



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 PM UTC

PDB ID : 1SX8 / pdb_00001sx8
Title : EcoRV bound to cognate DNA and Mn²⁺
Authors : Horton, N.C.; Perona, J.J.
Deposited on : 2004-03-30
Resolution : 2.15 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

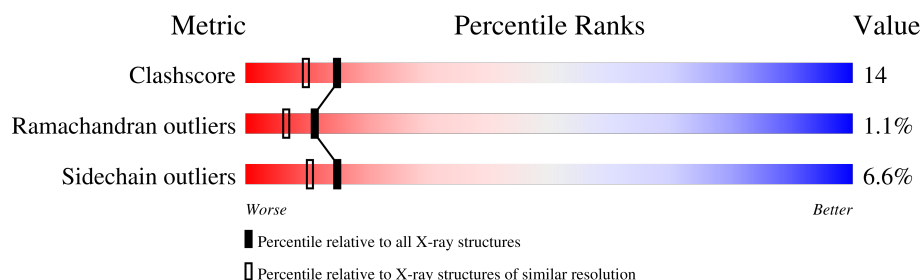
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	11	
1	D	11	
2	A	244	
2	B	244	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4379 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 5'-D(*C*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			202	99	36	58	9			
1	D	10	Total	C	N	O	P	0	0	0
			201	98	37	57	9			

- Molecule 2 is a protein called Type II restriction enzyme EcoRV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	241	Total	C	N	O	S	0	0	0
			1930	1245	318	366	1			
2	B	235	Total	C	N	O	S	0	0	0
			1888	1218	310	359	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	ALA	LYS	engineered mutation	UNP P04390
B	92	ALA	LYS	engineered mutation	UNP P04390

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mn	0	0
			3	3		
3	B	3	Total	Mn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	12	Total	O	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	8	Total 8	O 8	0	0
4	A	79	Total 79	O 79	0	0
4	B	53	Total 53	O 53	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: 5'-D(*C*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3'

Chain C: 



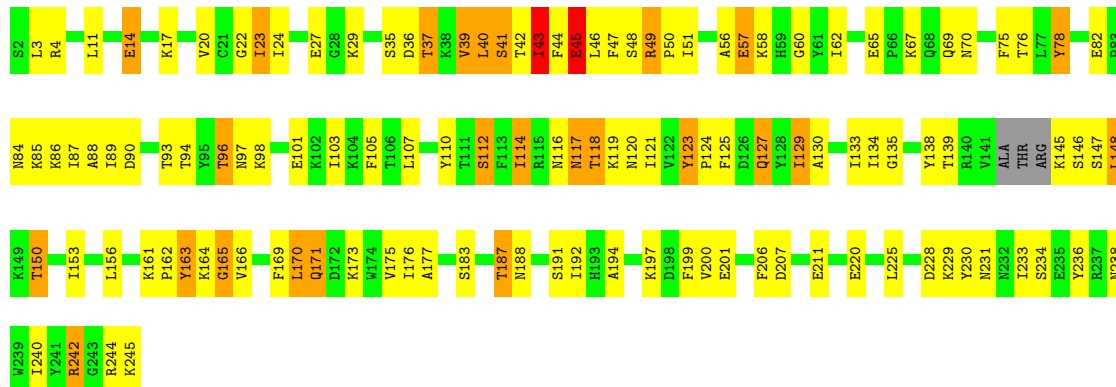
- Molecule 1: 5'-D(*C*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3'

Chain D: 

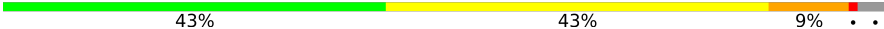


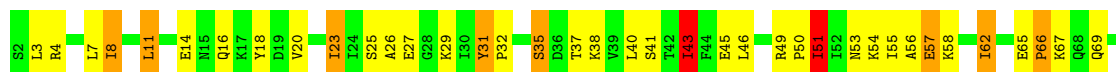
- Molecule 2: Type II restriction enzyme EcoRV

