Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:16 PM GMT

PDB ID	:	1SX8
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

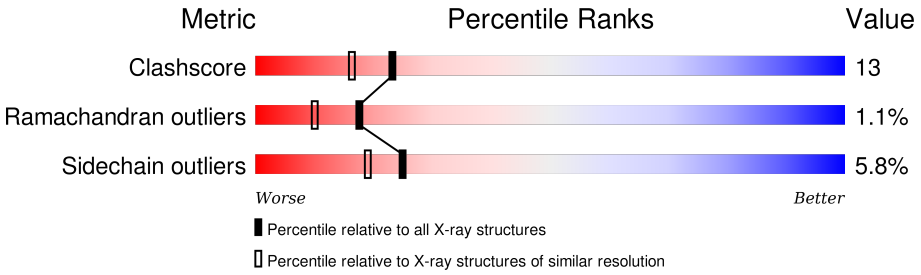
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	11	36% 18% 18% 18% 9%
1	D	11	18% 55% 9% 9% 9%
2	A	244	61% 33% 5%
2	B	244	55% 36% 5%

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	UNP P04390
B	92	ALA	LYS	ENGINEERED	UNP P04390

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	53	Total O 53 53	0	0
4	C	12	Total O 12 12	0	0
4	D	8	Total O 8 8	0	0

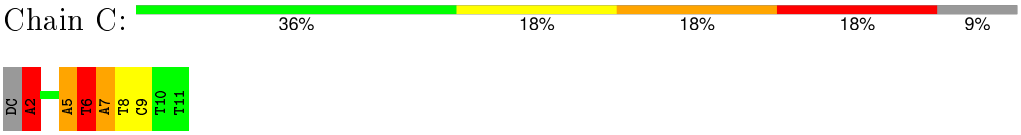
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

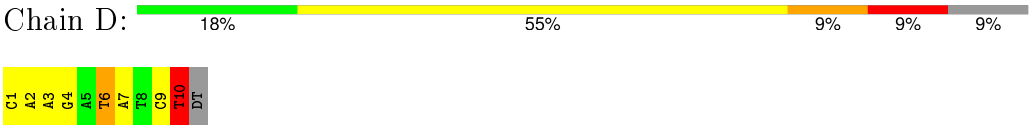
- Molecule 1: 5'-D(*C*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3'

Chain C:



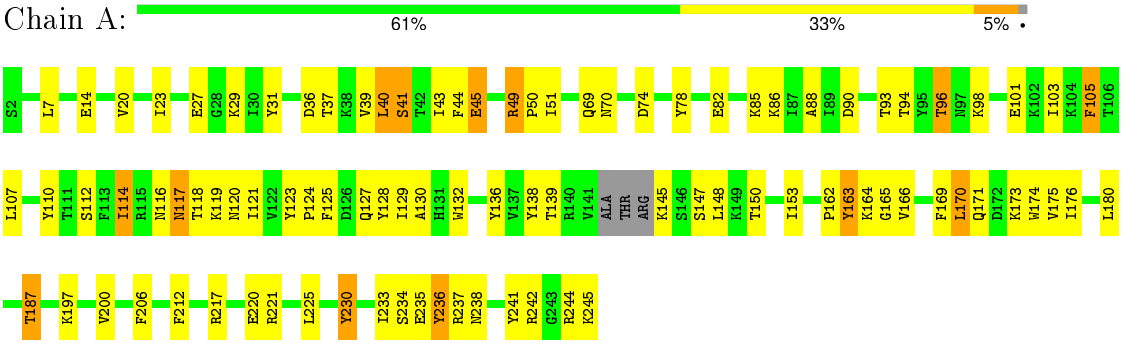
- Molecule 1: 5'-D(*C*AP*AP*GP*AP*TP*AP*TP*CP*TP*T)-3'

Chain D:



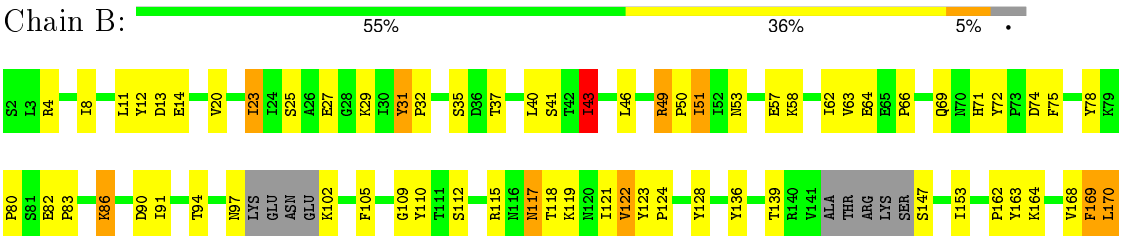
- Molecule 2: Type II restriction enzyme EcoRV

