Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:56 AM EDT

PDB ID	:	2RVE
Title	:	THE CRYSTAL STRUCTURE OF ECORV ENDONUCLEASE AND OF ITS COMPLEXES WITH COGNATE AND NON-COGNATE DNA SEGMENTS
Authors	:	Winkler, F.K.; Banner, D.W.; Oefner, C.; Tsernoglou, D.; Brown, R.S.; Heathman, S.P.; Bryan, R.K.; Martin, P.D.; Petratos, K.; Wilson, K.S.
Deposited on	:	1991-03-19
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

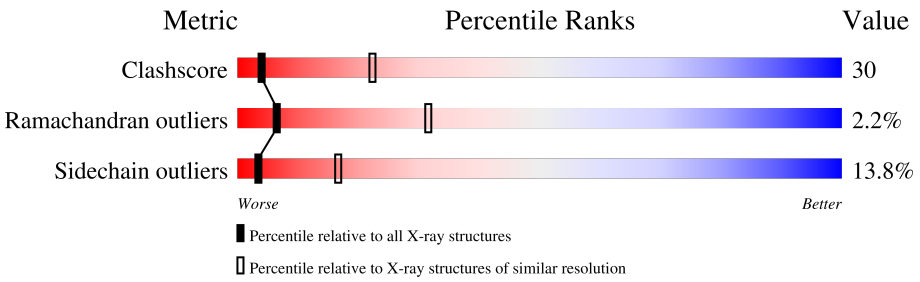
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	8	12% 12% 75%
1	D	8	38% 38% 25%
1	E	8	25% 38% 38%
1	F	8	12% 62% 25%
2	A	244	30% 45% 12% • 13%
2	B	244	34% 45% 8% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4240 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(*CP*GP*AP*GP*CP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	8	161	77	31	46	7	0	0	0
1	D	8	161	77	31	46	7	0	0	0
1	E	8	161	77	31	46	7	0	0	0
1	F	8	161	77	31	46	7	0	0	0

- Molecule 2 is a protein called PROTEIN (ECO RV (E.C.3.1.21.4)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	213	1768	1151	285	331	1	0	0	0
2	B	212	1760	1147	284	328	1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	7	7	7	0	0
3	D	4	4	4	0	0
3	E	6	6	6	0	0
3	F	1	1	1	0	0
3	A	23	23	23	0	0
3	B	27	27	27	0	0

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(*CP*GP*AP*GP*CP*TP*CP*G)-3')

Chain C: 12% 12% 75%

• Molecule 1: DNA (5'-D(*CP*GP*AP*GP*CP*TP*CP*G)-3')

Chain D: 38% 38% 25%

• Molecule 1: DNA (5'-D(*CP*GP*AP*GP*CP*TP*CP*G)-3')

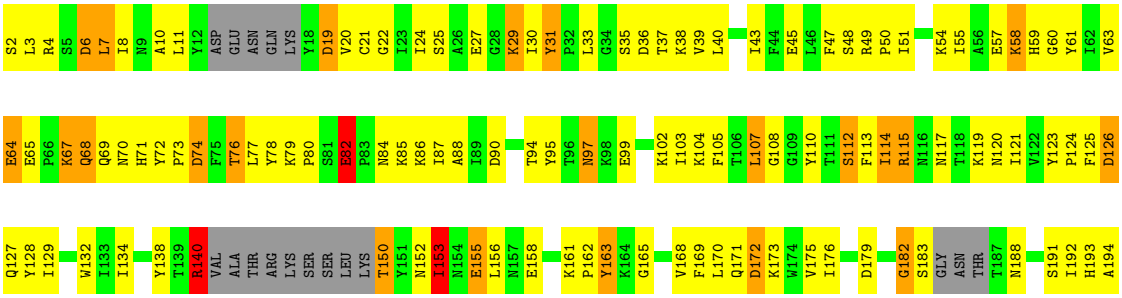
Chain E: 25% 38% 38%

• Molecule 1: DNA (5'-D(*CP*GP*AP*GP*CP*TP*CP*G)-3')

Chain F: 12% 62% 25%

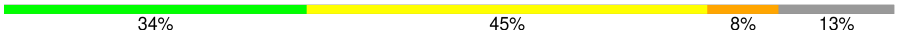
• Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