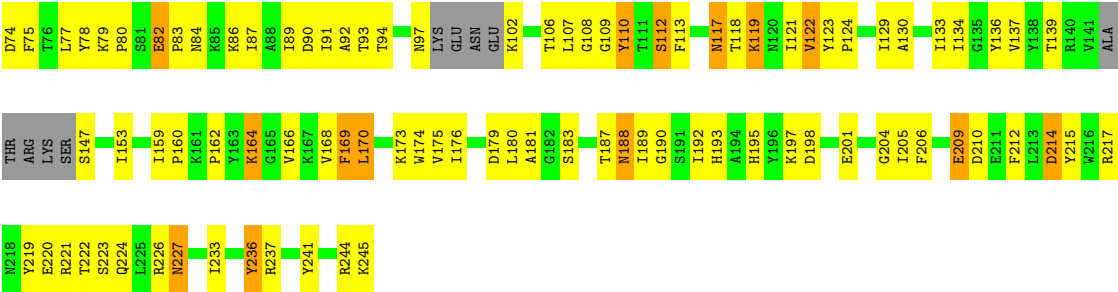
Chain A: 



- Molecule 2: Type II restriction enzyme EcoRV

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.80Å 49.10Å 63.70Å 96.90° 108.90° 107.10°	Depositor
Resolution (Å)	20.00 – 2.15	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.15)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4379	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.02	0/226	1.55	4/347 (1.2%)
1	D	1.07	0/225	1.39	3/345 (0.9%)
2	A	2.02	51/1980 (2.6%)	1.71	45/2692 (1.7%)
2	B	2.04	57/1936 (2.9%)	1.70	34/2631 (1.3%)
All	All	1.95	108/4367 (2.5%)	1.68	86/6015 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	2
2	B	0	2
All	All	0	6