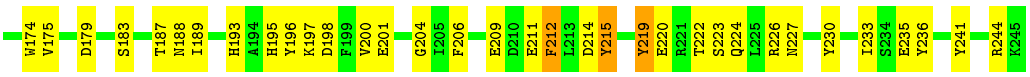
Chain A:



- Molecule 2: Type II restriction enzyme EcoRV

Chain B:




W174
V175
D179
S183
T187
N188
I189
H193
A194
H195
Y196
K197
D198
F199
V200
E201
G204
I205
F206
E209
D210
E211
F212
L213
D214
Y215
Y219
E220
R221
T222
S223
Q224
L225
R226
N227
Y230
I233
S234
E235
Y236
Y241
R244
K245

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	2.17	10/226 (4.4%)	1.57	2/347 (0.6%)
1	D	2.14	6/225 (2.7%)	1.50	1/345 (0.3%)
2	A	1.74	26/1980 (1.3%)	1.32	14/2692 (0.5%)
2	B	1.75	35/1936 (1.8%)	1.30	10/2631 (0.4%)
All	All	1.79	77/4367 (1.8%)	1.34	27/6015 (0.4%)

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 (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	6	DT	C2-N3	11.02	1.46	1.37
2	A	125	PHE	CE2-CZ	9.04	1.54	1.37
2	B	230	TYR	CE2-CZ	8.87	1.50	1.38
2	A	206	PHE	CD2-CE2	8.67	1.56	1.39
2	B	72	TYR	CD1-CE1	8.62	1.52	1.39
2	A	200	VAL	CB-CG1	8.25	1.70	1.52
2	A	169	PHE	CD2-CE2	7.69	1.54	1.39
2	A	235	GLU	CG-CD	7.53	1.63	1.51
2	B	72	TYR	CE2-CZ	7.36	1.48	1.38
2	A	236	TYR	CE1-CZ	7.24	1.48	1.38
2	B	230	TYR	CG-CD1	7.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	GLU	CD-OE1	7.03	1.33	1.25
1	C	8	DT	C4-O4	-7.03	1.17	1.23
1	C	6	DT	C4-C5	6.93	1.51	1.45
1	D	6	DT	C4-C5	6.83	1.51	1.45
2	B	41	SER	CA-CB	6.75	1.63	1.52
2	B	64	GLU	CG-CD	6.71	1.62	1.51
2	B	212	PHE	CD1-CE1	6.63	1.52	1.39
2	B	94	THR	CA-CB	6.57	1.70	1.53
2	B	23	ILE	CB-CG2	6.48	1.73	1.52
2	B	12	TYR	CG-CD2	6.47	1.47	1.39
1	D	6	DT	C4-O4	6.44	1.29	1.23
2	B	169	PHE	CG-CD1	6.35	1.48	1.38
2	A	244	ARG	CB-CG	6.34	1.69	1.52
2	B	12	TYR	CD2-CE2	6.29	1.48	1.39
1	C	6	DT	C5-C6	6.25	1.38	1.34
2	B	105	PHE	CE1-CZ	6.23	1.49	1.37
2	A	105	PHE	CE2-CZ	6.19	1.49	1.37
1	C	8	DT	N1-C2	6.16	1.43	1.38
2	A	212	PHE	CE1-CZ	6.16	1.49	1.37
2	A	136	TYR	CE1-CZ	6.13	1.46	1.38
2	A	88	ALA	CA-CB	6.12	1.65	1.52
2	B	211	GLU	CD-OE2	6.08	1.32	1.25
2	B	12	TYR	CE2-CZ	6.06	1.46	1.38
2	A	163	TYR	CB-CG	6.01	1.60	1.51
2	B	241	TYR	CE2-CZ	6.00	1.46	1.38
2	A	31	TYR	CD2-CE2	5.91	1.48	1.39
2	B	63	VAL	CB-CG1	5.87	1.65	1.52
2	B	136	TYR	CB-CG	5.79	1.60	1.51
2	B	215	TYR	CG-CD1	5.77	1.46	1.39
2	B	128	TYR	CD2-CE2	5.76	1.48	1.39
2	B	31	TYR	CE1-CZ	5.70	1.46	1.38
1	D	10	DT	C3'-O3'	5.67	1.51	1.44
2	A	230	TYR	CD2-CE2	-5.61	1.30	1.39
2	B	168	VAL	CA-CB	-5.58	1.43	1.54
2	B	196	TYR	CB-CG	-5.52	1.43	1.51
1	D	7	DA	C6-N6	-5.50	1.29	1.33
1	C	5	DA	C6-N1	5.49	1.39	1.35
2	A	163	TYR	CE2-CZ	5.47	1.45	1.38
2	B	219	TYR	CE1-CZ	5.46	1.45	1.38
2	A	128	TYR	CE1-CZ	5.45	1.45	1.38
2	B	200	VAL	CB-CG2	5.45	1.64	1.52