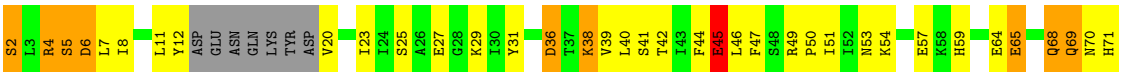
Chain A: 30% 45% 12% • 13%



- Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain B:





4 Data and refinement statistics (i)

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	68.50Å 79.60Å 66.40Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4240	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.62	3/180 (1.7%)	1.82	7/276 (2.5%)
1	D	1.70	0/180	1.82	5/276 (1.8%)
1	E	1.77	4/180 (2.2%)	2.18	5/276 (1.8%)
1	F	1.59	2/180 (1.1%)	2.01	8/276 (2.9%)
2	A	0.99	12/1814 (0.7%)	1.12	23/2455 (0.9%)
2	B	1.02	12/1806 (0.7%)	1.13	18/2444 (0.7%)
All	All	1.14	33/4340 (0.8%)	1.32	66/6003 (1.1%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	158	GLU	CD-OE2	7.23	1.33	1.25
2	A	57	GLU	CD-OE2	7.22	1.33	1.25
2	B	27	GLU	CD-OE2	7.03	1.33	1.25
1	C	1	DC	N1-C6	-6.96	1.32	1.37
2	B	64	GLU	CD-OE2	6.78	1.33	1.25
1	E	1	DC	N1-C6	-6.70	1.33	1.37
2	A	45	GLU	CD-OE2	6.58	1.32	1.25
2	B	65	GLU	CD-OE2	6.49	1.32	1.25
2	B	57	GLU	CD-OE2	6.44	1.32	1.25
2	B	101	GLU	CD-OE2	6.40	1.32	1.25
2	A	201	GLU	CD-OE2	6.34	1.32	1.25
2	A	27	GLU	CD-OE2	6.24	1.32	1.25
2	A	99	GLU	CD-OE2	6.22	1.32	1.25
1	F	3	DA	N3-C4	-6.20	1.31	1.34
2	A	82	GLU	CD-OE2	6.07	1.32	1.25
2	B	45	GLU	CD-OE2	6.02	1.32	1.25
2	B	158	GLU	CD-OE2	5.99	1.32	1.25
2	B	209	GLU	CD-OE2	5.83	1.32	1.25
2	B	220	GLU	CD-OE2	5.81	1.32	1.25
1	E	3	DA	P-O5'	-5.80	1.53	1.59
2	A	64	GLU	CD-OE2	5.76	1.31	1.25
1	E	1	DC	C3'-O3'	-5.60	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	220	GLU	CD-OE2	5.58	1.31	1.25
2	B	201	GLU	CD-OE2	5.54	1.31	1.25
2	A	65	GLU	CD-OE2	5.54	1.31	1.25
1	C	3	DA	C3'-O3'	-5.52	1.36	1.44
2	A	155	GLU	CD-OE2	5.35	1.31	1.25
2	B	235	GLU	CD-OE2	5.31	1.31	1.25
1	F	5	DC	C3'-O3'	-5.24	1.37	1.44
2	B	99	GLU	CD-OE2	5.20	1.31	1.25
1	C	3	DA	C6-N1	-5.14	1.31	1.35
2	A	209	GLU	CD-OE2	5.10	1.31	1.25
1	E	3	DA	N3-C4	-5.03	1.31	1.34

