2.26	0.50
1:B:153:ILE:HG13	1:B:153:ILE:O	2.11	0.50
1:B:156:LEU:HA	1:B:159:ILE:HD12	1.93	0.50
1:A:87:ILE:HG23	1:A:130:ALA:HB3	1.94	0.50
1:B:7:LEU:O	1:B:11:LEU:HG	2.11	0.50
1:A:201:GLU:OE1	1:A:201:GLU:HA	2.12	0.49
1:B:179:ASP:HB2	1:B:215:TYR:OH	2.11	0.49
1:B:196:TYR:CD2	1:B:197:LYS:HE2	2.47	0.49
1:A:42:THR:HG23	1:B:39:VAL:HG22	1.94	0.49
1:A:110:TYR:CD1	1:A:111:THR:HG23	2.47	0.49
1:A:40:LEU:HD11	1:A:163:TYR:CG	2.48	0.49
1:A:117:ASN:HD21	1:A:124:PRO:CB	2.10	0.49
1:A:67:LYS:HE3	1:A:68:GLN:CG	2.42	0.48
1:A:75:PHE:HE1	1:A:91:ILE:CD1	2.25	0.48
1:A:163:TYR:N	1:A:163:TYR:CD1	2.79	0.48
1:A:27:GLU:H	1:A:27:GLU:CD	2.17	0.48
1:A:43:ILE:HG12	1:B:23:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PRO:HB2	1:B:68:GLN:O	2.14	0.48
1:A:7:LEU:HD23	1:A:170:LEU:HD11	1.96	0.48
1:A:62:ILE:O	1:A:77:LEU:HA	2.14	0.48
1:A:72:TYR:CZ	1:A:73:PRO:HB3	2.47	0.48
1:B:23:ILE:O	1:B:30:ILE:HA	2.14	0.48
1:A:40:LEU:HD12	1:A:138:TYR:CE2	2.50	0.47
1:A:46:LEU:O	1:A:46:LEU:HD23	2.14	0.47
1:B:72:TYR:HD2	1:B:121:ILE:CD1	2.28	0.47
1:A:164:LYS:HG2	1:A:165:GLY:H	1.80	0.47
1:B:104:LYS:HB3	1:B:193:HIS:HD2	1.79	0.46
1:B:35:SER:HB2	1:B:140:ARG:HG3	1.95	0.46
1:A:83:PRO:O	1:A:86:LYS:NZ	2.46	0.46
1:B:2:SER:OG	1:B:5:SER:OG	2.29	0.46
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.64	0.46
1:B:95:TYR:CZ	1:B:140:ARG:NH1	2.84	0.46
1:B:163:TYR:CE1	1:B:166:VAL:CG2	2.99	0.45
1:A:24:ILE:HG13	1:A:25:SER:N	2.32	0.45
1:B:8:ILE:HG13	1:B:12:TYR:CE2	2.51	0.45
1:A:72:TYR:CG	1:A:73:PRO:HB3	2.52	0.45
1:B:194:ALA:HB1	1:B:198:ASP:OD2	2.17	0.45
1:A:192:ILE:HG22	1:A:205:ILE:HD12	1.98	0.44
1:A:54:LYS:HE3	1:A:54:LYS:HB2	1.59	0.44
1:A:124:PRO:HG2	1:A:127:GLN:NE2	2.32	0.44
1:A:218:ASN:HB2	1:A:230:TYR:OH	2.18	0.44
1:A:49:ARG:N	1:A:50:PRO:CD	2.79	0.44
1:A:8:ILE:HG23	1:A:12:TYR:CE2	2.52	0.44
1:A:95:TYR:CD1	1:A:95:TYR:C	2.91	0.44
1:A:140:ARG:HE	1:A:140:ARG:HB3	1.31	0.44
1:A:35:SER:O	1:A:36:ASP:HB3	2.18	0.44
1:A:74:ASP:HB2	1:A:89:ILE:O	2.17	0.44
1:A:20:VAL:HG12	1:A:21:CYS:N	2.32	0.43
1:A:238:ASN:O	1:A:241:TYR:N	2.51	0.43
1:B:67:LYS:HE3	1:B:67:LYS:HB2	1.88	0.43
1:A:75:PHE:CE1	1:A:91:ILE:CD1	3.00	0.43
1:B:104:LYS:HB3	1:B:193:HIS:CD2	2.53	0.43
1:B:74:ASP:HB2	1:B:89:ILE:O	2.18	0.43
1:A:11:LEU:HG	1:A:11:LEU:H	1.65	0.43