2	B	163	TYR	CG-CD1	5.39	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	174	TRP	CB-CG	5.39	1.59	1.50
2	A	238	ASN	CB-CG	5.36	1.63	1.51
2	A	132	TRP	CG-CD1	5.36	1.44	1.36
2	A	175	VAL	CA-CB	5.35	1.66	1.54
2	B	235	GLU	CD-OE1	5.34	1.31	1.25
2	A	241	TYR	CE2-CZ	5.33	1.45	1.38
2	B	122	VAL	CB-CG2	5.33	1.64	1.52
1	C	7	DA	N1-C2	5.32	1.39	1.34
2	B	163	TYR	CE1-CZ	5.29	1.45	1.38
2	B	121	ILE	CB-CG2	5.26	1.69	1.52
1	C	5	DA	N1-C2	5.25	1.39	1.34
2	A	236	TYR	CD2-CE2	5.18	1.47	1.39
1	C	2	DA	C6-N6	5.16	1.38	1.33
2	A	31	TYR	CD1-CE1	5.13	1.47	1.39
1	C	5	DA	N3-C4	5.10	1.38	1.34
2	B	109	GLY	CA-C	5.10	1.60	1.51
2	B	72	TYR	CG-CD2	5.07	1.45	1.39
2	A	49	ARG	CA-C	5.06	1.66	1.52
2	A	93	THR	C-O	5.05	1.32	1.23
1	D	10	DT	C4-C5	5.04	1.49	1.45
2	B	244	ARG	CD-NE	5.03	1.55	1.46
1	D	3	DA	C6-N6	5.03	1.38	1.33
2	A	125	PHE	CD1-CE1	5.03	1.49	1.39
2	B	75	PHE	CG-CD1	5.01	1.46	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	164	LYS	C-N-CA	-9.96	101.38	122.30
2	B	49	ARG	NE-CZ-NH2	-8.57	116.01	120.30
2	A	217	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	B	43	ILE	CG1-CB-CG2	-7.17	95.63	111.40
2	A	237	ARG	NE-CZ-NH1	-6.91	116.84	120.30
2	B	74	ASP	CB-CG-OD2	6.79	124.41	118.30
2	A	217	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	A	180	LEU	CB-CG-CD1	-6.42	100.09	111.00
2	B	13	ASP	CB-CG-OD1	-5.77	113.10	118.30
1	C	2	DA	O5'-C5'-C4'	5.76	125.39	111.00
2	B	115	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	B	170	LEU	CA-CB-CG	-5.67	102.25	115.30
2	A	221	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	8	DT	OP2-P-O3'	5.62	117.56	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	49	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	B	117	ASN	N-CA-C	5.57	126.05	111.00
2	B	86	LYS	CD-CE-NZ	-5.53	98.99	111.70
2	A	49	ARG	CG-CD-NE	-5.49	100.28	111.80
1	D	4	DG	C1'-O4'-C4'	-5.45	104.65	110.10
2	A	7	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	A	36	ASP	CB-CG-OD1	-5.27	113.56	118.30
2	A	187	THR	N-CA-C	5.26	125.20	111.00
2	A	74	ASP	CB-CG-OD1	5.25	123.02	118.30
2	A	163	TYR	CB-CA-C	-5.18	100.03	110.40
2	B	69	GLN	N-CA-C	5.15	124.92	111.00
2	B	91	ILE	CG1-CB-CG2	-5.14	100.10	111.40
2	A	166	VAL	N-CA-C	5.01	124.52	111.00

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 (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	202	0	116	6	0
1	D	201	0	115	5	0
2	A	1930	0	1814	56	0
2	B	1888	0	1778	58	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	12	0	0	1	0
4	D	8	0	0	0	0
All	All	4379	0	3823	108	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 13.