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1	DC	C2-N1-C1'	-17.46	99.59	118.80
1	E	1	DC	C6-N1-C1'	14.57	138.28	120.80
1	F	1	DC	C2-N1-C1'	-12.83	104.69	118.80
1	F	1	DC	C6-N1-C1'	11.06	134.07	120.80
1	C	1	DC	C2-N1-C1'	-9.77	108.06	118.80
1	E	2	DG	C4-N9-C1'	-9.76	113.81	126.50
1	E	2	DG	C8-N9-C1'	9.70	139.61	127.00
1	C	1	DC	C6-N1-C1'	7.60	129.92	120.80
2	B	214	ASP	CB-CG-OD2	-7.57	111.49	118.30
2	B	198	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	F	6	DT	C6-N1-C1'	7.21	131.21	120.40
2	A	207	ASP	CB-CG-OD1	7.14	124.73	118.30
2	A	198	ASP	CB-CG-OD2	-7.14	111.88	118.30
2	A	19	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	D	7	DC	O4'-C1'-N1	7.01	112.91	108.00
1	F	6	DT	C2-N1-C1'	-7.01	106.98	118.20
2	A	214	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	F	2	DG	O4'-C1'-C2'	-6.91	100.37	105.90
1	F	4	DG	P-O5'-C5'	-6.82	109.99	120.90
1	D	1	DC	C2-N1-C1'	-6.78	111.34	118.80
2	B	207	ASP	CB-CG-OD2	-6.77	112.21	118.30
2	A	172	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	D	4	DG	O4'-C1'-C2'	-6.58	100.64	105.90
1	E	7	DC	O4'-C1'-N1	6.49	112.54	108.00
2	A	6	ASP	CB-CG-OD1	6.44	124.09	118.30
2	B	36	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	A	207	ASP	CB-CG-OD2	-6.35	112.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	172	ASP	CB-CG-OD1	6.33	124.00	118.30
2	B	214	ASP	CB-CG-OD1	6.33	124.00	118.30
2	A	179	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	B	198	ASP	CB-CG-OD1	6.29	123.96	118.30
2	B	210	ASP	CB-CG-OD2	-6.27	112.65	118.30
2	B	74	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	A	126	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	A	140	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	B	172	ASP	CB-CG-OD1	6.03	123.72	118.30
2	B	179	ASP	CB-CG-OD2	-5.97	112.93	118.30
2	A	198	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	8	DG	C4-N9-C1'	5.94	134.22	126.50
2	A	214	ASP	CB-CG-OD1	5.94	123.64	118.30
2	B	6	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	7	DC	C2-N1-C1'	-5.88	112.33	118.80
2	A	6	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	172	ASP	CB-CG-OD2	-5.85	113.04	118.30
2	A	179	ASP	CB-CG-OD1	5.83	123.55	118.30
1	F	7	DC	P-O5'-C5'	-5.82	111.59	120.90
1	C	8	DG	C8-N9-C1'	-5.78	119.48	127.00
2	B	74	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	2	DG	O4'-C1'-N9	5.64	111.95	108.00
1	C	4	DG	P-O3'-C3'	5.59	126.40	119.70
2	A	230	TYR	N-CA-C	5.54	125.95	111.00
1	F	2	DG	C1'-O4'-C4'	-5.52	104.58	110.10
2	A	74	ASP	CB-CG-OD1	5.48	123.24	118.30
1	D	1	DC	C6-N1-C1'	5.47	127.37	120.80
2	A	36	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	126	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	36	ASP	CB-CG-OD1	5.37	123.13	118.30
2	A	210	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	A	36	ASP	CB-CG-OD1	5.30	123.07	118.30
2	A	126	ASP	CB-CG-OD1	5.29	123.06	118.30
2	A	210	ASP	CB-CG-OD1	5.26	123.04	118.30
2	B	207	ASP	CB-CG-OD1	5.23	123.01	118.30
2	A	115	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	B	179	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	7	DC	C1'-O4'-C4'	-5.07	105.03	110.10
2	B	4	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	C	161	0	91	7	0
1	D	161	0	91	7	0
1	E	161	0	91	5	0
1	F	161	0	91	1	0
2	A	1768	0	1718	131	0
2	B	1760	0	1714	94	0
3	A	23	0	0	5	0
3	B	27	0	0	2	0
3	C	7	0	0	0	0
3	D	4	0	0	1	0
3	E	6	0	0	1	0
3	F	1	0	0	0	0
All	All	4240	0	3796	232	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 30.