1:A:45:GLU:O	1:A:48:SER:HB2	2.18	0.43
1:A:98:LYS:HB2	1:A:101:GLU:OE2	2.18	0.43
1:B:162:PRO:HD2	1:B:163:TYR:H	1.82	0.43
1:A:244:ARG:O	1:A:245:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HG3	1:A:68:GLN:H	1.78	0.42
1:A:94:THR:CG2	1:A:105:PHE:CE1	2.99	0.42
1:A:10:ALA:HB1	1:A:51:ILE:CG2	2.49	0.42
1:A:25:SER:HA	1:B:20:VAL:HA	2.02	0.42
1:A:100:ASN:HA	1:A:100:ASN:HD22	1.62	0.42
1:A:20:VAL:CG2	1:A:47:PHE:CZ	3.02	0.42
1:A:237:ARG:O	1:A:240:ILE:HB	2.20	0.42
1:A:243:GLY:O	1:A:245:LYS:HE2	2.19	0.42
1:B:21:CYS:CA	1:B:161:LYS:HE3	2.50	0.42
1:B:164:LYS:HG3	1:B:164:LYS:O	2.18	0.42
1:B:205:ILE:HG12	1:B:206:PHE:N	2.34	0.42
1:A:121:ILE:CG1	1:A:122:VAL:N	2.82	0.42
1:A:197:LYS:HB3	1:A:197:LYS:HE2	1.80	0.42
1:A:72:TYR:HA	1:A:73:PRO:HA	1.68	0.42
1:B:21:CYS:CB	1:B:161:LYS:NZ	2.77	0.42
1:A:18:TYR:HD2	1:A:47:PHE:CD2	2.38	0.42
1:A:137:VAL:O	1:A:166:VAL:HA	2.20	0.42
1:B:72:TYR:HA	1:B:73:PRO:HA	1.70	0.42
1:A:119:LYS:C	1:A:119:LYS:HD2	2.39	0.41
1:B:163:TYR:CE1	1:B:166:VAL:HG23	2.54	0.41
1:B:102:LYS:CB	1:B:102:LYS:NZ	2.84	0.41
1:B:11:LEU:HA	1:B:11:LEU:HD23	1.85	0.41
1:B:156:LEU:HA	1:B:159:ILE:CD1	2.49	0.41
1:B:54:LYS:HB2	1:B:54:LYS:HE2	1.69	0.41
1:A:102:LYS:HD2	1:A:194:ALA:HA	2.01	0.41
1:A:98:LYS:H	1:A:101:GLU:CD	2.24	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.80	0.41
1:B:162:PRO:CD	1:B:163:TYR:N	2.84	0.41
1:B:99:GLU:O	1:B:100:ASN:HB2	2.20	0.41
1:A:151:TYR:N	1:A:151:TYR:CD1	2.88	0.41
1:A:171:GLN:OE1	1:A:171:GLN:HA	2.21	0.41
1:A:67:LYS:HG3	1:A:68:GLN:CG	2.42	0.41
1:A:174:TRP:CE2	1:A:175:VAL:HG23	2.55	0.41
1:B:214:ASP:OD2	1:B:236:TYR:HE2	2.04	0.41
1:A:124:PRO:HD2	1:A:127:GLN:HE22	1.86	0.41
1:B:106:THR:O	1:B:107:LEU:HD23	2.21	0.41
1:B:95:TYR:HB3	1:B:138:TYR:CE1	2.53	0.41
1:A:33:LEU:HD22	1:A:39:VAL:HG11	2.02	0.41
1:A:49:ARG:N	1:A:50:PRO:HD3	2.35	0.40
1:A:67:LYS:NZ	1:A:68:GLN:CG	2.83	0.40
1:B:103:ILE:O	1:B:193:HIS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:ND2	1:A:244:ARG:NH2	2.67	0.40
1:A:121:ILE:HD11	1:A:128:TYR:CE2	2.56	0.40
1:A:155:GLU:O	1:A:159:ILE:HG13	2.21	0.40
1:A:64:GLU:N	1:A:76:THR:O	2.46	0.40
1:A:161:LYS:HA	1:A:162:PRO:HD3	1.93	0.40
1:B:6:ASP:HB3	1:B:55:ILE:HD12	2.03	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)
1:B:172:ASP:OD1	1:B:242:ARG:NH2[4_445]	2.18	0.02

