



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:58 PM UTC

PDB ID : 4RVE / pdb_00004rve
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.; Wilso, K.S.
Deposited on : 1993-02-18
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 ⓘ 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

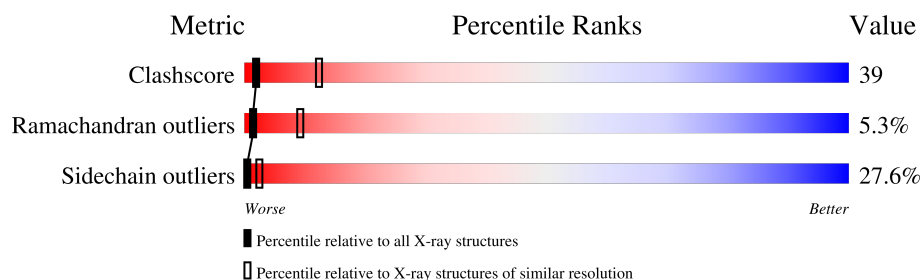
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	10	30% 30% 40%
1	E	10	50% 50%
1	F	10	50% 30% 20%
2	A	244	30% 47% 18% ..
2	B	244	32% 43% 20% ..
2	C	244	32% 45% 18% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6590 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(*GP*GP*GP*AP*TP*AP*TP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	E	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	F	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	240	Total	C	N	O	S	202	0	0
			1987	1280	330	376	1			
2	B	240	Total	C	N	O	S	205	0	0
			1987	1280	330	376	1			
2	C	240	Total	C	N	O	S	204	0	0
			1987	1280	330	376	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	O	0	0
			1	1		
3	E	2	Total	O	0	0
			2	2		
3	F	1	Total	O	0	0
			1	1		
3	A	7	Total	O	0	0
			7	7		
3	B	4	Total	O	0	0
			4	4		
3	C	8	Total	O	0	0
			8	8		

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.

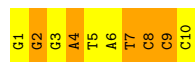
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*TP*AP*TP*CP*CP*C)-3')

Chain D: 



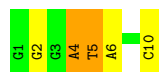
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*TP*AP*TP*CP*CP*C)-3')

Chain E: 

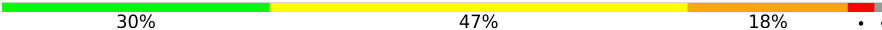


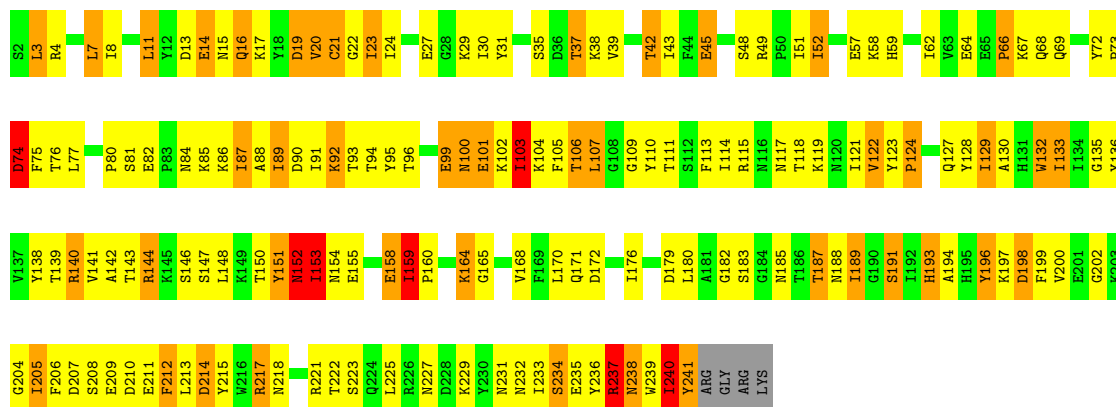
- Molecule 1: DNA (5'-D(*GP*GP*GP*AP*TP*AP*TP*CP*CP*C)-3')

Chain F: 

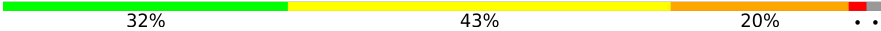


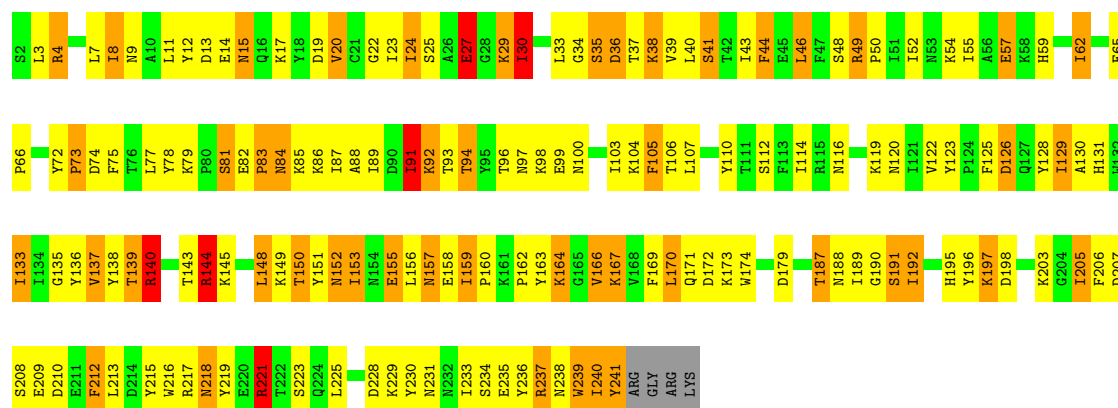
- Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain A: 

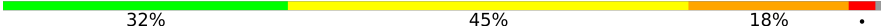


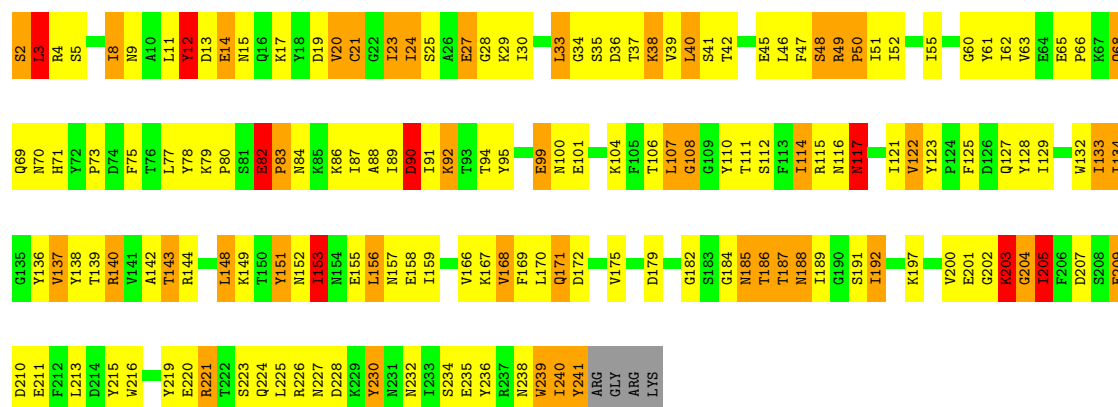
- Molecule 2: PROTEIN (ECO RV (E.C.3.1.21.4))

Chain B: 



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

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.20 Å 78.40 Å 371.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	D	0.91	0/226	1.71	12/347 (3.5%)
1	E	0.98	0/226	1.62	9/347 (2.6%)
1	F	0.94	0/226	1.89	11/347 (3.2%)
2	A	1.31	3/2038 (0.1%)	1.67	32/2760 (1.2%)
2	B	1.37	5/2038 (0.2%)	1.70	35/2760 (1.3%)
2	C	1.33	4/2038 (0.2%)	1.67	37/2760 (1.3%)
All	All	1.30	12/6792 (0.2%)	1.69	136/9321 (1.5%)

