



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:55 AM UTC

PDB ID : 1RVE / pdb_00001rve
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 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

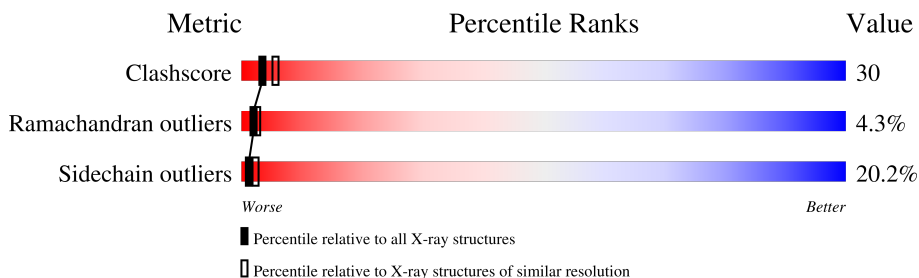
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

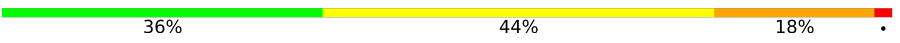
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 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	245	 36% 44% 18% •
1	B	245	 46% 40% 14%

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.

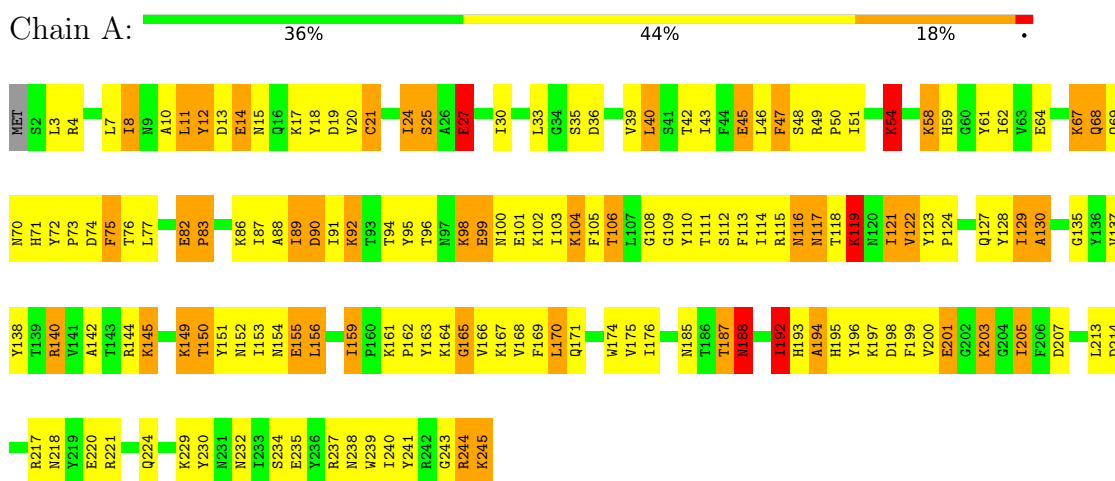
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	30	Total	O	0	0
			30	30		