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	242/245 (99%)	208 (86%)	25 (10%)	9 (4%)		
1	B	242/245 (99%)	213 (88%)	17 (7%)	12 (5%)		
All	All	484/490 (99%)	421 (87%)	42 (9%)	21 (4%)		

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	14	GLU
1	A	17	LYS
1	A	185	ASN
1	B	18	TYR
1	B	19	ASP
1	B	117	ASN

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Mol	Chain	Res	Type
1	B	142	ALA
1	B	144	ARG
1	B	147	SER
1	B	183	SER
1	B	186	THR
1	B	226	ARG
1	B	227	ASN
1	A	117	ASN
1	A	165	GLY
1	B	225	LEU
1	A	142	ALA
1	A	145	LYS
1	A	196	TYR
1	B	49	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	220/221 (100%)	179 (81%)	41 (19%)	1	2
1	B	220/221 (100%)	183 (83%)	37 (17%)	2	4
All	All	440/442 (100%)	362 (82%)	78 (18%)	2	3

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	11	LEU
1	A	13	ASP
1	A	14	GLU
1	A	15	ASN
1	A	24	ILE
1	A	25	SER
1	A	27	GLU
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	45	GLU
1	A	54	LYS
1	A	68	GLN
1	A	69	GLN
1	A	70	ASN
1	A	82	GLU
1	A	89	ILE
1	A	90	ASP
1	A	92	LYS
1	A	98	LYS
1	A	106	THR
1	A	114	ILE
1	A	116	ASN
1	A	119	LYS
1	A	121	ILE
1	A	129	ILE
1	A	140	ARG
1	A	144	ARG
1	A	145	LYS
1	A	149	LYS
1	A	150	THR
1	A	155	GLU
1	A	156	LEU
1	A	188	ASN
1	A	201	GLU
1	A	205	ILE
1	A	207	ASP
1	A	221	ARG
1	A	224	GLN
1	A	235	GLU
1	A	237	ARG
1	A	245	LYS
1	B	3	LEU
1	B	5	SER
1	B	14	GLU
1	B	16	GLN
1	B	17	LYS
1	B	18	TYR
1	B	21	CYS
1	B	24	ILE
1	B	27	GLU
1	B	37	THR

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Mol	Chain	Res	Type
1	B	46	LEU
1	B	48	SER
1	B	54	LYS
1	B	79	LYS
1	B	81	SER
1	B	86	LYS
1	B	104	LYS
1	B	112	SER
1	B	114	ILE
1	B	144	ARG
1	B	145	LYS
1	B	146	SER
1	B	153	ILE
1	B	180	LEU
1	B	185	ASN
1	B	188	ASN
1	B	197	LYS
1	B	203	LYS
1	B	205	ILE
1	B	220	GLU
1	B	221	ARG
1	B	222	THR
1	B	223	SER
1	B	226	ARG
1	B	234	SER
1	B	236	TYR
1	B	240	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	69	GLN
1	A	100	ASN
1	A	120	ASN
1	A	188	ASN
1	A	193	HIS
1	A	195	HIS
1	A	218	ASN
1	A	238	ASN
1	B	9	ASN
1	B	53	ASN

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Mol	Chain	Res	Type
1	B	71	HIS
1	B	117	ASN
1	B	193	HIS

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 carbohydrates 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.