All (232) 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)
2:A:19:ASP:HB3	2:A:161:LYS:HE3	1.41	1.02
2:A:73:PRO:HG3	2:A:88:ALA:HB1	1.46	0.97
2:B:2:SER:HB3	2:B:5:SER:HB3	1.46	0.94
2:A:85:LYS:HG2	2:A:129:ILE:HD13	1.60	0.81
2:A:29:LYS:HE3	2:A:150:THR:OG1	1.80	0.81
2:B:98:LYS:HG2	2:B:101:GLU:OE1	1.83	0.78
2:B:68:GLN:HG3	2:B:71:HIS:CE1	2.19	0.78
2:B:4:ARG:HB3	2:B:132:TRP:CH2	2.18	0.77
2:A:19:ASP:CB	2:A:161:LYS:HE3	2.15	0.76
2:A:22:GLY:HA2	2:A:33:LEU:HD23	1.66	0.76
2:A:73:PRO:CG	2:A:88:ALA:HB1	2.14	0.76
2:B:20:VAL:HG23	2:B:47:PHE:CZ	2.21	0.76
2:B:164:LYS:HD3	2:B:165:GLY:N	2.01	0.75
2:A:67:LYS:HG3	3:A:247:HOH:O	1.85	0.75
2:B:78:TYR:HB3	2:B:86:LYS:HG2	1.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LYS:HB3	2:B:129:ILE:HD13	1.68	0.74
2:A:119:LYS:HG2	2:A:120:ASN:OD1	1.88	0.74
2:A:85:LYS:CG	2:A:129:ILE:HD13	2.18	0.73
2:B:107:LEU:HD22	2:B:133:ILE:HD12	1.71	0.72
2:A:124:PRO:HD2	2:A:127:GLN:NE2	2.02	0.72
2:B:2:SER:HB3	2:B:5:SER:CB	2.21	0.70
2:B:2:SER:CB	2:B:5:SER:HB3	2.21	0.70
2:B:36:ASP:OD1	2:B:38:LYS:HB2	1.93	0.69
2:A:94:THR:HG22	2:A:105:PHE:CE1	2.28	0.69
2:A:19:ASP:HB3	2:A:161:LYS:CE	2.21	0.69
2:B:161:LYS:HD3	3:B:270:HOH:O	1.92	0.69
2:A:172:ASP:O	2:A:176:ILE:HG22	1.93	0.68
2:A:40:LEU:HD23	2:A:43:ILE:HD12	1.76	0.68
2:B:113:PHE:HD2	2:B:125:PHE:CD2	2.13	0.67
2:A:173:LYS:HE2	3:A:260:HOH:O	1.94	0.67
2:B:68:GLN:HG3	2:B:71:HIS:CG	2.30	0.66
2:B:176:ILE:O	2:B:192:ILE:HG23	1.95	0.66
2:A:68:GLN:HG3	2:A:71:HIS:CD2	2.29	0.66
2:A:55:ILE:HD13	2:A:58:LYS:HD3	1.76	0.66
2:A:176:ILE:O	2:A:192:ILE:HG23	1.96	0.66
2:A:218:ASN:HB2	2:A:230:TYR:OH	1.95	0.66
2:B:173:LYS:NZ	3:B:259:HOH:O	2.29	0.65
2:A:152:ASN:OD1	2:A:155:GLU:HG3	1.97	0.64
2:A:6:ASP:OD2	2:A:59:HIS:NE2	2.26	0.64
2:A:117:ASN:ND2	2:A:126:ASP:OD2	2.29	0.64
2:A:29:LYS:HD3	3:A:261:HOH:O	1.97	0.64
2:B:107:LEU:HD22	2:B:133:ILE:CD1	2.27	0.64
2:A:104:LYS:HB3	2:A:193:HIS:ND1	2.13	0.64
2:A:87:ILE:HG21	2:A:132:TRP:CH2	2.33	0.63
2:B:88:ALA:HB2	2:B:128:TYR:CE1	2.33	0.63
2:A:88:ALA:HB2	2:A:128:TYR:CD1	2.34	0.63
1:D:7:DC:H4'	2:B:119:LYS:HE2	1.81	0.62
2:A:22:GLY:HA2	2:A:33:LEU:CD2	2.29	0.62
2:B:79:LYS:HB3	2:B:80:PRO:HD2	1.81	0.62
2:B:113:PHE:HD2	2:B:125:PHE:HD2	1.47	0.62
1:E:1:DC:H2"	1:E:2:DG:H5'	1.82	0.62
2:A:103:ILE:N	2:A:194:ALA:O	2.32	0.62
2:B:93:THR:CG2	2:B:138:TYR:HE1	2.12	0.61
2:A:123:TYR:HB2	2:A:128:TYR:CE2	2.35	0.61
2:B:78:TYR:CB	2:B:86:LYS:HG2	2.30	0.61
2:B:152:ASN:OD1	2:B:154:ASN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLN:HG3	2:B:71:HIS:CD2	2.35	0.60
2:B:81:SER:O	2:B:83:PRO:HD3	2.01	0.60