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
2	B	1	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	21	CYS	CA-C	-8.88	1.45	1.52
2	B	140	ARG	CA-C	-7.05	1.43	1.52
2	B	105	PHE	CA-C	-6.31	1.44	1.52
2	A	118	THR	CA-C	-6.12	1.46	1.52
2	C	240	ILE	CA-C	5.49	1.59	1.52
2	C	55	ILE	CA-CB	-5.46	1.47	1.54
2	A	217	ARG	CA-C	-5.35	1.45	1.52
2	C	45	GLU	CD-OE2	5.33	1.35	1.25
2	C	90	ASP	CG-OD2	5.17	1.35	1.25
2	B	83	PRO	N-CA	-5.09	1.43	1.47
2	B	139	THR	CA-C	-5.09	1.46	1.52
2	B	34	GLY	N-CA	-5.04	1.40	1.45

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4	DA	C8-N9-C1'	-12.15	108.82	127.05
1	F	4	DA	C4-N9-C1'	11.48	144.27	127.05
1	F	5	DT	C2-N1-C1'	-9.11	105.69	119.35
2	A	159	ILE	N-CA-CB	9.09	118.53	110.08
1	F	5	DT	C6-N1-C1'	8.51	132.12	119.35
2	B	143	THR	N-CA-C	-8.21	101.34	113.40
2	A	37	THR	N-CA-C	8.18	119.83	111.07
1	E	10	DC	C2-N1-C1'	8.16	131.93	119.70
1	D	2	DG	C8-N9-C1'	8.15	139.22	127.00
2	A	159	ILE	N-CA-C	8.13	116.91	108.95
2	B	187	THR	N-CA-CB	-8.12	100.01	111.62
2	B	44	PHE	CA-CB-CG	-8.10	105.70	113.80
2	B	30	ILE	N-CA-C	7.97	120.06	108.58
1	E	10	DC	C6-N1-C1'	-7.81	107.99	119.70
1	D	2	DG	C4-N9-C1'	-7.65	115.52	127.00
1	D	2	DG	P-O3'-C3'	7.61	131.61	120.20
2	A	129	ILE	CB-CA-C	-7.42	102.20	111.92
2	A	124	PRO	N-CA-CB	7.29	110.12	103.19
2	B	126	ASP	N-CA-C	7.26	120.25	111.82
2	B	152	ASN	CA-CB-CG	7.21	119.81	112.60
1	D	9	DC	C2-N1-C1'	-7.18	108.93	119.70
2	A	67	LYS	N-CA-C	-7.16	104.17	113.12
2	B	116	ASN	CA-CB-CG	-7.15	105.45	112.60
2	A	27	GLU	N-CA-C	-7.11	104.21	113.17
2	B	19	ASP	N-CA-C	7.10	119.48	110.61
2	C	188	ASN	N-CA-C	7.01	120.39	110.50
2	C	112	SER	N-CA-C	6.93	114.46	108.78
2	A	209	GLU	N-CA-C	-6.92	104.70	113.01
1	D	3	DG	C8-N9-C1'	6.90	137.35	127.00
2	C	122	VAL	N-CA-C	6.87	116.96	110.30
2	A	107	LEU	N-CA-C	6.72	119.84	107.73
2	A	14	GLU	N-CA-C	-6.69	105.11	113.20
2	C	127	GLN	N-CA-C	-6.67	105.71	114.31
1	D	3	DG	C4-N9-C1'	-6.65	117.02	127.00
2	B	159	ILE	CA-C-N	6.63	126.39	119.76
2	B	159	ILE	C-N-CA	6.63	126.39	119.76
1	F	4	DA	C5'-C4'-C3'	6.60	124.80	114.90
2	C	17	LYS	N-CA-C	6.55	118.30	111.03
2	A	152	ASN	CA-CB-CG	-6.48	106.12	112.60
1	E	2	DG	C4-N9-C1'	6.45	136.67	127.00
2	A	193	HIS	CA-CB-CG	-6.44	107.36	113.80
2	C	50	PRO	CA-C-N	6.39	128.61	120.56
2	C	50	PRO	C-N-CA	6.39	128.61	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	117	ASN	CA-C-N	-6.38	110.34	120.17
2	A	117	ASN	C-N-CA	-6.38	110.34	120.17
2	C	33	LEU	N-CA-C	6.35	119.13	110.55
1	F	2	DG	C8-N9-C1'	6.26	136.38	127.00
2	C	188	ASN	CA-CB-CG	-6.25	106.35	112.60
2	B	99	GLU	N-CA-C	6.25	119.55	110.42
2	B	36	ASP	N-CA-CB	6.11	119.11	109.71
2	B	24	ILE	N-CA-C	6.10	116.91	108.12
2	B	91	ILE	N-CA-C	6.07	116.91	108.89
2	B	129	ILE	CA-C-O	6.04	124.21	118.90
1	D	9	DC	C6-N1-C1'	6.00	128.70	119.70
2	C	107	LEU	N-CA-C	5.99	120.43	113.18
2	C	187	THR	N-CA-C	5.96	119.76	111.90
2	B	96	THR	N-CA-CB	5.95	121.90	111.55
1	F	5	DT	P-O5'-C5'	-5.93	111.11	120.00
2	A	222	THR	N-CA-C	5.91	117.77	108.96
2	C	82	GLU	CA-C-N	5.88	127.19	119.84
2	C	82	GLU	C-N-CA	5.88	127.19	119.84
1	D	3	DG	P-O5'-C5'	-5.88	111.19	120.00
1	F	10	DC	P-O5'-C5'	-5.87	111.20	120.00
2	C	3	LEU	N-CA-C	-5.80	104.96	111.28
2	B	14	GLU	N-CA-C	-5.79	106.25	113.38
2	A	122	VAL	N-CA-C	5.79	118.32	111.09
2	C	116	ASN	CA-CB-CG	-5.78	106.82	112.60
2	B	112	SER	N-CA-C	5.77	113.51	108.78
1	E	7	DT	C4'-C3'-O3'	-5.71	101.44	110.00
2	C	186	THR	N-CA-C	5.70	120.09	113.20
2	A	106	THR	N-CA-CB	5.68	119.47	110.84
2	A	103	ILE	N-CA-C	5.64	118.25	108.95
2	B	219	TYR	CB-CA-C	-5.62	102.14	111.41
2	A	74	ASP	N-CA-CB	5.61	118.15	110.01
1	D	1	DG	C8-N9-C1'	5.60	135.41	127.00
1	E	9	DC	P-O3'-C3'	5.60	128.60	120.20
2	B	85	LYS	N-CA-C	-5.60	101.16	109.11
2	A	187	THR	N-CA-C	5.59	118.01	111.02
2	C	21	CYS	N-CA-CB	5.58	118.02	110.59
2	C	205	ILE	N-CA-C	5.56	116.79	112.12
2	A	74	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	84	ASN	N-CA-C	-5.53	105.98	114.16
2	A	218	ASN	CB-CA-C	5.52	118.35	109.07
2	A	124	PRO	CB-CA-C	5.52	118.64	110.85
2	A	198	ASP	O-C-N	5.50	127.95	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	ARG	N-CA-C	5.49	122.49	110.80
2	C	34	GLY	N-CA-C	-5.49	106.21	112.79
2	C	24	ILE	N-CA-C	5.48	116.02	108.12
1	D	5	DT	P-O5'-C5'	5.47	128.21	120.00
2	B	79	LYS	CA-C-N	5.45	124.91	119.24
2	B	79	LYS	C-N-CA	5.45	124.91	119.24
2	C	12	TYR	N-CA-C	5.44	118.45	110.30
1	F	6	DA	P-O3'-C3'	5.43	128.34	120.20
2	B	207	ASP	N-CA-C	5.43	119.16	112.54
2	C	19	ASP	N-CA-C	5.41	117.88	107.44
2	A	240	ILE	CA-C-N	5.40	131.42	121.70
2	A	240	ILE	C-N-CA	5.40	131.42	121.70
1	E	8	DC	P-O3'-C3'	-5.40	112.10	120.20
2	B	98	LYS	CA-C-N	5.38	129.95	121.56
2	B	98	LYS	C-N-CA	5.38	129.95	121.56
2	C	204	GLY	CA-C-N	5.35	128.39	122.77
2	C	204	GLY	C-N-CA	5.35	128.39	122.77
2	B	27	GLU	CB-CG-CD	5.35	121.69	112.60
2	A	59	HIS	CA-CB-CG	5.32	119.12	113.80
2	B	143	THR	CA-C-N	5.32	131.71	121.54
2	B	143	THR	C-N-CA	5.32	131.71	121.54
2	C	156	LEU	N-CA-C	5.31	117.81	111.71
2	B	74	ASP	CA-CB-CG	-5.27	107.33	112.60
2	A	66	PRO	CA-N-CD	-5.25	104.64	112.00
2	C	117	ASN	N-CA-C	5.25	121.99	110.80
2	C	90	ASP	CA-CB-CG	5.20	117.80	112.60
2	C	210	ASP	CA-C-N	5.20	127.24	120.28
2	C	210	ASP	C-N-CA	5.20	127.24	120.28
2	B	239	TRP	CA-CB-CG	5.19	123.46	113.60
2	C	108	GLY	N-CA-C	5.19	118.18	110.60
1	E	4	DA	C5'-C4'-C3'	5.18	122.67	114.90
1	D	1	DG	C4-N9-C1'	-5.17	119.25	127.00
2	B	221	ARG	N-CA-C	5.16	119.63	113.23
1	D	7	DT	C4'-C3'-O3'	-5.16	102.27	110.00
2	A	3	LEU	O-C-N	5.15	127.66	122.09
2	A	198	ASP	CA-CB-CG	-5.14	107.46	112.60
2	B	62	ILE	CB-CA-C	5.12	119.04	111.31
1	F	4	DA	C2'-C3'-O3'	-5.12	103.82	111.50
2	A	159	ILE	CB-CA-C	-5.11	105.37	110.89
2	C	230	TYR	N-CA-CB	5.08	119.98	110.99
2	C	139	THR	CA-C-N	-5.08	114.24	121.50
2	C	139	THR	C-N-CA	-5.08	114.24	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	ILE	N-CA-C	-5.07	105.65	110.42
1	E	2	DG	C8-N9-C1'	-5.05	119.43	127.00
1	F	2	DG	C4-N9-C1'	-5.04	119.43	127.00
2	C	200	VAL	CB-CA-C	-5.03	105.35	112.14
2	A	132	TRP	N-CA-C	5.03	117.94	109.95
2	C	39	VAL	N-CA-C	-5.02	106.78	111.45
2	C	20	VAL	N-CA-CB	-5.01	100.74	111.37
2	C	153	ILE	N-CA-C	5.01	119.77	109.34
1	E	7	DT	P-O5'-C5'	-5.01	112.49	120.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	240	ILE	CA