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	49	ARG	CA-C	10.54	1.66	1.52
2	B	94	THR	CA-CB	9.98	1.70	1.53
2	B	168	VAL	CA-CB	-8.92	1.43	1.54
2	A	175	VAL	CA-CB	8.30	1.66	1.54
2	B	173	LYS	CA-C	8.18	1.63	1.52
2	A	11	LEU	N-CA	7.92	1.55	1.46
2	A	88	ALA	CA-CB	7.63	1.65	1.53
2	A	75	PHE	C-O	7.49	1.32	1.23
2	A	207	ASP	C-O	-7.47	1.14	1.24
2	A	93	THR	C-O	7.39	1.32	1.23
2	A	207	ASP	CA-C	-7.34	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	87	ILE	CA-CB	7.34	1.64	1.54
2	A	231	ASN	CA-C	7.25	1.62	1.52
2	B	66	PRO	CA-C	7.22	1.61	1.52
2	A	177	ALA	C-O	7.13	1.32	1.23
2	B	241	TYR	C-O	-7.01	1.16	1.24
2	B	210	ASP	N-CA	6.93	1.54	1.46
2	B	113	PHE	C-O	6.88	1.32	1.24
2	B	11	LEU	C-O	6.83	1.32	1.24
2	B	74	ASP	N-CA	6.82	1.54	1.46
2	B	109	GLY	CA-C	6.73	1.60	1.52
2	A	183	SER	N-CA	6.63	1.54	1.46
2	B	77	LEU	CA-C	-6.62	1.44	1.52
2	A	211	GLU	CA-C	6.62	1.61	1.52
2	B	237	ARG	CA-C	6.57	1.61	1.52
2	B	133	ILE	N-CA	-6.57	1.38	1.46
2	B	134	ILE	N-CA	6.46	1.53	1.46
2	B	176	ILE	CA-CB	6.46	1.62	1.54
2	B	107	LEU	CA-C	-6.42	1.44	1.52
2	A	45	GLU	N-CA	-6.38	1.38	1.46
2	B	159	ILE	CA-C	6.38	1.59	1.52
2	B	209	GLU	CA-C	6.34	1.61	1.52
2	A	135	GLY	CA-C	6.31	1.56	1.52
2	B	8	ILE	CA-C	6.26	1.60	1.52
2	A	127	GLN	N-CA	6.26	1.54	1.46
2	B	51	ILE	CA-C	6.25	1.60	1.52
2	B	244	ARG	CD-NE	6.25	1.55	1.46
2	B	169	PHE	N-CA	6.25	1.53	1.45
2	B	112	SER	C-O	6.23	1.31	1.24
2	B	181	ALA	CA-CB	-6.18	1.43	1.53
2	B	23	ILE	CB-CG2	6.17	1.73	1.52
2	B	41	SER	CA-CB	6.16	1.63	1.53
2	B	54	LYS	CA-C	6.14	1.60	1.52
2	B	133	ILE	CA-CB	6.12	1.61	1.53
2	B	212	PHE	N-CA	6.11	1.53	1.46
2	A	146	SER	CA-C	6.10	1.60	1.52
2	A	161	LYS	CA-C	-6.06	1.44	1.52
2	A	134	ILE	C-O	6.03	1.30	1.23
2	B	91	ILE	CA-CB	6.03	1.62	1.54
2	A	206	PHE	CD2-CE2	5.98	1.56	1.38
2	B	136	TYR	CA-CB	5.94	1.64	1.53
2	A	211	GLU	C-O	5.88	1.30	1.24
2	B	89	ILE	N-CA	-5.85	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	GLN	CA-C	5.84	1.60	1.52
2	B	57	GLU	C-O	-5.81	1.17	1.24
2	A	238	ASN	N-CA	5.76	1.53	1.46
2	B	210	ASP	C-O	-5.75	1.17	1.24
2	A	244	ARG	CB-CG	5.74	1.69	1.52
2	B	26	ALA	CA-C	5.73	1.60	1.52
2	A	43	ILE	CA-C	5.72	1.59	1.52
2	A	194	ALA	C-O	-5.69	1.17	1.23
2	B	93	THR	CA-CB	5.68	1.64	1.54
2	A	199	PHE	CA-C	5.61	1.59	1.52
2	B	217	ARG	C-O	-5.58	1.16	1.24
2	A	57	GLU	CA-C	5.56	1.60	1.52
2	A	3	LEU	CA-C	5.55	1.59	1.52
2	B	87	ILE	CA-CB	-5.54	1.47	1.54
2	B	160	PRO	CA-C	5.53	1.59	1.52
2	A	89	ILE	C-O	-5.50	1.18	1.24