2:A:61:TYR:HE2	2:A:79:LYS:HZ2	1.50	0.60
2:B:121:ILE:HG12	2:B:123:TYR:O	2.01	0.60
2:A:60:GLY:O	2:A:79:LYS:HG2	2.02	0.59
2:A:203:LYS:HG3	3:A:268:HOH:O	2.01	0.59
2:A:59:HIS:O	2:A:79:LYS:NZ	2.33	0.59
2:A:138:TYR:HD2	2:A:163:TYR:HB2	1.68	0.59
2:A:162:PRO:HD2	2:A:163:TYR:CD2	2.38	0.58
2:B:38:LYS:CE	2:B:38:LYS:HA	2.32	0.58
2:A:86:LYS:HE3	2:A:123:TYR:CD1	2.37	0.58
2:B:12:TYR:HE1	2:B:168:VAL:O	1.87	0.58
2:B:138:TYR:HB3	2:B:166:VAL:HG22	1.85	0.57
2:B:38:LYS:HA	2:B:38:LYS:HE3	1.85	0.57
2:A:172:ASP:HB2	2:A:175:VAL:HG23	1.85	0.57
2:A:85:LYS:HG2	2:A:129:ILE:CD1	2.31	0.56
2:A:153:ILE:HD12	2:A:153:ILE:O	2.06	0.56
2:B:213:LEU:O	2:B:217:ARG:HG3	2.06	0.56
2:A:24:ILE:HG13	2:A:30:ILE:HG12	1.87	0.56
2:A:121:ILE:HG12	2:A:123:TYR:O	2.06	0.56
2:A:163:TYR:CD2	2:A:163:TYR:N	2.74	0.55
2:A:213:LEU:O	2:A:217:ARG:HG3	2.07	0.55
2:A:21:CYS:SG	2:A:156:LEU:HD22	2.47	0.55
2:A:85:LYS:CB	2:A:129:ILE:HD13	2.37	0.55
2:A:115:ARG:NH1	2:A:217:ARG:O	2.40	0.54
2:A:58:LYS:HG3	2:A:58:LYS:O	2.06	0.54
2:A:171:GLN:NE2	2:A:199:PHE:O	2.35	0.54
1:C:7:DC:H42	1:D:2:DG:H1	1.56	0.54
2:A:38:LYS:HB3	2:B:38:LYS:HD2	1.89	0.54
2:B:119:LYS:HG3	2:B:120:ASN:OD1	2.07	0.54
2:B:95:TYR:HB3	2:B:138:TYR:CE2	2.43	0.53
1:C:7:DC:H1'	1:C:8:DG:C8	2.43	0.53
2:A:114:ILE:O	2:A:217:ARG:NH1	2.41	0.53
2:B:93:THR:HG22	2:B:138:TYR:HE1	1.73	0.53
2:A:102:LYS:HD3	2:A:193:HIS:CD2	2.43	0.53
2:B:68:GLN:HG3	2:B:71:HIS:ND1	2.21	0.53
1:D:7:DC:C4'	2:B:119:LYS:HE2	2.39	0.53
2:B:49:ARG:NH2	2:B:65:GLU:OE2	2.41	0.53
2:A:84:ASN:HD22	2:A:84:ASN:N	2.07	0.53
2:A:31:TYR:HB2	2:B:46:LEU:HD21	1.92	0.52
2:A:236:TYR:O	2:A:239:TRP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:LYS:HA	2:A:129:ILE:HG23	1.92	0.52
2:B:109:GLY:HA2	2:B:188:ASN:HA	1.91	0.52
2:A:213:LEU:HD13	2:A:217:ARG:NH2	2.25	0.52
2:A:207:ASP:O	2:A:208:SER:HB3	2.10	0.51
2:B:104:LYS:HD2	2:B:193:HIS:HD2	1.76	0.51
2:B:102:LYS:HG3	2:B:195:HIS:CE1	2.44	0.51
2:A:171:GLN:HG3	2:A:172:ASP:N	2.24	0.51
2:A:211:GLU:OE2	2:A:237:ARG:NH2	2.39	0.51
2:B:6:ASP:OD2	2:B:59:HIS:NE2	2.34	0.51
2:A:87:ILE:HG21	2:A:132:TRP:CZ3	2.46	0.51
2:B:73:PRO:HG3	2:B:88:ALA:HB1	1.92	0.51
2:B:111:THR:HG22	2:B:111:THR:O	2.10	0.51
1:D:6:DT:H72	3:D:18:HOH:O	2.11	0.50
2:B:74:ASP:HB2	2:B:90:ASP:HA	1.93	0.50
1:F:3:DA:H2"	1:F:4:DG:C8	2.46	0.50
1:E:6:DT:H1'	1:E:7:DC:H5'	1.94	0.49
2:B:239:TRP:CZ3	2:B:240:ILE:HD13	2.47	0.49
2:A:238:ASN:C	2:A:240:ILE:H	2.15	0.49
2:A:10:ALA:HB1	3:A:255:HOH:O	2.13	0.49
2:A:103:ILE:HG13	2:A:199:PHE:CE2	2.48	0.49
2:B:102:LYS:HE2	2:B:193:HIS:ND1	2.26	0.49
2:A:124:PRO:HG2	2:A:127:GLN:HE21	1.78	0.49