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	D	202	0	114	9	0
1	E	202	0	114	14	0
1	F	202	0	114	3	0
2	A	1987	0	1945	165	0
2	B	1987	0	1945	155	0
2	C	1987	0	1945	124	0
3	A	7	0	0	2	0
3	B	4	0	0	0	0
3	C	8	0	0	2	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
All	All	6590	0	6177	442	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 39.

All (442) 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:D:7:DT:H4'	2:B:37:THR:HG21	1.35	1.05
2:C:192:ILE:HD11	2:C:205:ILE:HG13	1.39	1.03
1:E:7:DT:H4'	2:A:37:THR:HG21	1.35	1.03
2:A:11:LEU:HD23	2:A:51:ILE:HG21	1.38	1.00
2:C:171:GLN:HE21	2:C:172:ASP:N	1.58	0.99
2:C:11:LEU:HD11	2:C:134:ILE:HD13	1.45	0.94
2:C:171:GLN:NE2	2:C:172:ASP:H	1.68	0.91
2:B:238:ASN:HA	2:B:241:TYR:HE1	1.32	0.91
1:D:7:DT:H4'	2:B:37:THR:CG2	2.01	0.91
2:A:62:ILE:HD12	2:A:80:PRO:HG3	1.52	0.89
2:C:185:ASN:HD22	2:C:186:THR:N	1.72	0.88
2:C:171:GLN:HE21	2:C:172:ASP:H	0.88	0.87
2:A:11:LEU:CD2	2:A:51:ILE:HG21	2.05	0.86
2:A:106:THR:HG22	2:A:182:GLY:HA3	1.57	0.85
1:E:7:DT:H4'	2:A:37:THR:CG2	2.08	0.83
2:B:213:LEU:HD22	2:B:217:ARG:NH2	1.94	0.83
2:B:170:LEU:HD12	2:B:171:GLN:N	1.94	0.82
2:B:151:TYR:CG	2:B:159:ILE:HD11	2.14	0.82
2:B:170:LEU:HD12	2:B:171:GLN:H	1.43	0.81
2:B:122:VAL:HG12	2:B:123:TYR:CD1	2.15	0.81
2:C:25:SER:OG	2:C:27:GLU:HG2	1.82	0.80
2:A:179:ASP:C	2:A:180:LEU:HD23	2.06	0.80
2:C:185:ASN:HD22	2:C:186:THR:H	1.30	0.80
2:A:31:TYR:CD1	2:B:46:LEU:HD11	2.17	0.79
2:B:81:SER:O	2:B:83:PRO:HD3	1.82	0.78
2:A:86:LYS:HB2	2:A:127:GLN:O	1.83	0.78
2:A:123:TYR:HB3	2:A:127:GLN:HE21	1.49	0.77
2:C:2:SER:N	2:C:5:SER:HG	1.83	0.77
2:A:39:VAL:HG12	2:A:43:ILE:CD1	2.16	0.76
2:C:151:TYR:HB3	2:C:155:GLU:HB2	1.67	0.76
2:C:152:ASN:OD1	2:C:155:GLU:HG3	1.84	0.76
1:E:6:DA:C2'	1:E:7:DT:H5'	2.16	0.76
2:C:232:ASN:OD1	2:C:235:GLU:HG3	1.85	0.76
2:A:206:PHE:CE1	2:A:233:ILE:HD12	2.21	0.75
2:A:85:LYS:HG3	2:A:129:ILE:HD11	1.67	0.75
2:B:240:ILE:N	2:B:240:ILE:HD12	2.01	0.74
1:E:8:DC:H2''	1:E:9:DC:C6	2.21	0.74
2:A:206:PHE:CD2	2:A:212:PHE:HB2	2.23	0.73
2:A:49:ARG:HB2	2:A:75:PHE:HZ	1.53	0.73
2:C:23:ILE:CD1	2:C:33:LEU:HD21	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:TYR:O	2:C:239:TRP:HB3	1.89	0.73
2:A:132:TRP:C	2:A:133:ILE:HD13	2.13	0.72
2:A:196:TYR:O	2:A:199:PHE:HB2	1.89	0.72
2:A:233:ILE:HG22	3:A:773:HOH:O	1.88	0.72
2:C:8:ILE:HG23	2:C:12:TYR:CE1	2.24	0.72
2:A:42:THR:HG21	2:B:39:VAL:HG21	1.71	0.72
2:C:23:ILE:HD11	2:C:33:LEU:HD21	1.72	0.72
2:B:197:LYS:HE3	2:B:198:ASP:OD1	1.90	0.71
2:B:151:TYR:CB	2:B:159:ILE:HD11	2.19	0.71
2:C:27:GLU:CD	2:C:27:GLU:H	1.99	0.71
2:A:85:LYS:CB	2:A:129:ILE:HD11	2.21	0.70
2:C:37:THR:HA	2:C:40:LEU:HB2	1.71	0.70
2:C:4:ARG:HB2	2:C:132:TRP:CH2	2.26	0.70
2:C:62:ILE:HD11	2:C:80:PRO:HG3	1.73	0.70
2:B:233:ILE:O	2:B:237:ARG:HG3	1.92	0.69
2:B:135:GLY:HA3	2:B:169:PHE:CE2	2.26	0.69
1:E:4:DA:H5'	2:A:119:LYS:NZ	2.07	0.69
2:B:238:ASN:HA	2:B:241:TYR:CE1	2.22	0.68
2:A:85:LYS:CG	2:A:129:ILE:HD11	2.23	0.67
2:B:8:ILE:CG2	2:B:12:TYR:HE2	2.07	0.67
2:B:236:TYR:O	2:B:239:TRP:HB3	1.94	0.67
2:C:49:ARG:NH1	2:C:49:ARG:HG3	2.08	0.67
1:E:7:DT:C4'	2:A:37:THR:HG21	2.18	0.67
2:A:207:ASP:HB2	2:A:211:GLU:OE1	1.94	0.67
2:B:40:LEU:HD23	2:B:43:ILE:HD13	1.77	0.66
2:A:89:ILE:HD13	2:A:132:TRP:HE3	1.58	0.66
2:C:49:ARG:N	2:C:50:PRO:HD2	2.10	0.66
2:B:149:LYS:HD3	2:B:151:TYR:CZ	2.30	0.66
2:A:39:VAL:HG12	2:A:43:ILE:HD11	1.76	0.66
2:B:231:ASN:ND2	2:B:235:GLU:OE1	2.29	0.66
2:A:171:GLN:HG3	2:A:172:ASP:N	2.11	0.66
2:A:238:ASN:OD1	2:A:238:ASN:N	2.29	0.65
2:C:202:GLY:O	2:C:204:GLY:N	2.30	0.65
2:B:39:VAL:O	2:B:43:ILE:HD12	1.96	0.65
2:A:87:ILE:HG12	2:A:130:ALA:HB3	1.77	0.65
2:B:105:PHE:H	2:B:191:SER:HB3	1.62	0.65
2:B:179:ASP:OD1	2:B:179:ASP:N	2.30	0.65
2:C:49:ARG:HG3	2:C:49:ARG:HH11	1.61	0.65
2:A:85:LYS:HG3	2:A:129:ILE:CD1	2.28	0.64
2:B:100:ASN:ND2	2:B:195:HIS:HD2	1.96	0.64