2	A	24	ILE	CA-CB	5.50	1.64	1.55
2	A	171	GLN	C-O	5.49	1.30	1.23
2	A	200	VAL	N-CA	5.48	1.52	1.46
2	A	42	THR	CA-C	5.48	1.59	1.52
2	A	90	ASP	N-CA	-5.46	1.39	1.45
2	A	134	ILE	CA-C	5.42	1.59	1.52
2	A	191	SER	C-O	5.42	1.30	1.23
2	A	187	THR	C-O	5.42	1.30	1.24
2	B	130	ALA	C-O	5.41	1.31	1.23
2	B	137	VAL	CA-CB	5.41	1.63	1.55
2	B	119	LYS	C-O	5.39	1.30	1.24
2	A	200	VAL	CB-CG1	5.34	1.70	1.52
2	A	169	PHE	CD2-CE2	5.33	1.54	1.38
2	B	236	TYR	CA-C	5.32	1.59	1.52
2	A	89	ILE	N-CA	-5.31	1.39	1.46
2	B	31	TYR	CA-C	5.31	1.58	1.52
2	A	14	GLU	CA-C	5.31	1.59	1.52
2	B	180	LEU	C-O	5.30	1.30	1.24
2	A	125	PHE	CE2-CZ	5.29	1.54	1.38
2	A	123	TYR	C-O	5.29	1.29	1.24
2	B	122	VAL	CA-CB	5.28	1.61	1.54
2	A	58	LYS	C-O	5.27	1.30	1.24
2	B	181	ALA	CA-C	5.27	1.59	1.52
2	A	23	ILE	N-CA	-5.27	1.39	1.46
2	A	165	GLY	C-O	-5.25	1.16	1.23
2	B	107	LEU	CG-CD2	5.22	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	ALA	C-O	5.21	1.30	1.24
2	A	76	THR	CA-CB	5.20	1.60	1.53
2	B	129	ILE	CA-CB	5.19	1.60	1.54
2	A	47	PHE	N-CA	-5.16	1.40	1.46
2	B	170	LEU	CA-C	5.16	1.58	1.52
2	B	7	LEU	CG-CD1	5.12	1.69	1.52
2	A	112	SER	CA-C	5.12	1.59	1.52
2	B	164	LYS	C-O	5.10	1.30	1.23
2	B	55	ILE	C-O	-5.09	1.18	1.24
2	A	56	ALA	CA-C	5.07	1.59	1.52
2	A	200	VAL	CA-C	5.06	1.58	1.52
2	B	190	GLY	C-O	5.05	1.30	1.23
2	B	121	ILE	CB-CG2	5.03	1.69	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	166	VAL	N-CA-C	11.55	124.52	108.93
2	B	65	GLU	CA-C-N	-11.45	109.09	120.31
2	B	65	GLU	C-N-CA	-11.45	109.09	120.31
2	A	164	LYS	CA-C-N	-10.22	101.38	121.41
2	A	164	LYS	C-N-CA	-10.22	101.38	121.41
2	B	82	GLU	CA-C-N	9.88	129.50	119.82
2	B	82	GLU	C-N-CA	9.88	129.50	119.82
1	C	2	DA	O5'-C5'-C4'	9.73	125.39	110.80
2	B	69	GLN	N-CA-C	9.70	124.92	113.18
2	B	35	SER	N-CA-C	7.74	123.20	112.45
1	C	6	DT	C4'-C3'-O3'	7.45	121.17	110.00
2	B	221	ARG	N-CA-C	7.33	120.14	111.71
2	A	3	LEU	N-CA-C	-7.31	103.25	111.07
2	A	48	SER	N-CA-C	7.30	119.32	111.36
2	B	38	LYS	N-CA-C	-7.19	102.55	111.75
2	A	161	LYS	CA-C-N	7.17	128.81	119.84
2	A	161	LYS	C-N-CA	7.17	128.81	119.84
2	B	117	ASN	N-CA-C	7.16	126.05	110.80
2	A	148	LEU	N-CA-C	6.87	121.27	113.02
2	A	240	ILE	N-CA-C	-6.85	104.09	110.53
2	A	67	LYS	N-CA-C	-6.83	104.91	113.18
2	A	187	THR	N-CA-C	6.76	125.20	110.80
2	B	106	THR	N-CA-C	-6.60	98.96	109.59
2	B	3	LEU	N-CA-C	-6.58	103.37	111.33
2	B	67	LYS	N-CA-C	-6.45	101.69	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	GLU	N-CA-C	6.36	120.88	113.18