2:A:163:TYR:N	2:A:163:TYR:HD2	2.10	0.49
2:B:49:ARG:HB3	2:B:50:PRO:HD3	1.94	0.49
2:B:25:SER:HB3	2:B:31:TYR:HE2	1.78	0.49
2:A:48:SER:C	2:A:50:PRO:HD2	2.33	0.49
2:B:112:SER:HB2	2:B:119:LYS:O	2.13	0.49
1:C:4:DG:OP1	2:B:69:GLN:HB2	2.13	0.48
2:A:88:ALA:HB2	2:A:128:TYR:CE1	2.49	0.48
2:B:113:PHE:CD2	2:B:125:PHE:HD2	2.30	0.48
2:B:122:VAL:HG12	2:B:123:TYR:CD2	2.49	0.48
1:C:1:DC:H2'	1:C:2:DG:C8	2.48	0.48
1:E:4:DG:H5"	2:A:68:GLN:HB2	1.95	0.48
2:A:134:ILE:HG13	2:A:170:LEU:HD12	1.96	0.48
2:A:76:THR:HG1	2:A:128:TYR:HH	1.60	0.48
2:B:118:THR:O	2:B:121:ILE:HG22	2.13	0.48
2:B:171:GLN:CG	2:B:176:ILE:HG23	2.44	0.48
2:B:68:GLN:HG3	2:B:71:HIS:NE2	2.28	0.47
2:A:162:PRO:HD2	2:A:163:TYR:HD2	1.79	0.47
2:A:85:LYS:CG	2:A:129:ILE:HG21	2.44	0.47
2:A:213:LEU:HD13	2:A:217:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DC:N4	1:D:2:DG:H1	2.13	0.47
2:A:39:VAL:HG21	2:B:42:THR:HG21	1.97	0.47
2:A:63:VAL:HG22	2:A:77:LEU:CD1	2.44	0.47
2:B:41:SER:O	2:B:44:PHE:N	2.46	0.47
2:B:45:GLU:OE2	2:B:91:ILE:HB	2.15	0.47
2:B:49:ARG:HB3	2:B:50:PRO:CD	2.45	0.47
2:A:43:ILE:HG22	2:A:47:PHE:CE2	2.50	0.47
2:A:162:PRO:HD2	2:A:163:TYR:CE2	2.50	0.47
2:B:68:GLN:CG	2:B:71:HIS:CG	2.98	0.47
1:D:7:DC:C5'	2:B:119:LYS:HE2	2.45	0.46
2:A:95:TYR:CD2	2:A:140:ARG:HG3	2.51	0.46
2:B:72:TYR:OH	2:B:131:HIS:ND1	2.30	0.46
2:A:94:THR:CG2	2:A:105:PHE:CE1	2.98	0.46
2:B:102:LYS:HB3	2:B:193:HIS:CE1	2.50	0.46
2:A:153:ILE:CD1	2:A:156:LEU:HD11	2.46	0.46
2:A:43:ILE:CG2	2:A:47:PHE:CE2	2.99	0.45
1:E:2:DG:O5'	1:E:2:DG:H2'	2.16	0.45
2:A:94:THR:OG1	2:A:95:TYR:N	2.49	0.45
2:A:162:PRO:O	2:A:163:TYR:HB3	2.17	0.45
2:A:3:LEU:HD12	2:A:3:LEU:O	2.16	0.45
2:A:43:ILE:HG22	2:A:47:PHE:CD2	2.51	0.45
2:A:172:ASP:HB2	2:A:175:VAL:CG2	2.47	0.45
2:A:11:LEU:HD23	2:A:51:ILE:HG21	1.97	0.45
2:B:83:PRO:O	2:B:86:LYS:NZ	2.44	0.45
2:B:73:PRO:CG	2:B:88:ALA:HB1	2.46	0.45
1:E:2:DG:N3	3:E:60:HOH:O	2.36	0.45
2:B:113:PHE:HB3	2:B:121:ILE:HB	1.98	0.45
2:A:40:LEU:HD23	2:A:40:LEU:HA	1.70	0.45
2:A:168:VAL:HG12	2:A:169:PHE:N	2.32	0.45
2:B:156:LEU:HD12	2:B:156:LEU:HA	1.57	0.45
2:A:161:LYS:HB3	2:A:162:PRO:CD	2.47	0.45
2:B:69:GLN:O	2:B:70:ASN:HB2	2.17	0.45
2:A:107:LEU:HD21	2:A:191:SER:HB3	1.98	0.44
2:B:49:ARG:O	2:B:53:ASN:HB2	2.17	0.44
2:A:11:LEU:HB3	2:A:168:VAL:HG11	1.99	0.44
2:A:85:LYS:HG3	2:A:129:ILE:HG21	1.99	0.44
2:A:112:SER:HB3	2:A:113:PHE:H	1.55	0.44
2:B:85:LYS:HA	2:B:129:ILE:HG23	1.98	0.44
2:A:68:GLN:CG	2:A:71:HIS:CD2	3.00	0.44
2:B:171:GLN:HG3	2:B:176:ILE:HG23	2.00	0.44
2:A:4:ARG:O	2:A:8:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:24:ILE:HG13	2:A:30:ILE:CG1	2.47	0.43