2:C:66:PRO:HD3	3:C:754:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:DA:H4'	2:B:120:ASN:ND2	2.12	0.64
2:A:3:LEU:HD12	2:A:3:LEU:O	1.96	0.64
2:A:24:ILE:HG22	2:B:22:GLY:O	1.97	0.64
2:A:73:PRO:HG2	2:A:75:PHE:O	1.97	0.64
2:C:49:ARG:NH2	2:C:65:GLU:OE1	2.30	0.64
2:A:123:TYR:HB3	2:A:127:GLN:NE2	2.12	0.63
2:B:3:LEU:O	2:B:7:LEU:HB2	1.97	0.63
2:C:207:ASP:N	2:C:211:GLU:OE1	2.27	0.63
2:B:8:ILE:HG22	2:B:12:TYR:HE2	1.62	0.63
2:A:179:ASP:O	2:A:180:LEU:HD23	1.98	0.63
2:C:49:ARG:NE	2:C:65:GLU:OE2	2.27	0.63
2:B:107:LEU:HD22	2:B:133:ILE:CD1	2.29	0.63
2:C:62:ILE:O	2:C:77:LEU:HA	1.99	0.63
2:A:49:ARG:HB2	2:A:75:PHE:CZ	2.33	0.62
2:A:105:PHE:HB2	2:A:191:SER:HB3	1.80	0.62
2:B:210:ASP:N	2:B:210:ASP:OD1	2.29	0.62
2:A:58:LYS:HG3	2:A:58:LYS:O	2.00	0.62
2:B:91:ILE:C	2:B:92:LYS:HG2	2.25	0.62
2:B:100:ASN:HD21	2:B:195:HIS:HD2	1.48	0.62
2:B:159:ILE:HG23	2:B:160:PRO:HD2	1.82	0.62
2:A:4:ARG:HH12	2:A:172:ASP:CG	2.06	0.62
2:C:108:GLY:O	2:C:188:ASN:HA	2.00	0.61
2:A:194:ALA:HB1	2:A:198:ASP:OD2	2.00	0.61
2:A:31:TYR:CE1	2:A:150:THR:HG21	2.35	0.61
2:A:106:THR:HG22	2:A:182:GLY:CA	2.29	0.61
2:A:164:LYS:HE2	2:A:165:GLY:H	1.65	0.61
1:D:4:DA:N6	2:A:185:ASN:OD1	2.29	0.61
2:B:155:GLU:O	2:B:158:GLU:N	2.29	0.61
2:A:102:LYS:HD2	2:A:193:HIS:HD2	1.66	0.60
2:A:42:THR:O	2:A:45:GLU:HB2	2.01	0.60
2:B:77:LEU:O	2:B:78:TYR:HB3	2.01	0.60
2:C:137:VAL:O	2:C:166:VAL:HA	1.99	0.60
2:A:68:GLN:N	2:A:68:GLN:OE1	2.33	0.60
2:B:151:TYR:HB2	2:B:159:ILE:HD11	1.82	0.60
2:A:135:GLY:O	2:A:168:VAL:HA	2.02	0.60
2:C:82:GLU:N	2:C:83:PRO:HD3	2.17	0.60
2:C:153:ILE:O	2:C:153:ILE:HG13	2.01	0.59
2:B:29:LYS:NZ	2:B:150:THR:HG22	2.17	0.59
2:B:46:LEU:O	2:B:46:LEU:HG	2.01	0.59
2:A:91:ILE:O	2:A:92:LYS:HD3	2.02	0.59
2:B:179:ASP:HB2	2:B:215:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:109:GLY:HA2	2:A:187:THR:O	2.02	0.59
1:D:3:DG:O6	2:A:183:SER:HB2	2.03	0.59
2:C:107:LEU:N	2:C:189:ILE:O	2.29	0.59
2:A:20:VAL:HA	2:B:25:SER:HA	1.85	0.59
2:C:49:ARG:HH21	2:C:65:GLU:CD	2.10	0.59
2:A:171:GLN:HG2	2:A:176:ILE:CG2	2.33	0.58
2:A:31:TYR:CD1	2:A:150:THR:HG22	2.38	0.58
2:A:113:PHE:CB	2:A:121:ILE:HD12	2.33	0.58
2:A:153:ILE:HG13	2:B:153:ILE:HD13	1.85	0.58
2:C:47:PHE:O	2:C:50:PRO:HG2	2.02	0.58
2:A:91:ILE:HD12	2:A:91:ILE:N	2.18	0.58
2:B:40:LEU:HD23	2:B:43:ILE:CD1	2.32	0.58
2:B:191:SER:OG	2:B:192:ILE:N	2.36	0.58
2:A:122:VAL:HG12	2:A:123:TYR:CD2	2.38	0.58
2:A:187:THR:O	2:A:187:THR:HG22	2.04	0.58
2:B:3:LEU:HD23	2:B:87:ILE:HD13	1.86	0.58
2:A:152:ASN:O	2:A:155:GLU:N	2.35	0.57
2:B:7:LEU:HD12	2:B:55:ILE:HG13	1.86	0.57
2:A:48:SER:O	2:A:52:ILE:HG13	2.04	0.57
2:A:179:ASP:OD1	2:A:179:ASP:N	2.36	0.57
2:B:187:THR:O	2:B:187:THR:HG22	2.03	0.57
2:A:85:LYS:CA	2:A:129:ILE:HD11	2.35	0.57
2:A:113:PHE:CG	2:A:121:ILE:HD12	2.39	0.57
2:A:164:LYS:HE2	2:A:165:GLY:N	2.20	0.57
2:B:36:ASP:OD1	2:B:38:LYS:HB2	2.05	0.57
2:A:214:ASP:HB3	2:A:236:TYR:OH	2.05	0.57
2:B:88:ALA:HB2	2:B:128:TYR:CD2	2.40	0.57
2:C:151:TYR:CD1	2:C:151:TYR:N	2.72	0.57
2:B:195:HIS:HB3	2:B:197:LYS:HE2	1.86	0.57
2:B:54:LYS:O	2:B:57:GLU:HB3	2.04	0.57
2:B:221:ARG:HH11	2:B:221:ARG:CG	2.18	0.56
2:B:29:LYS:HZ2	2:B:150:THR:HG22	1.70	0.56
2:B:174:TRP:CH2	2:B:208:SER:HA	2.39	0.56
2:B:195:HIS:CB	2:B:197:LYS:HE2	2.36	0.56
2:C:12:TYR:OH	2:C:169:PHE:HA	2.05	0.56
2:C:75:PHE:HE2	2:C:91:ILE:CD1	2.19	0.56
2:C:4:ARG:HB2	2:C:132:TRP:CZ2	2.40	0.56
2:B:189:ILE:HG22	2:B:190:GLY:N	2.19	0.56
2:C:80:PRO:O	2:C:83:PRO:HD3	2.06	0.56
2:B:37:THR:O	2:B:41:SER:OG	2.23	0.56
2:A:213:LEU:HD13	2:A:217:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:DA:H5'	2:A:119:LYS:HZ2	1.71	0.55
2:A:211:GLU:OE2	2:A:237:ARG:NH2	2.34	0.55
2:B:174:TRP:CZ3	2:B:208:SER:HA	2.41	0.55
2:A:102:LYS:HB3	2:A:193:HIS:CD2	2.41	0.55
2:C:4:ARG:O	2:C:8:ILE:HG13	2.07	0.55
2:C:171:GLN:NE2	2:C:171:GLN:HA	2.19	0.55
2:B:33:LEU:HB2	2:B:162:PRO:HG3	1.88	0.55