3 Residue-property plots

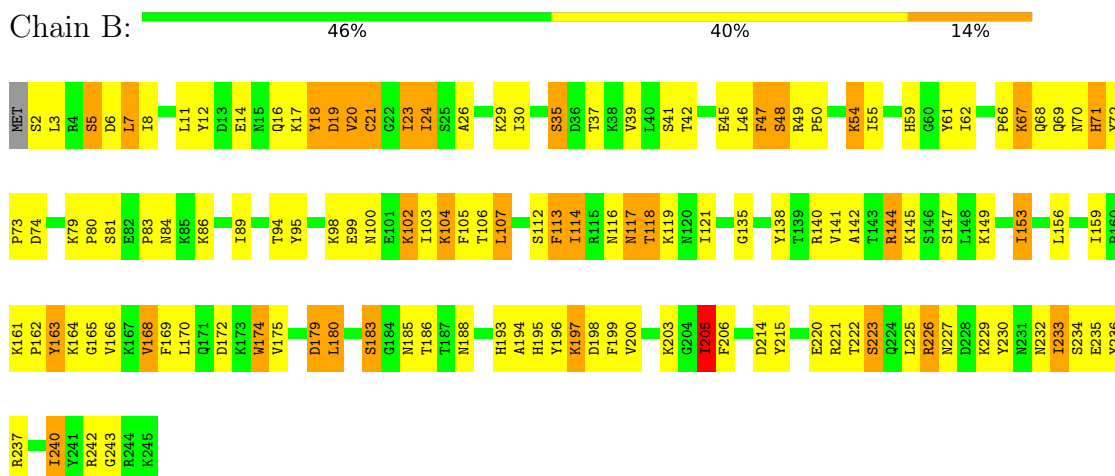
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 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	58.20Å 71.70Å 130.60Å 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	1.34	7/2074 (0.3%)	1.55	24/2804 (0.9%)
1	B	1.43	10/2074 (0.5%)	1.55	21/2804 (0.7%)
All	All	1.39	17/4148 (0.4%)	1.55	45/5608 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	TYR	CA-C	-10.89	1.40	1.52
1	B	7	LEU	C-N	-7.05	1.26	1.34
1	A	21	CYS	CA-C	-7.03	1.45	1.52
1	B	205	ILE	CA-CB	-6.71	1.46	1.54
1	B	200	VAL	N-CA	-6.28	1.39	1.46
1	B	47	PHE	N-CA	-6.20	1.39	1.46
1	B	168	VAL	CA-C	-5.97	1.45	1.52
1	B	174	TRP	C-N	-5.81	1.26	1.33
1	B	35	SER	C-N	5.62	1.41	1.33
1	B	21	CYS	CA-C	-5.59	1.45	1.52
1	A	58	LYS	CA-C	-5.52	1.45	1.52
1	B	118	THR	CA-C	-5.52	1.45	1.52
1	A	150	THR	N-CA	-5.41	1.39	1.45
1	A	75	PHE	CA-C	-5.25	1.46	1.52
1	A	244	ARG	CA-C	-5.21	1.45	1.53
1	A	99	GLU	CA-C	5.20	1.59	1.52
1	A	200	VAL	N-CA	-5.16	1.39	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LYS	N-CA-C	-9.03	104.33	114.62
1	B	205	ILE	CB-CA-C	-8.72	102.11	110.65
1	A	122	VAL	N-CA-C	8.48	118.56	110.42
1	A	119	LYS	N-CA-C	8.09	121.43	108.41
1	A	188	ASN	N-CA-C	7.99	121.92	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ALA	N-CA-C	7.43	118.05	108.24
1	A	187	THR	N-CA-C	-7.13	104.45	113.72
1	A	159	ILE	N-CA-C	7.05	114.69	108.63
1	A	122	VAL	CB-CA-C	7.01	120.94	111.97
1	B	84	ASN	CA-CB-CG	-6.78	105.82	112.60
1	A	140	ARG	CA-C-N	-6.42	114.11	123.10
1	A	140	ARG	C-N-CA	-6.42	114.11	123.10
1	A	192	ILE	N-CA-C	-6.36	103.02	110.21
1	A	12	TYR	N-CA-C	6.17	118.86	110.35
1	B	48	SER	N-CA-C	5.92	118.22	111.11
1	B	233	ILE	N-CA-C	5.92	116.10	110.42
1	A	192	ILE	CB-CA-C	-5.90	104.84	111.45
1	B	69	GLN	N-CA-C	5.87	119.63	112.23
1	B	59	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	47	PHE	CA-C-N	5.72	127.87	120.44
1	A	47	PHE	C-N-CA	5.72	127.87	120.44
1	B	7	LEU	CA-C-N	-5.68	111.21	120.64
1	B	7	LEU	C-N-CA	-5.68	111.21	120.64
1	B	47	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	113	PHE	CA-CB-CG	-5.57	108.23	113.80
1	A	4	ARG	N-CA-C	5.50	116.96	110.97
1	A	27	GLU	N-CA-C	-5.49	106.08	112.89
1	B	84	ASN	N-CA-C	5.44	119.61	112.92
1	B	163	TYR	N-CA-C	5.44	117.34	109.07
1	B	223	SER	N-CA-C	-5.42	105.92	112.54
1	A	130	ALA	N-CA-C	5.42	118.29	109.24
1	A	82	GLU	N-CA-C	5.32	118.30	108.94
1	A	83	PRO	CA-C-N	-5.27	113.14	122.26
1	A	83	PRO	C-N-CA	-5.27	113.14	122.26
1	B	67	LYS	CA-C-N	5.18	130.37	122.65
1	B	67	LYS	C-N-CA	5.18	130.37	122.65
1	A	54	LYS	CB-CA-C	5.08	118.13	109.24
1	B	149	LYS	CA-C-N	-5.07	114.59	122.09
1	B	149	LYS	C-N-CA	-5.07	114.59	122.09
1	A	12	TYR	CA-C-N	5.04	131.17	121.54
1	A	12	TYR	C-N-CA	5.04	131.17	121.54
1	B	71	HIS	N-CA-C	5.04	117.78	109.72
1	B	179	ASP	CA-CB-CG	-5.04	107.56	112.60
1	B	19	ASP	CA-C-N	5.03	127.90	120.91
1	B	19	ASP	C-N-CA	5.03	127.90	120.91

There are no chirality outliers.