2	A	62	ILE	CB-CA-C	-6.29	104.67	111.59
2	A	65	GLU	N-CA-C	-6.27	102.79	110.31
1	D	8	DT	C2'-C3'-O3'	-6.24	102.14	111.50
2	B	217	ARG	N-CA-C	-6.22	104.95	112.54
2	B	92	ALA	N-CA-C	-6.21	99.60	109.23
2	A	228	ASP	N-CA-C	6.20	120.58	112.89
2	B	62	ILE	N-CA-C	-6.17	99.69	108.58
2	B	205	ILE	CB-CA-C	-6.17	104.61	110.65
1	D	6	DT	C4'-C3'-O3'	6.15	119.22	110.00
2	A	84	ASN	N-CA-C	-6.14	104.96	112.88
2	B	192	ILE	N-CA-C	-6.13	103.28	110.21
2	A	163	TYR	CB-CA-C	-6.07	100.03	110.95
2	B	227	ASN	N-CA-C	6.00	119.86	112.54
2	A	78	TYR	N-CA-C	5.95	117.45	108.46
2	A	97	ASN	N-CA-C	-5.94	105.12	112.90
2	B	79	LYS	CA-C-N	5.85	125.99	119.32
2	B	79	LYS	C-N-CA	5.85	125.99	119.32
1	D	10	DT	C4'-C3'-O3'	5.84	118.76	110.00
2	B	133	ILE	CB-CA-C	-5.82	103.11	111.19
2	B	57	GLU	N-CA-C	-5.81	104.85	111.07
2	B	110	TYR	N-CA-C	-5.80	104.76	112.94
2	A	42	THR	N-CA-C	-5.76	104.70	110.97
2	A	4	ARG	N-CA-C	5.70	117.18	110.97
2	A	133	ILE	CB-CA-C	-5.67	102.72	110.77
2	A	37	THR	N-CA-C	5.66	122.86	110.80
2	B	113	PHE	N-CA-C	5.59	118.14	111.71
2	A	229	LYS	CA-C-O	5.55	122.94	119.55
2	A	242	ARG	CA-C-N	-5.53	115.00	122.63
2	A	242	ARG	C-N-CA	-5.53	115.00	122.63
2	A	164	LYS	O-C-N	-5.52	115.25	122.59
1	C	6	DT	N1-C1'-C2'	-5.46	105.31	113.50
2	B	89	ILE	N-CA-C	5.42	115.66	107.75
2	A	22	GLY	CA-C-N	-5.41	114.56	122.68
2	A	22	GLY	C-N-CA	-5.41	114.56	122.68
2	B	75	PHE	N-CA-C	5.38	117.84	108.76
2	A	62	ILE	N-CA-C	-5.34	104.23	110.05
2	A	49	ARG	CG-CD-NE	-5.33	100.28	112.00
2	B	245	LYS	CA-C-O	-5.33	111.74	120.80
2	A	188	ASN	CB-CA-C	-5.32	100.53	109.48
2	B	108	GLY	CA-C-O	-5.28	118.35	122.52
2	B	214	ASP	N-CA-C	-5.28	105.58	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	39	VAL	N-CA-C	-5.27	105.57	110.53
2	A	17	LYS	N-CA-C	5.25	119.75	113.23
2	A	11	LEU	CA-C-O	5.24	126.11	120.55
2	B	122	VAL	N-CA-C	5.21	115.99	110.72
2	A	192	ILE	N-CA-C	-5.21	104.32	110.21
2	A	156	LEU	N-CA-C	5.21	116.95	111.28
2	A	60	GLY	N-CA-C	5.20	122.79	115.30
2	A	118	THR	N-CA-C	5.20	119.37	112.30
2	B	18	TYR	N-CA-C	5.19	117.91	109.24
2	A	161	LYS	CB-CA-C	-5.18	103.35	109.47
2	B	45	GLU	CA-C-O	-5.17	115.39	120.82
2	B	84	ASN	N-CA-C	5.12	119.62	113.17
2	A	46	LEU	CA-C-N	5.11	127.13	120.28
2	A	46	LEU	C-N-CA	5.11	127.13	120.28
1	C	8	DT	N1-C1'-C2'	5.04	121.06	113.50
2	A	36	ASP	CA-C-N	5.02	131.13	121.54
2	A	36	ASP	C-N-CA	5.02	131.13	121.54
2	B	43	ILE	CG1-CB-CG2	-5.02	95.63	110.70
2	A	150	THR	N-CA-C	-5.01	103.04	110.46