2:C:11:LEU:HD11	2:C:134:ILE:CD1	2.29	0.55
2:A:86:LYS:O	2:A:128:TYR:HA	2.07	0.55
2:A:102:LYS:HD3	2:A:194:ALA:HA	1.88	0.55
2:B:221:ARG:HH11	2:B:221:ARG:HG2	1.72	0.55
2:B:49:ARG:HB2	2:B:75:PHE:HE2	1.72	0.54
2:B:229:LYS:HG2	2:B:230:TYR:CD2	2.41	0.54
2:A:31:TYR:CG	2:B:46:LEU:HD11	2.42	0.54
2:C:36:ASP:OD1	2:C:38:LYS:HB2	2.08	0.54
2:C:220:GLU:HA	2:C:220:GLU:OE1	2.07	0.54
2:B:72:TYR:CE2	2:B:73:PRO:HB3	2.43	0.54
1:E:8:DC:H2''	1:E:9:DC:H6	1.69	0.53
2:A:64:GLU:OE1	2:A:123:TYR:OH	2.27	0.53
2:A:24:ILE:O	2:A:24:ILE:HG23	2.07	0.53
2:A:151:TYR:HD1	2:A:151:TYR:H	1.56	0.53
2:C:188:ASN:N	2:C:188:ASN:HD22	2.06	0.53
2:A:64:GLU:N	2:A:76:THR:O	2.41	0.53
2:A:88:ALA:C	2:A:89:ILE:HG12	2.33	0.53
2:A:233:ILE:HG23	2:A:234:SER:N	2.23	0.53
2:A:237:ARG:O	2:A:240:ILE:HG22	2.09	0.53
2:C:62:ILE:CD1	2:C:80:PRO:HG3	2.39	0.53
2:C:30:ILE:HD12	2:C:152:ASN:C	2.33	0.53
2:A:171:GLN:NE2	2:A:202:GLY:CA	2.72	0.53
2:B:78:TYR:CD2	2:B:86:LYS:HD3	2.44	0.53
2:B:33:LEU:HB2	2:B:162:PRO:CG	2.39	0.52
2:B:100:ASN:ND2	2:B:195:HIS:CD2	2.77	0.52
2:B:119:LYS:O	2:B:120:ASN:HB2	2.09	0.52
2:A:39:VAL:CG1	2:A:43:ILE:HD11	2.39	0.52
2:B:192:ILE:HD11	2:B:205:ILE:HB	1.91	0.52
2:C:110:TYR:CD1	2:C:111:THR:HG23	2.44	0.52
2:C:3:LEU:HD23	2:C:87:ILE:CD1	2.39	0.52
2:C:106:THR:HG22	2:C:182:GLY:HA3	1.91	0.52
2:C:171:GLN:NE2	2:C:172:ASP:N	2.39	0.52
2:B:171:GLN:HG3	2:B:172:ASP:N	2.24	0.52
2:A:206:PHE:CD1	2:A:233:ILE:HD12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:TRP:HB3	2:C:170:LEU:HD11	1.92	0.52
2:B:138:TYR:CD1	2:B:138:TYR:N	2.78	0.52
2:A:4:ARG:NH1	2:A:172:ASP:OD1	2.29	0.52
2:A:179:ASP:HB2	2:A:215:TYR:OH	2.10	0.51
2:A:239:TRP:C	2:A:241:TYR:H	2.17	0.51
2:B:229:LYS:O	2:B:230:TYR:HB3	2.11	0.51
2:B:241:TYR:CD1	2:B:241:TYR:N	2.78	0.51
2:C:86:LYS:HE2	2:C:123:TYR:CE2	2.44	0.51
2:B:20:VAL:O	2:B:20:VAL:HG12	2.09	0.51
2:B:157:ASN:OD1	2:B:157:ASN:N	2.38	0.51
2:C:209:GLU:O	2:C:209:GLU:HG3	2.10	0.51
2:A:151:TYR:CG	2:A:159:ILE:HG12	2.45	0.51
2:B:94:THR:O	2:B:137:VAL:HA	2.10	0.51
2:A:93:THR:HG22	2:A:136:TYR:HB2	1.93	0.51
2:C:238:ASN:O	2:C:240:ILE:N	2.44	0.51
2:A:171:GLN:HE22	2:A:202:GLY:HA3	1.75	0.51
2:C:216:TRP:HZ3	2:C:219:TYR:CD2	2.28	0.51
2:A:214:ASP:OD2	2:A:236:TYR:OH	2.26	0.51
2:A:121:ILE:HG23	2:A:123:TYR:O	2.10	0.51
2:B:221:ARG:NH1	2:B:221:ARG:CB	2.74	0.51
2:C:107:LEU:HB2	2:C:189:ILE:HG22	1.93	0.51
2:C:197:LYS:HE2	2:C:201:GLU:OE2	2.11	0.51
2:C:27:GLU:CD	2:C:27:GLU:N	2.68	0.51
2:B:25:SER:HB2	2:B:27:GLU:OE2	2.11	0.50
1:D:4:DA:H4'	2:B:120:ASN:CG	2.35	0.50
2:C:83:PRO:O	2:C:86:LYS:NZ	2.43	0.50
2:C:92:LYS:HE3	2:C:106:THR:O	2.11	0.50
2:A:39:VAL:HG12	2:A:43:ILE:HD12	1.90	0.50
2:B:189:ILE:HG23	2:B:216:TRP:CZ2	2.46	0.50
2:A:39:VAL:O	2:A:43:ILE:HD12	2.12	0.50
2:B:35:SER:HB3	2:B:140:ARG:NH1	2.27	0.50
2:B:36:ASP:OD1	2:B:38:LYS:N	2.42	0.50
2:B:238:ASN:CA	2:B:241:TYR:HE1	2.15	0.50
2:A:102:LYS:HD2	2:A:193:HIS:O	2.12	0.50
2:B:62:ILE:N	2:B:78:TYR:O	2.26	0.50
2:C:171:GLN:NE2	2:C:171:GLN:CA	2.75	0.50
2:A:3:LEU:HD12	2:A:3:LEU:C	2.36	0.50
2:B:62:ILE:O	2:B:77:LEU:HA	2.11	0.50
2:B:240:ILE:HG22	2:B:240:ILE:O	2.12	0.50
1:D:9:DC:H42	1:E:2:DG:H1	1.60	0.49
2:C:11:LEU:CD1	2:C:134:ILE:HD13	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:138:TYR:HE1	2:A:140:ARG:HB3	1.77	0.49
2:B:174:TRP:CD1	2:B:209:GLU:HB2	2.46	0.49
2:B:206:PHE:HE1	2:B:215:TYR:CB	2.26	0.49
2:C:77:LEU:HD13	2:C:89:ILE:HD12	1.94	0.49
2:C:88:ALA:HB2	2:C:128:TYR:CD1	2.48	0.49
2:B:240:ILE:HD12	2:B:240:ILE:H	1.74	0.49
2:A:153:ILE:CG1	2:B:153:ILE:HD13	2.43	0.49
2:C:114:ILE:HD12	2:C:213:LEU:CD2	2.43	0.49
2:C:172:ASP:HB2	2:C:175:VAL:HG23	1.95	0.49
2:C:95:TYR:CD1	2:C:140:ARG:HG2	2.47	0.49
1:F:4:DA:H2''	1:F:5:DT:O5'	2.13	0.49
2:A:103:ILE:O	2:A:193:HIS:HA	2.13	0.49
2:A:7:LEU:HD12	2:A:7:LEU:O	2.13	0.48
1:F:5:DT:H73	2:C:186:THR:HB	1.95	0.48
2:A:94:THR:HG22	2:A:105:PHE:CZ	2.48	0.48