All (108) 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: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
2:A:27:GLU:CD	2:A:27:GLU:H	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:DC:H2'	1:D:10:DT:H71	1.91	0.52
2:B:222:THR:HG22	2:B:223:SER:N	2.24	0.52
2:B:220:GLU:HB2	2:B:226:ARG:HG2	1.92	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:29:LYS:HD3	2:B:31:TYR:OH	2.11	0.51
2:B:25:SER:HB2	2:B:27:GLU:OE1	2.09	0.51
2:B:174:TRP:CG	2:B:209:GLU:HB2	2.46	0.51
2:A:49:ARG:HB3	2:A:50:PRO:CD	2.41	0.51
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: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:B:222:THR:HG22	2:B:224:GLN:N	2.26	0.47
2:A:170:LEU:HD23	2:A:171:GLN:N	2.29	0.47
2:A:124:PRO:HD2	2:A:127:GLN:CD	2.34	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:B:195:HIS:O	2:B:198:ASP:HB2	2.15	0.46
2:B:49:ARG:CB	2:B:50:PRO:HD3	2.40	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:230:TYR:CD1	2:A:236:TYR:HB2	2.51	0.46
2:A:163:TYR:C	2:A:163:TYR:CD1	2.89	0.46
2:A:170:LEU:C	2:A:170:LEU:HD23	2.35	0.45
2:B:222:THR:CG2	2:B:223:SER:N	2.78	0.45
2:A:14:GLU:CD	2:A:51:ILE:HD11	2.36	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:145:LYS:C	2:A:147:SER:H	2.20	0.45
2:A:139:THR:H	2:A:165:GLY:H	1.65	0.44
2:B:27:GLU:H	2:B:27:GLU:CD	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ILE:HG22	2:B:153:ILE:O	2.17	0.44
2:B:66:PRO:HB3	2:B:122:VAL:HG22	1.98	0.44
2:A:27:GLU:CD	2:A:27:GLU:N	2.71	0.44
2:A:121:ILE:HG12	2:A:123:TYR:O	2.18	0.44
2:B:31:TYR:HA	2:B:32:PRO:HD3	1.88	0.43
2:A:220:GLU:HB3	2:A:225:LEU:HB2	2.00	0.43
2:A:23:ILE:CD1	2:B:43:ILE:HG23	2.48	0.43
2:B:31:TYR:CD1	2:B:31:TYR:N	2.87	0.43
2:A:23:ILE:HA	2:B:23:ILE:HA	2.00	0.43
1:C:7:DA:H3'	4:C:18:HOH:O	2.18	0.43
2:A:41:SER:O	2:A:45:GLU:HB2	2.18	0.43
2:A:242:ARG:O	2:A:245:LYS:HE3	2.18	0.43
2:A:78:TYR:HB3	2:A:86:LYS:HG2	2.01	0.43
2:A:145:LYS:C	2:A:147:SER:N	2.71	0.42
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:B:123:TYR:O	2:B:124:PRO:C	2.58	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:A:220:GLU:OE2	2:A:220:GLU:HA	2.20	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:116:ASN:O	2:A:117:ASN:C	2.57	0.41
2:A:107:LEU:O	2:A:173:LYS:HE3	2.19	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:40:LEU:HD23	2:A:138:TYR:CZ	2.55	0.41
2:B:169:PHE:CD1	2:B:169:PHE:C	2.94	0.41
2:A:165:GLY:HA3	4:A:274:HOH:O	2.20	0.41
2:A:170:LEU:C	2:A:170:LEU:CD2	2.90	0.40
2:B:110:TYR:HB3	2:B:189:ILE:HG13	2.03	0.40
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%)	15 8
2	B	229/244 (94%)	212 (93%)	15 (7%)	2 (1%)	21 13
All	All	466/488 (96%)	434 (93%)	27 (6%)	5 (1%)	17 10

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%)	189 (95%)	10 (5%)	30 25
2	B	196/219 (90%)	183 (93%)	13 (7%)	21 14
All	All	395/438 (90%)	372 (94%)	23 (6%)	25 19

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	40	LEU

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Mol	Chain	Res	Type
2	A	41	SER
2	A	45	GLU
2	A	69	GLN
2	A	90	ASP
2	A	96	THR
2	A	114	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	71	HIS
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	212	PHE
2	B	227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	69	GLN
2	B	16	GLN
2	B	53	ASN
2	B	84	ASN
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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.