2:B:8:ILE:CG2	2:B:12:TYR:CE2	3.01	0.43
2:A:113:PHE:CD1	2:A:121:ILE:HB	2.52	0.43
2:A:19:ASP:CA	2:A:161:LYS:HE3	2.49	0.43
2:A:86:LYS:HE3	2:A:123:TYR:CG	2.52	0.43
2:A:238:ASN:N	2:A:238:ASN:HD22	2.16	0.43
2:B:159:ILE:HA	2:B:160:PRO:HD2	1.90	0.43
2:B:39:VAL:HG23	2:B:40:LEU:N	2.33	0.43
2:A:64:GLU:HB2	2:A:76:THR:HB	2.00	0.43
2:A:76:THR:O	2:A:76:THR:HG22	2.19	0.43
2:A:161:LYS:HB3	2:A:162:PRO:HD2	2.00	0.43
2:B:134:ILE:HG12	2:B:170:LEU:HD12	2.00	0.43
2:A:31:TYR:N	2:A:31:TYR:CD2	2.87	0.43
2:B:171:GLN:HG2	2:B:176:ILE:CG2	2.49	0.43
2:A:72:TYR:HA	2:A:73:PRO:HA	1.63	0.42
2:B:46:LEU:O	2:B:50:PRO:HD2	2.18	0.42
2:A:61:TYR:HA	2:A:78:TYR:O	2.20	0.42
2:A:6:ASP:HB3	2:A:55:ILE:HD12	2.00	0.42
2:B:8:ILE:HG23	2:B:12:TYR:CE2	2.54	0.42
2:A:97:ASN:HD21	2:A:140:ARG:NH1	2.17	0.42
2:B:95:TYR:HB3	2:B:138:TYR:CZ	2.54	0.42
2:A:79:LYS:O	2:A:82:GLU:N	2.50	0.42
2:A:233:ILE:O	2:A:237:ARG:HD2	2.19	0.42
2:B:36:ASP:O	2:B:39:VAL:HG22	2.19	0.42
2:B:240:ILE:HD13	2:B:240:ILE:HA	1.61	0.42
2:A:97:ASN:HD21	2:A:140:ARG:HH12	1.68	0.42
2:A:7:LEU:HA	2:A:7:LEU:HD23	1.76	0.41
2:A:110:TYR:HD2	2:A:115:ARG:HH21	1.66	0.41
1:C:3:DA:OP1	2:A:37:THR:HB	2.21	0.41
2:A:108:GLY:O	2:A:188:ASN:HA	2.20	0.41
2:A:69:GLN:O	2:A:70:ASN:HB2	2.20	0.41
2:A:182:GLY:HA3	2:A:188:ASN:OD1	2.20	0.41
2:B:72:TYR:HA	2:B:73:PRO:HA	1.89	0.41
2:B:206:PHE:CE1	2:B:233:ILE:CD1	3.03	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.97	0.41
2:A:197:LYS:HA	2:A:197:LYS:HD3	1.81	0.41
2:B:136:TYR:CD1	2:B:168:VAL:HG12	2.55	0.41
2:A:20:VAL:CG2	2:B:23:ILE:CG2	2.99	0.41
2:A:108:GLY:O	2:A:188:ASN:HB2	2.21	0.41
2:B:92:LYS:O	2:B:135:GLY:HA2	2.21	0.41
2:B:162:PRO:HD2	2:B:163:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:LEU:CD2	2:A:51:ILE:HG21	2.50	0.41
2:A:40:LEU:CD2	2:A:43:ILE:HD12	2.48	0.41
2:A:211:GLU:CD	2:A:237:ARG:HH21	2.24	0.41
2:B:92:LYS:HE3	2:B:106:THR:O	2.21	0.41
2:A:55:ILE:HD13	2:A:55:ILE:HA	1.89	0.41
1:C:5:DC:N4	1:D:4:DG:H1	2.18	0.40
2:A:213:LEU:HD23	2:A:213:LEU:HA	1.91	0.40
2:A:33:LEU:HD11	2:A:43:ILE:HD11	2.03	0.40
2:A:95:TYR:HA	2:A:138:TYR:O	2.21	0.40
2:A:233:ILE:O	2:A:233:ILE:HG13	2.20	0.40
2:A:49:ARG:N	2:A:50:PRO:CD	2.85	0.40
2:B:7:LEU:O	2:B:11:LEU:HG	2.21	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
2	A	203/244 (83%)	169 (83%)	27 (13%)	7 (3%)	3 20
2	B	202/244 (83%)	173 (86%)	27 (13%)	2 (1%)	15 53
All	All	405/488 (83%)	342 (84%)	54 (13%)	9 (2%)	6 31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	112	SER
2	A	182	GLY
2	A	239	TRP
2	B	117	ASN
2	A	125	PHE
2	B	165	GLY