2:C:215:TYR:CE1	2:C:230:TYR:CE1	3.01	0.48
2:A:171:GLN:HG2	2:A:176:ILE:HG23	1.95	0.48
2:A:231:ASN:O	2:A:232:ASN:HB3	2.12	0.48
2:B:163:TYR:N	2:B:163:TYR:CD1	2.81	0.48
2:C:69:GLN:HB2	3:C:762:HOH:O	2.14	0.48
2:C:77:LEU:O	2:C:78:TYR:HB3	2.13	0.48
2:A:19:ASP:O	2:B:25:SER:HB2	2.12	0.48
2:B:77:LEU:N	2:B:77:LEU:HD12	2.28	0.48
2:B:233:ILE:HG23	2:B:234:SER:N	2.27	0.48
2:B:49:ARG:NE	2:B:65:GLU:OE1	2.39	0.48
2:C:216:TRP:CZ3	2:C:219:TYR:CD2	3.02	0.48
2:A:179:ASP:OD2	2:A:232:ASN:HB2	2.12	0.48
2:A:31:TYR:CE1	2:A:150:THR:CG2	2.97	0.48
2:B:81:SER:C	2:B:83:PRO:HD3	2.38	0.48
2:B:221:ARG:NH1	2:B:221:ARG:HB3	2.29	0.48
2:B:3:LEU:HD23	2:B:87:ILE:CD1	2.45	0.47
2:B:49:ARG:HB3	2:B:49:ARG:NH1	2.28	0.47
2:C:156:LEU:HD12	2:C:156:LEU:HA	1.73	0.47
2:A:35:SER:HB2	2:A:140:ARG:HD3	1.96	0.47
2:B:174:TRP:CZ3	2:B:208:SER:CA	2.98	0.47
2:B:233:ILE:CG2	2:B:234:SER:N	2.78	0.47
2:A:89:ILE:HD13	2:A:132:TRP:CE3	2.45	0.47
2:A:91:ILE:N	2:A:91:ILE:CD1	2.78	0.47
1:D:4:DA:H2''	1:D:5:DT:O5'	2.15	0.47
2:A:21:CYS:N	2:B:24:ILE:O	2.39	0.47
2:A:152:ASN:O	2:A:154:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ILE:CG2	2:B:190:GLY:N	2.78	0.46
2:C:3:LEU:CD2	2:C:87:ILE:HD12	2.45	0.46
2:C:60:GLY:O	2:C:79:LYS:HG2	2.15	0.46
1:E:6:DA:H2''	1:E:7:DT:H5'	1.96	0.46
2:A:211:GLU:OE2	2:A:233:ILE:HD11	2.15	0.46
2:B:221:ARG:CG	2:B:221:ARG:NH1	2.77	0.46
2:C:170:LEU:HG	2:C:171:GLN:N	2.29	0.46
2:C:38:LYS:HB2	2:C:38:LYS:HE2	1.76	0.46
2:C:82:GLU:N	2:C:83:PRO:CD	2.78	0.46
2:A:233:ILE:CG2	2:A:234:SER:N	2.78	0.46
2:B:155:GLU:O	2:B:158:GLU:HB2	2.15	0.46
2:A:87:ILE:CG1	2:A:130:ALA:HB3	2.46	0.46
2:A:180:LEU:HD23	2:A:180:LEU:N	2.21	0.46
2:B:49:ARG:HB2	2:B:75:PHE:CE2	2.51	0.46
2:B:57:GLU:C	2:B:59:HIS:H	2.24	0.46
2:B:72:TYR:CD2	2:B:73:PRO:HB3	2.51	0.46
2:A:110:TYR:CD1	2:A:111:THR:HG23	2.51	0.46
2:A:124:PRO:HD2	2:A:127:GLN:NE2	2.31	0.46
2:B:151:TYR:N	2:B:151:TYR:CD1	2.84	0.46
2:B:236:TYR:O	2:B:239:TRP:N	2.49	0.46
2:C:75:PHE:HB2	2:C:89:ILE:HB	1.98	0.45
2:C:62:ILE:CG2	2:C:63:VAL:N	2.79	0.45
2:C:114:ILE:HD13	2:C:114:ILE:HA	1.63	0.45
2:B:29:LYS:NZ	2:B:150:THR:CG2	2.80	0.45
2:A:22:GLY:O	2:B:24:ILE:HG22	2.16	0.45
2:A:133:ILE:HD13	2:A:133:ILE:N	2.30	0.45
2:B:140:ARG:HG3	2:B:140:ARG:O	2.15	0.45
2:A:153:ILE:HG21	2:B:153:ILE:HD11	1.99	0.45
2:A:239:TRP:C	2:A:241:TYR:N	2.73	0.45
1:F:5:DT:C7	2:C:186:THR:HB	2.45	0.45
2:A:89:ILE:CD1	2:A:132:TRP:CE3	2.99	0.45
2:C:48:SER:O	2:C:52:ILE:HG13	2.15	0.45
2:C:86:LYS:O	2:C:129:ILE:HG12	2.16	0.45
2:B:123:TYR:HB2	2:B:128:TYR:CE1	2.51	0.45
2:C:136:TYR:HA	2:C:167:LYS:O	2.17	0.45
2:C:156:LEU:HD12	2:C:159:ILE:HD12	1.98	0.45
2:A:164:LYS:HB2	2:A:164:LYS:HE3	1.47	0.45
2:A:238:ASN:O	2:A:241:TYR:N	2.46	0.45
2:B:44:PHE:CD2	2:B:93:THR:HG21	2.52	0.45
2:A:110:TYR:CD1	2:A:111:THR:CG2	3.00	0.45
2:B:8:ILE:HG23	2:B:12:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:240:ILE:C	2:C:241:TYR:CD1	2.95	0.45
2:A:49:ARG:O	2:A:49:ARG:HG2	2.14	0.44
2:A:193:HIS:CD2	2:A:193:HIS:C	2.95	0.44
2:B:66:PRO:HB3	2:B:122:VAL:CG2	2.47	0.44
1:D:4:DA:H5'	2:B:119:LYS:NZ	2.32	0.44
2:B:221:ARG:CB	2:B:221:ARG:CZ	2.96	0.44
2:B:40:LEU:HA	2:B:43:ILE:HD12	1.98	0.44
1:E:6:DA:H2'	1:E:7:DT:H5'	1.94	0.44
2:C:62:ILE:HG22	2:C:63:VAL:N	2.32	0.44
2:B:86:LYS:O	2:B:128:TYR:HA	2.17	0.44
2:C:51:ILE:H	2:C:51:ILE:HG13	1.57	0.44
2:C:73:PRO:HG2	2:C:75:PHE:O	2.16	0.44
2:C:136:TYR:CD1	2:C:168:VAL:HG23	2.52	0.44
2:A:153:ILE:HB	2:B:153:ILE:CD1	2.48	0.44
2:A:171:GLN:NE2	2:A:202:GLY:HA3	2.32	0.44
2:A:208:SER:C	2:A:210:ASP:N	2.74	0.44
2:B:135:GLY:HA3	2:B:169:PHE:CZ	2.52	0.44
2:B:137:VAL:O	2:B:166:VAL:HA	2.17	0.44
2:B:139:THR:HB	2:B:164:LYS:HB3	2.00	0.44
2:C:169:PHE:CD1	2:C:169:PHE:C	2.96	0.44
2:C:238:ASN:C	2:C:240:ILE:N	2.75	0.44
2:A:31:TYR:CD1	2:A:150:THR:CG2	3.01	0.44
2:B:7:LEU:HD12	2:B:7:LEU:HA	1.78	0.44
2:C:49:ARG:CB	2:C:50:PRO:CD	2.96	0.44
2:A:95:TYR:O	2:A:96:THR:HG23	2.17	0.43