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	219	TYR	Sidechain
2	B	78	TYR	Sidechain
1	C	2	DA	Sidechain
1	C	6	DT	Sidechain
1	D	10	DT	Sidechain
1	D	6	DT	Sidechain

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	C	202	0	116	6	0
1	D	201	0	115	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1930	0	1814	57	0
2	B	1888	0	1778	60	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	79	0	0	2	0
4	B	53	0	0	2	0
4	C	12	0	0	1	0
4	D	8	0	0	0	0
All	All	4379	0	3823	110	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 14.

All (110) 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:23:ILE:HG22	2:B:23:ILE:HG22	1.39	1.04
2:B:62:ILE:HD11	2:B:80:PRO:HG3	1.47	0.94
2:A:82:GLU:HG3	2:A:85:LYS:HB2	1.52	0.90
2:B:11:LEU:HD23	2:B:51:ILE:HD12	1.56	0.84
2:A:110:TYR:HA	2:A:114:ILE:HG21	1.64	0.79
2:B:49:ARG:HB2	2:B:50:PRO:HD3	1.69	0.74
2:B:4:ARG:O	2:B:8:ILE:HG13	1.87	0.74
2:B:222:THR:HG22	2:B:224:GLN:H	1.55	0.71
1:D:9:DC:H5'	2:B:37:THR:HG21	1.73	0.71
2:A:20:VAL:HG11	2:B:23:ILE:HD12	1.72	0.70
2:B:53:ASN:O	2:B:57:GLU:HG3	1.92	0.68
2:B:58:LYS:O	2:B:58:LYS:HG2	1.93	0.67
2:B:8:ILE:HG23	4:B:254:HOH:O	1.94	0.67
2:B:62:ILE:CD1	2:B:80:PRO:HG3	2.24	0.65
2:B:57:GLU:HG2	4:B:299:HOH:O	1.98	0.64
2:A:27:GLU:H	2:A:27:GLU:CD	2.04	0.64
2:A:116:ASN:O	2:A:118:THR:N	2.31	0.63
2:A:148:LEU:HD13	2:B:53:ASN:ND2	2.13	0.63
2:A:96:THR:HG22	2:A:139:THR:HA	1.84	0.59
1:C:6:DT:O4'	2:A:70:ASN:HA	2.03	0.58
2:A:124:PRO:HD2	2:A:127:GLN:NE2	2.18	0.58
1:D:9:DC:C5'	2:B:37:THR:HG21	2.33	0.57
2:A:119:LYS:HG2	2:A:120:ASN:OD1	2.05	0.56
1:C:9:DC:H5''	2:A:37:THR:OG1	2.04	0.56
2:A:98:LYS:O	2:A:101:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:103:ILE:HG22	4:A:300:HOH:O	2.04	0.56
2:A:20:VAL:CG1	2:B:23:ILE:HD12	2.35	0.55
2:B:112:SER:HA	2:B:119:LYS:HD2	1.88	0.54
2:A:29:LYS:HE2	2:A:150:THR:HG21	1.90	0.54
2:B:206:PHE:CE1	2:B:233:ILE:HD13	2.43	0.53
1:D:1:DC:H2''	1:D:2:DA:C8	2.44	0.52
2:A:124:PRO:HD2	2:A:127:GLN:CD	2.34	0.52
1:D:9:DC:H2'	1:D:10:DT:H71	1.91	0.52
2:B:220:GLU:HB2	2:B:226:ARG:HG2	1.92	0.51
2:B:222:THR:HG22	2:B:223:SER:N	2.24	0.51
2:B:29:LYS:HD3	2:B:31:TYR:OH	2.11	0.51
2:B:86:LYS:HE3	2:B:123:TYR:CD1	2.45	0.51
2:B:174:TRP:CD1	2:B:209:GLU:HB2	2.46	0.51
2:B:25:SER:HB2	2:B:27:GLU:OE1	2.09	0.51
2:A:49:ARG:HB3	2:A:50:PRO:CD	2.41	0.51
2:A:170:LEU:C	2:A:170:LEU:HD23	2.35	0.51
2:B:174:TRP:CG	2:B:209:GLU:HB2	2.46	0.51
2:A:14:GLU:CD	2:A:51:ILE:HD11	2.36	0.51
2:A:163:TYR:C	2:A:163:TYR:CD1	2.89	0.50
2:A:233:ILE:HG23	2:A:234:SER:N	2.27	0.50
2:A:49:ARG:HB3	2:A:50:PRO:HD3	1.92	0.50
2:A:242:ARG:CZ	2:A:245:LYS:O	2.60	0.49
2:B:214:ASP:OD2	2:B:236:TYR:OH	2.19	0.49
2:A:145:LYS:C	2:A:147:SER:H	2.20	0.49
2:B:27:GLU:H	2:B:27:GLU:CD	2.21	0.49
2:A:39:VAL:HG13	2:B:46:LEU:HD11	1.93	0.49
2:B:222:THR:O	2:B:226:ARG:HG3	2.13	0.49
2:B:183:SER:OG	2:B:188:ASN:HB2	2.13	0.48
1:C:9:DC:OP1	2:A:94:THR:HA	2.14	0.48
2:A:40:LEU:HD23	2:A:138:TYR:CE2	2.48	0.48
2:B:139:THR:HB	2:B:164:LYS:HG3	1.95	0.48
2:A:27:GLU:CD	2:A:27:GLU:N	2.71	0.47
2:A:170:LEU:HD23	2:A:171:GLN:N	2.29	0.47
2:B:222:THR:HG22	2:B:224:GLN:N	2.26	0.47
2:B:83:PRO:O	2:B:86:LYS:HE2	2.13	0.47
2:A:23:ILE:HD12	2:B:43:ILE:HG23	1.97	0.47