There are no planarity outliers.

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	2023	0	1987	143	0
1	B	2023	0	1987	82	1
2	A	19	0	0	0	0
2	B	30	0	0	2	0
All	All	4095	0	3974	216	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 30.

All (216) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:C	1:A:188:ASN:HB2	2.13	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:198:ASP:CG	1:A:203:LYS:HZ2	1.99	0.70
1:A:39:VAL:HG22	1:B:42:THR:HG22	1.74	0.69
1:A:201:GLU:HG2	1:A:203:LYS:HE2	1.73	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:179:ASP:C	1:B:180:LEU:HD23	2.18	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: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:73:PRO:HG3	1:A:88:ALA:HB1	1.78	0.65
1:A:232:ASN:OD1	1:A:234:SER:N	2.30	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
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: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:170:LEU:C	1:B:170:LEU:HD23	2.27	0.59
1:B:237:ARG:O	1:B:240:ILE:HG12	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:THR:CG2	1:A:103:ILE:HG22	2.35	0.56
1:A:218:ASN:ND2	1:A:244:ARG:HH22	1.99	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:46:LEU:C	1:A:46:LEU:HD23	2.31	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:7:LEU:O	1:A:10:ALA:HB3	2.08	0.54
1:A:99:GLU:O	1:A:100:ASN:HB2	2.07	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
1:A:27:GLU:CD	1:A:27:GLU:H	2.17	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:B:162:PRO:CD	1:B:163:TYR:H	2.23	0.52
1:A:121:ILE:HG12	1:A:123:TYR:O	2.09	0.52
1:A:153:ILE:HD13	1:B:153:ILE:HD13	1.92	0.52
1:A:239:TRP:CZ3	1:A:244:ARG:NH1	2.78	0.52
1:B:243:GLY:N	2:B:273:HOH:O	2.43	0.52
1:B:102:LYS:HB2	1:B:102:LYS:NZ	2.25	0.51
1:A:42:THR:CG2	1:B:39:VAL:HG22	2.40	0.51
1:B:8:ILE:HG13	1:B:8:ILE:O	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:67:LYS:HZ2	1:A:68:GLN:HG3	1.73	0.51
1:A:117:ASN:HD22	1:A:118:THR:HG23	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:A:201:GLU:OE1	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:43:ILE:HG12	1:B:23:ILE:CD1	2.43	0.48
1:A:95:TYR:CD1	1:A:95:TYR:C	2.91	0.48
1:A:163:TYR:N	1:A:163:TYR:CD1	2.79	0.48
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:HD23	1:A:46:LEU:O	2.14	0.47
1:A:112:SER:OG	1:A:113:PHE:N	2.43	0.47
1:A:119:LYS:C	1:A:119:LYS:HD2	2.39	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:35:SER:HB2	1:B:140:ARG:HG3	1.95	0.46
1:B:104:LYS:HB3	1:B:193:HIS:HD2	1.79	0.46
1:A:98:LYS:H	1:A:101:GLU:CD	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:LYS:HE3	1:A:54:LYS:HB2	1.59	0.44
1:A:192:ILE:HG22	1:A:205:ILE:HD12	1.98	0.44
1:A:115:ARG:HH21	1:A:217:ARG:C	2.25	0.44
1:A:49:ARG:N	1:A:50:PRO:CD	2.79	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:8:ILE:HG23	1:A:12:TYR:CE2	2.52	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:140:ARG:HE	1:A:140:ARG:HB3	1.31	0.44
1:A:238:ASN:O	1:A:241:TYR:N	2.51	0.43
1:B:67:LYS:HB2	1:B:67:LYS:HE3	1.88	0.43
1:A:75:PHE:CE1	1:A:91:ILE:CD1	3.00	0.43
1:B:74:ASP:HB2	1:B:89:ILE:O	2.18	0.43
1:B:104:LYS:HB3	1:B:193:HIS:CD2	2.53	0.43
1:A:11:LEU:H	1:A:11:LEU:HG	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:B:165:GLY:C	1:B:166:VAL:HG23	2.43	0.43
1:A:244:ARG:O	1:A:245:LYS:HG3	2.19	0.43
1:A:20:VAL:HG12	1:A:21:CYS:N	2.32	0.42
1:A:67:LYS:HG3	1:A:68:GLN:H	1.78	0.42
1:A:198:ASP:OD1	1:A:203:LYS:NZ	2.27	0.42
1:A:10:ALA:HB1	1:A:51:ILE:CG2	2.49	0.42
1:A:94:THR:CG2	1:A:105:PHE:CE1	2.99	0.42
1:A:25:SER:HA	1:B:20:VAL:HA	2.02	0.42
1:A:20:VAL:CG2	1:A:47:PHE:CZ	3.02	0.42
1:A:100:ASN:HD22	1:A:100:ASN:HA	1.62	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:O	1:B:164:LYS:HG3	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:72:TYR:HA	1:A:73:PRO:HA	1.68	0.42
1:A:197:LYS:HB3	1:A:197:LYS:HE2	1.80	0.42
1:B:21:CYS:CB	1:B:161:LYS:NZ	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:163:TYR:CE1	1:B:166:VAL:HG23	2.54	0.41
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.85	0.41
1:B:54:LYS:HE2	1:B:54:LYS:HB2	1.69	0.41
1:B:102:LYS:NZ	1:B:102:LYS:CB	2.84	0.41
1:B:156:LEU:HA	1:B:159:ILE:CD1	2.49	0.41
1:A:102:LYS:HD2	1:A:194:ALA:HA	2.01	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.80	0.41
1:B:99:GLU:O	1:B:100:ASN:HB2	2.20	0.41
1:B:162:PRO:CD	1:B:163:TYR:N	2.84	0.41
1:A:67:LYS:HG3	1:A:68:GLN:CG	2.42	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: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:70:ASN:C	1:B:71:HIS:HD2	2.29	0.41
1:B:95:TYR:HB3	1:B:138:TYR:CE1	2.53	0.41
1:B:106:THR:O	1:B:107:LEU:HD23	2.21	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:95:TYR:CD2	1:B:95:TYR:C	3.00	0.40
1:B:103:ILE:O	1:B:193:HIS:HD2	2.04	0.40
1:A:218:ASN:ND2	1:A:244:ARG:NH2	2.67	0.40
1:A:64:GLU:N	1:A:76:THR:O	2.46	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: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%)	2	3
1	B	242/245 (99%)	213 (88%)	17 (7%)	12 (5%)	1	2
All	All	484/490 (99%)	421 (87%)	42 (9%)	21 (4%)	2	2