2:A:171:GLN:CG	2:A:172:ASP:N	2.80	0.43
2:A:233:ILE:CD1	2:A:237:ARG:NH2	2.81	0.43
2:B:107:LEU:HD22	2:B:133:ILE:HD11	2.00	0.43
2:B:229:LYS:HG2	2:B:230:TYR:HD2	1.83	0.43
2:A:138:TYR:CE1	2:A:140:ARG:HB3	2.53	0.43
2:B:4:ARG:NH1	2:B:172:ASP:OD1	2.48	0.43
2:C:170:LEU:O	2:C:171:GLN:HB2	2.18	0.43
2:A:72:TYR:CD1	2:A:72:TYR:C	2.96	0.43
2:A:93:THR:HA	2:A:136:TYR:O	2.18	0.43
2:A:110:TYR:CZ	2:A:187:THR:HG23	2.53	0.43
2:C:49:ARG:N	2:C:50:PRO:CD	2.80	0.43
2:C:86:LYS:HE2	2:C:123:TYR:CD2	2.53	0.43
2:C:121:ILE:HG12	2:C:122:VAL:N	2.32	0.43
2:A:132:TRP:O	2:A:133:ILE:HD13	2.18	0.43
2:A:159:ILE:HG22	2:A:160:PRO:N	2.33	0.43
2:A:73:PRO:HG3	2:A:88:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:TYR:CD1	2:A:151:TYR:N	2.85	0.43
2:A:211:GLU:CD	2:A:237:ARG:HH21	2.22	0.43
2:C:82:GLU:O	2:C:84:ASN:N	2.51	0.43
2:C:187:THR:HG22	2:C:187:THR:O	2.19	0.43
2:B:11:LEU:HD23	2:B:11:LEU:HA	1.84	0.43
2:B:86:LYS:HE2	2:B:123:TYR:CE2	2.53	0.43
2:A:7:LEU:HD12	2:A:7:LEU:C	2.42	0.43
2:B:136:TYR:HA	2:B:167:LYS:O	2.19	0.43
2:B:196:TYR:CD1	2:B:196:TYR:C	2.96	0.43
2:B:206:PHE:CE1	2:B:215:TYR:CB	3.02	0.43
2:A:42:THR:CG2	2:B:39:VAL:HG21	2.46	0.42
2:B:122:VAL:HG12	2:B:123:TYR:CE1	2.52	0.42
2:A:77:LEU:HD12	2:A:77:LEU:N	2.35	0.42
2:A:205:ILE:HG22	2:A:206:PHE:N	2.34	0.42
2:B:110:TYR:HB3	2:B:189:ILE:HG13	2.01	0.42
2:C:138:TYR:HB3	2:C:166:VAL:HG22	2.02	0.42
2:A:66:PRO:HD3	2:A:74:ASP:O	2.20	0.42
2:A:158:GLU:O	2:A:160:PRO:HD3	2.20	0.42
2:B:39:VAL:HG12	2:B:43:ILE:HD11	2.01	0.42
2:C:221:ARG:H	2:C:221:ARG:HG2	1.46	0.42
2:A:140:ARG:O	2:A:140:ARG:HG3	2.20	0.42
2:B:7:LEU:HD23	2:B:170:LEU:HD22	2.01	0.42
2:A:171:GLN:NE2	2:A:202:GLY:HA2	2.34	0.42
2:B:169:PHE:CD1	2:B:169:PHE:C	2.96	0.42
2:C:68:GLN:OE1	2:C:71:HIS:CG	2.73	0.42
2:C:179:ASP:OD1	2:C:179:ASP:N	2.51	0.42
2:A:80:PRO:C	2:A:82:GLU:H	2.28	0.42
2:A:189:ILE:HD13	2:A:212:PHE:HE2	1.84	0.42
2:A:233:ILE:C	2:A:235:GLU:N	2.78	0.42
2:C:24:ILE:HG23	2:C:24:ILE:O	2.18	0.42
2:C:138:TYR:CD1	2:C:138:TYR:C	2.97	0.42
1:E:1:DG:H2''	1:E:2:DG:C8	2.54	0.42
1:E:5:DT:C4	1:E:6:DA:N7	2.88	0.42
2:A:105:PHE:HB2	2:A:191:SER:CB	2.47	0.42
2:B:49:ARG:N	2:B:50:PRO:HD2	2.35	0.42
2:C:203:LYS:HA	2:C:203:LYS:HD2	1.82	0.41
2:B:30:ILE:CD1	2:B:156:LEU:HD21	2.50	0.41
2:C:75:PHE:HE2	2:C:91:ILE:HD12	1.84	0.41
2:B:218:ASN:OD1	2:B:218:ASN:N	2.53	0.41
2:B:27:GLU:H	2:B:27:GLU:CD	2.29	0.41
2:B:130:ALA:C	2:B:131:HIS:CD2	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:92:LYS:O	2:A:135:GLY:HA2	2.21	0.41
2:A:159:ILE:HA	2:A:160:PRO:HD3	1.86	0.41
2:A:233:ILE:HD11	2:A:237:ARG:NH2	2.35	0.41
2:B:8:ILE:CG2	2:B:12:TYR:CE2	2.97	0.41
2:C:77:LEU:CD1	2:C:89:ILE:HD12	2.50	0.41
2:A:110:TYR:CE1	2:A:187:THR:HG23	2.56	0.41
2:A:23:ILE:O	2:A:30:ILE:HG23	2.21	0.41
2:B:100:ASN:HD21	2:B:195:HIS:CD2	2.33	0.41
2:B:212:PHE:CD1	2:B:212:PHE:C	2.99	0.41
2:C:68:GLN:HB2	2:C:71:HIS:ND1	2.35	0.41
2:C:235:GLU:O	2:C:239:TRP:HB2	2.21	0.41
2:C:240:ILE:HG22	2:C:240:ILE:O	2.20	0.41
1:E:2:DG:C6	1:E:3:DG:C6	3.09	0.41
2:A:138:TYR:CD1	2:A:138:TYR:C	2.99	0.41
2:C:40:LEU:HD23	2:C:40:LEU:HA	1.82	0.41
2:C:78:TYR:CD1	2:C:78:TYR:C	2.96	0.41
2:C:90:ASP:HB3	2:C:133:ILE:CD1	2.51	0.41
2:A:153:ILE:O	2:A:153:ILE:HG12	2.19	0.41
2:A:179:ASP:HB2	2:A:232:ASN:HA	2.03	0.41
2:B:8:ILE:O	2:B:12:TYR:CD2	2.74	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.76	0.41
2:C:24:ILE:HA	2:C:29:LYS:O	2.21	0.41
2:C:117:ASN:OD1	2:C:117:ASN:O	2.39	0.41
2:A:204:GLY:HA3	3:A:767:HOH:O	2.20	0.40
2:C:187:THR:O	2:C:187:THR:CG2	2.70	0.40
2:B:8:ILE:HG23	2:B:12:TYR:CE2	2.55	0.40
2:C:61:TYR:CD1	2:C:79:LYS:HG3	2.56	0.40
2:A:77:LEU:N	2:A:77:LEU:CD1	2.84	0.40
2:A:189:ILE:HD13	2:A:212:PHE:CE2	2.56	0.40
2:B:55:ILE:C	2:B:57:GLU:N	2.80	0.40
2:B:78:TYR:CD1	2:B:78:TYR:C	2.99	0.40
2:C:11:LEU:HD23	2:C:11:LEU:HA	1.78	0.40
2:C:77:LEU:HD13	2:C:89:ILE:CD1	2.50	0.40