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Mol	Chain	Res	Type
2	A	153	ILE
2	A	80	PRO
2	A	165	GLY

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
2	A	192/220 (87%)	165 (86%)	27 (14%)	3 16
2	B	191/220 (87%)	165 (86%)	26 (14%)	3 17
All	All	383/440 (87%)	330 (86%)	53 (14%)	3 17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	SER
2	A	7	LEU
2	A	25	SER
2	A	29	LYS
2	A	31	TYR
2	A	35	SER
2	A	54	LYS
2	A	58	LYS
2	A	67	LYS
2	A	68	GLN
2	A	74	ASP
2	A	76	THR
2	A	82	GLU
2	A	90	ASP
2	A	97	ASN
2	A	107	LEU
2	A	114	ILE
2	A	140	ARG
2	A	150	THR
2	A	153	ILE

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Mol	Chain	Res	Type
2	A	163	TYR
2	A	183	SER
2	A	203	LYS
2	A	218	ASN
2	A	231	ASN
2	A	237	ARG
2	A	238	ASN
2	B	2	SER
2	B	5	SER
2	B	29	LYS
2	B	38	LYS
2	B	45	GLU
2	B	51	ILE
2	B	54	LYS
2	B	68	GLN
2	B	69	GLN
2	B	81	SER
2	B	90	ASP
2	B	91	ILE
2	B	94	THR
2	B	112	SER
2	B	114	ILE
2	B	116	ASN
2	B	139	THR
2	B	150	THR
2	B	156	LEU
2	B	157	ASN
2	B	180	LEU
2	B	220	GLU
2	B	231	ASN
2	B	234	SER
2	B	240	ILE
2	B	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	68	GLN
2	A	71	HIS
2	A	84	ASN
2	A	97	ASN
2	A	127	GLN

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Mol	Chain	Res	Type
2	A	218	ASN
2	A	238	ASN
2	B	69	GLN
2	B	70	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.