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
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%)	175 (80%)	45 (20%)	1	2
1	B	220/221 (100%)	176 (80%)	44 (20%)	1	2
All	All	440/442 (100%)	351 (80%)	89 (20%)	1	2

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	11	LEU
1	A	14	GLU
1	A	15	ASN
1	A	24	ILE
1	A	25	SER
1	A	27	GLU
1	A	40	LEU
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	104	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	144	ARG
1	A	145	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	LYS
1	A	150	THR
1	A	155	GLU
1	A	156	LEU
1	A	167	LYS
1	A	170	LEU
1	A	176	ILE
1	A	187	THR
1	A	188	ASN
1	A	192	ILE
1	A	201	GLU
1	A	203	LYS
1	A	205	ILE
1	A	207	ASP
1	A	221	ARG
1	A	224	GLN
1	A	235	GLU
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	20	VAL
1	B	23	ILE
1	B	24	ILE
1	B	29	LYS
1	B	37	THR
1	B	46	LEU
1	B	48	SER
1	B	54	LYS
1	B	62	ILE
1	B	79	LYS
1	B	81	SER
1	B	86	LYS
1	B	98	LYS
1	B	102	LYS
1	B	104	LYS
1	B	107	LEU
1	B	112	SER
1	B	114	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	117	ASN
1	B	141	VAL
1	B	144	ARG
1	B	145	LYS
1	B	153	ILE
1	B	180	LEU
1	B	183	SER
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	229	LYS
1	B	234	SER
1	B	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	100	ASN
1	A	117	ASN
1	A	120	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
1	B	71	HIS
1	B	117	ASN
1	B	193	HIS

5.3.3 RNA ⓘ

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.