There are no symmetry-related clashes.

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	238/244 (98%)	190 (80%)	34 (14%)	14 (6%)	1	7
2	B	238/244 (98%)	191 (80%)	40 (17%)	7 (3%)	3	20
2	C	238/244 (98%)	190 (80%)	31 (13%)	17 (7%)	1	4
All	All	714/732 (98%)	571 (80%)	105 (15%)	38 (5%)	1	9

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	99	GLU
2	A	101	GLU
2	A	144	ARG
2	A	151	TYR
2	A	153	ILE
2	B	15	ASN
2	B	144	ARG
2	B	145	LYS
2	C	13	ASP
2	C	83	PRO
2	C	99	GLU
2	C	117	ASN
2	C	142	ALA
2	C	143	THR
2	C	148	LEU
2	A	15	ASN
2	A	16	GLN
2	A	100	ASN
2	A	196	TYR
2	A	237	ARG
2	B	13	ASP
2	B	35	SER
2	B	125	PHE
2	B	148	LEU

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Mol	Chain	Res	Type
2	C	184	GLY
2	C	227	ASN
2	C	239	TRP
2	A	142	ALA
2	A	143	THR
2	C	14	GLU
2	C	125	PHE
2	C	203	LYS
2	C	228	ASP
2	C	191	SER
2	A	13	ASP
2	A	141	VAL
2	C	82	GLU
2	C	28	GLY

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	217/220 (99%)	155 (71%)	62 (29%)	0	2
2	B	217/220 (99%)	156 (72%)	61 (28%)	0	2
2	C	217/220 (99%)	160 (74%)	57 (26%)	0	3
All	All	651/660 (99%)	471 (72%)	180 (28%)	0	2

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	7	LEU
2	A	8	ILE
2	A	11	LEU
2	A	14	GLU
2	A	16	GLN
2	A	17	LYS
2	A	19	ASP
2	A	20	VAL

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Mol	Chain	Res	Type
2	A	23	ILE
2	A	29	LYS
2	A	38	LYS
2	A	42	THR
2	A	45	GLU
2	A	52	ILE
2	A	57	GLU
2	A	69	GLN
2	A	74	ASP
2	A	81	SER
2	A	84	ASN
2	A	87	ILE
2	A	89	ILE
2	A	90	ASP
2	A	92	LYS
2	A	99	GLU
2	A	100	ASN
2	A	101	GLU
2	A	103	ILE
2	A	104	LYS
2	A	107	LEU
2	A	114	ILE
2	A	115	ARG
2	A	133	ILE
2	A	139	THR
2	A	140	ARG
2	A	144	ARG
2	A	146	SER
2	A	147	SER
2	A	148	LEU
2	A	152	ASN
2	A	153	ILE
2	A	158	GLU
2	A	159	ILE
2	A	164	LYS
2	A	170	LEU
2	A	188	ASN
2	A	189	ILE
2	A	191	SER
2	A	197	LYS
2	A	200	VAL
2	A	205	ILE

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Mol	Chain	Res	Type
2	A	212	PHE
2	A	214	ASP
2	A	221	ARG
2	A	223	SER
2	A	225	LEU
2	A	227	ASN
2	A	229	LYS
2	A	234	SER
2	A	237	ARG
2	A	238	ASN
2	A	240	ILE
2	A	241	TYR
2	B	4	ARG
2	B	8	ILE
2	B	9	ASN
2	B	15	ASN
2	B	17	LYS
2	B	20	VAL
2	B	23	ILE
2	B	27	GLU
2	B	29	LYS
2	B	30	ILE
2	B	38	LYS
2	B	41	SER
2	B	46	LEU
2	B	48	SER
2	B	49	ARG
2	B	57	GLU
2	B	73	PRO
2	B	81	SER
2	B	82	GLU
2	B	84	ASN
2	B	89	ILE
2	B	91	ILE
2	B	92	LYS
2	B	94	THR
2	B	97	ASN
2	B	103	ILE
2	B	104	LYS
2	B	106	THR
2	B	114	ILE
2	B	126	ASP

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Mol	Chain	Res	Type
2	B	129	ILE
2	B	133	ILE
2	B	137	VAL
2	B	140	ARG
2	B	144	ARG
2	B	148	LEU
2	B	150	THR
2	B	152	ASN
2	B	153	ILE
2	B	155	GLU
2	B	157	ASN
2	B	164	LYS
2	B	166	VAL
2	B	167	LYS
2	B	170	LEU
2	B	173	LYS
2	B	188	ASN
2	B	191	SER
2	B	192	ILE
2	B	197	LYS
2	B	203	LYS
2	B	205	ILE
2	B	212	PHE
2	B	218	ASN
2	B	221	ARG
2	B	223	SER
2	B	225	LEU
2	B	228	ASP
2	B	237	ARG
2	B	240	ILE
2	B	241	TYR
2	C	2	SER
2	C	3	LEU
2	C	8	ILE
2	C	9	ASN
2	C	12	TYR
2	C	14	GLU
2	C	15	ASN
2	C	20	VAL
2	C	21	CYS
2	C	23	ILE
2	C	27	GLU

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Mol	Chain	Res	Type
2	C	35	SER
2	C	38	LYS
2	C	40	LEU
2	C	41	SER
2	C	42	THR
2	C	46	LEU
2	C	48	SER
2	C	49	ARG
2	C	68	GLN
2	C	70	ASN
2	C	82	GLU
2	C	90	ASP
2	C	92	LYS
2	C	94	THR
2	C	99	GLU
2	C	100	ASN
2	C	101	GLU
2	C	104	LYS
2	C	114	ILE
2	C	115	ARG
2	C	133	ILE
2	C	134	ILE
2	C	137	VAL
2	C	140	ARG
2	C	143	THR
2	C	144	ARG
2	C	148	LEU
2	C	149	LYS
2	C	151	TYR
2	C	153	ILE
2	C	157	ASN
2	C	158	GLU
2	C	168	VAL
2	C	171	GLN
2	C	185	ASN
2	C	192	ILE
2	C	203	LYS
2	C	205	ILE
2	C	209	GLU
2	C	221	ARG
2	C	223	SER
2	C	224	GLN

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Mol	Chain	Res	Type
2	C	225	LEU
2	C	226	ARG
2	C	234	SER
2	C	241	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	69	GLN
2	A	127	GLN
2	B	97	ASN
2	B	193	HIS
2	B	195	HIS
2	B	238	ASN
2	C	171	GLN
2	C	185	ASN
2	C	188	ASN
2	C	193	HIS
2	C	218	ASN
2	C	238	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.