2:B:175:VAL:O	2:B:204:GLY:HA3	2.15	0.47
2:A:43:ILE:HG22	2:A:44:PHE:N	2.27	0.47
2:A:145:LYS:C	2:A:147:SER:N	2.71	0.46
2:B:195:HIS:O	2:B:198:ASP:HB2	2.15	0.46
2:B:123:TYR:O	2:B:124:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ARG:CB	2:B:50:PRO:HD3	2.40	0.46
2:A:116:ASN:O	2:A:117:ASN:C	2.57	0.46
2:B:122:VAL:HG12	2:B:123:TYR:CD2	2.51	0.46
2:B:66:PRO:HB3	2:B:122:VAL:CG2	2.46	0.46
2:A:82:GLU:CD	2:A:85:LYS:HE2	2.41	0.46
2:A:230:TYR:CD1	2:A:236:TYR:HB2	2.51	0.46
2:B:169:PHE:C	2:B:169:PHE:CD1	2.94	0.46
2:A:170:LEU:C	2:A:170:LEU:CD2	2.90	0.45
2:B:222:THR:CG2	2:B:223:SER:N	2.78	0.45
2:A:171:GLN:HG2	2:A:176:ILE:CG2	2.46	0.45
1:C:5:DA:H2'	1:C:6:DT:C6	2.52	0.45
2:A:148:LEU:CD1	2:B:53:ASN:ND2	2.79	0.45
2:A:139:THR:H	2:A:165:GLY:H	1.65	0.44
2:B:66:PRO:HB3	2:B:122:VAL:HG22	1.98	0.44
2:A:121:ILE:HG12	2:A:123:TYR:O	2.18	0.44
2:B:27:GLU:CD	2:B:27:GLU:N	2.76	0.44
2:A:148:LEU:HD13	2:B:53:ASN:CG	2.43	0.43
2:A:220:GLU:HB3	2:A:225:LEU:HB2	2.00	0.43
2:B:31:TYR:HA	2:B:32:PRO:HD3	1.88	0.43
2:A:23:ILE:CD1	2:B:43:ILE:HG23	2.48	0.43
2:B:153:ILE:O	2:B:153:ILE:HG22	2.17	0.43
2:B:31:TYR:N	2:B:31:TYR:CD1	2.87	0.43
1:C:7:DA:H3'	4:C:18:HOH:O	2.18	0.43
2:A:23:ILE:HA	2:B:23:ILE:HA	2.00	0.43
2:A:41:SER:O	2:A:45:GLU:HB2	2.18	0.43
2:A:78:TYR:HB3	2:A:86:LYS:HG2	2.01	0.43
2:A:242:ARG:O	2:A:245:LYS:HE3	2.18	0.43
2:B:197:LYS:O	2:B:201:GLU:HG3	2.19	0.42
2:A:23:ILE:HD12	2:B:20:VAL:HG11	2.02	0.42
2:A:129:ILE:HD12	2:A:130:ALA:N	2.34	0.42
2:A:94:THR:HG22	2:A:105:PHE:CE2	2.55	0.42
2:A:23:ILE:CG2	2:B:23:ILE:HG22	2.29	0.41
2:A:112:SER:HA	2:A:119:LYS:HD2	2.01	0.41
2:B:14:GLU:HG2	2:B:51:ILE:HD13	2.02	0.41
2:B:102:LYS:HD2	2:B:193:HIS:CE1	2.55	0.41
2:A:107:LEU:O	2:A:173:LYS:HE3	2.19	0.41
2:A:40:LEU:HD23	2:A:138:TYR:CZ	2.55	0.41
2:A:110:TYR:CA	2:A:114:ILE:HG21	2.43	0.41
2:B:8:ILE:HG12	2:B:170:LEU:HB3	2.02	0.41
2:A:165:GLY:HA3	4:A:274:HOH:O	2.20	0.41
2:B:110:TYR:HB3	2:B:189:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:DA:H3'	2:B:223:SER:OG	2.22	0.40
1:D:9:DC:H2'	1:D:10:DT:C7	2.51	0.40
2:B:179:ASP:HB2	2:B:215:TYR:OH	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	237/244 (97%)	222 (94%)	12 (5%)	3 (1%)	9	5
2	B	229/244 (94%)	212 (93%)	15 (7%)	2 (1%)	14	9
All	All	466/488 (96%)	434 (93%)	27 (6%)	5 (1%)	11	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	117	ASN
2	B	117	ASN
2	A	162	PRO
2	A	187	THR
2	B	187	THR

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	199/219 (91%)	186 (94%)	13 (6%)	15	11
2	B	196/219 (90%)	183 (93%)	13 (7%)	15	10
All	All	395/438 (90%)	369 (93%)	26 (7%)	15	10

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	35	SER
2	A	40	LEU
2	A	41	SER
2	A	43	ILE
2	A	45	GLU
2	A	57	GLU
2	A	69	GLN
2	A	96	THR
2	A	114	ILE
2	A	129	ILE
2	A	153	ILE
2	A	170	LEU
2	A	197	LYS
2	B	35	SER
2	B	40	LEU
2	B	43	ILE
2	B	51	ILE
2	B	82	GLU
2	B	90	ASP
2	B	97	ASN
2	B	118	THR
2	B	147	SER
2	B	162	PRO
2	B	166	VAL
2	B	188	ASN
2	B	227	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	15	ASN
2	A	157	ASN
2	B	16	GLN
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	84	ASN
2	B	127	GLN
2	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.