Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:35 PM GMT

PDB ID	:	1BHM
Title	:	RESTRICTION ENDONUCLEASE BAMHI COMPLEX WITH DNA
Authors	:	Aggarwal, A.K.; Newman, M.
Deposited on	:	1995-07-12
Resolution	:	2.20 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 (i) symbol.

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

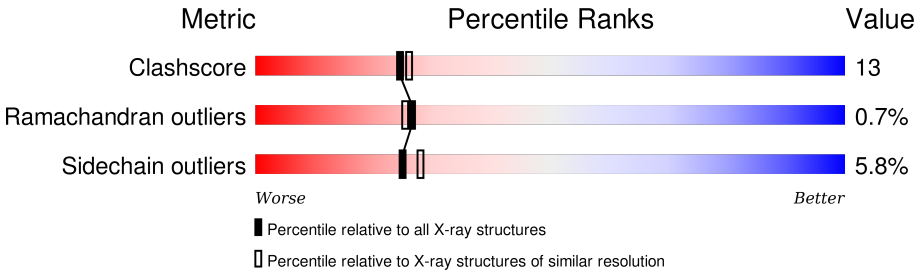
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	12	75% 25%
1	D	12	8% 50% 33% 8%
2	A	213	53% 34% 6% 7%
2	B	213	64% 25% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3886 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(*TP*AP*TP*GP*GP*AP*TP*CP*CP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			243	118	44	70	11			
1	D	11	Total	C	N	O	P	0	0	0
			222	108	39	65	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	198	Total	C	N	O	S	0	0	0
			1559	1005	246	300	8			
2	B	208	Total	C	N	O	S	0	0	0
			1647	1060	262	317	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	1	0
			79	79		
3	B	89	Total	O	0	0
			89	89		
3	C	24	Total	O	0	0
			24	24		
3	D	23	Total	O	0	0
			23	23		

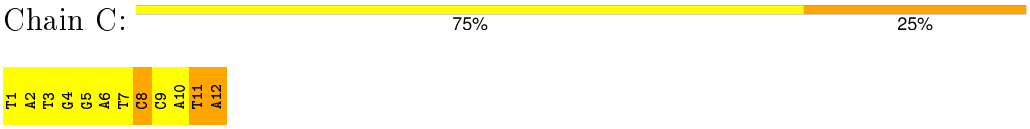
3 Residue-property plots (i)

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: DNA (5'-D(*TP*AP*TP*GP*GP*AP*TP*CP*CP*AP*TP*A)-3')

Chain C:

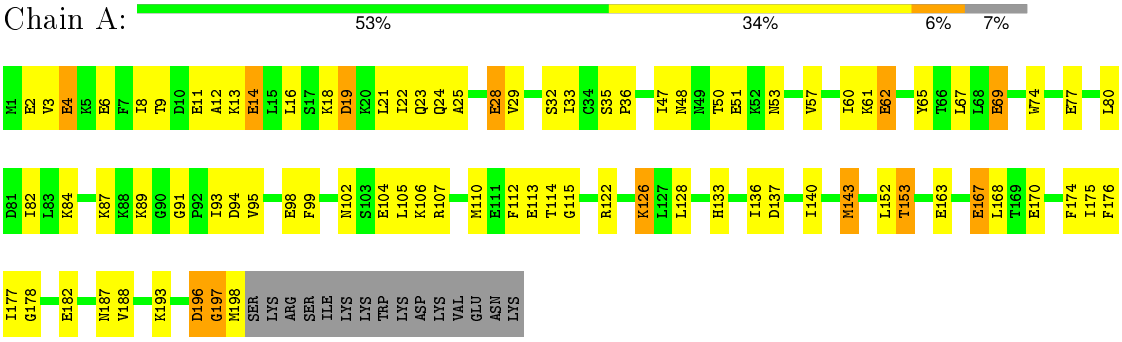


- Molecule 1: DNA (5'-D(*TP*AP*TP*GP*GP*AP*TP*CP*CP*AP*TP*A)-3')

Chain D:

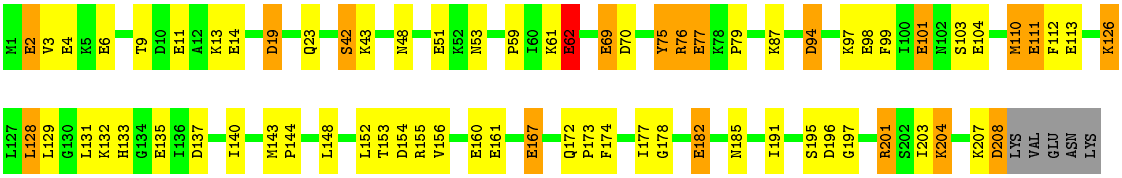
- Molecule 2: PROTEIN (BAMHI (E.C.3.1.21.4))

Chain A:



- Molecule 2: PROTEIN (BAMHI (E.C.3.1.21.4))

Chain B:



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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.80Å 81.90Å 68.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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	C	2.65	13/272 (4.8%)	2.83	33/418 (7.9%)
1	D	2.26	9/248 (3.6%)	2.88	37/381 (9.7%)
2	A	1.20	19/1592 (1.2%)	1.40	10/2158 (0.5%)
2	B	1.33	17/1682 (1.0%)	1.50	18/2279 (0.8%)
All	All	1.49	58/3794 (1.5%)	1.74	98/5236 (1.9%)

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	A	1	0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	62	GLU	CD-OE1	13.62	1.40	1.25
1	C	11	DT	C5-C6	-12.69	1.25	1.34
1	C	11	DT	C5-C7	11.97	1.57	1.50
2	B	135	GLU	CD-OE1	9.84	1.36	1.25
2	A	2	GLU	CD-OE1	9.19	1.35	1.25
2	B	104	GLU	CD-OE1	8.42	1.34	1.25
2	A	28	GLU	CD-OE1	8.27	1.34	1.25
1	D	11	DT	C5-C7	-8.24	1.45	1.50
1	D	11	DT	C3'-O3'	8.18	1.54	1.44
2	A	170	GLU	CD-OE1	8.17	1.34	1.25
2	B	113	GLU	CD-OE1	-7.71	1.17	1.25
2	A	113	GLU	CD-OE2	-7.67	1.17	1.25
2	A	104	GLU	CD-OE1	7.66	1.34	1.25
2	B	4	GLU	CD-OE2	7.57	1.33	1.25
2	B	101	GLU	CD-OE1	7.42	1.33	1.25
2	A	182	GLU	CD-OE1	7.33	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	62	GLU	CD-OE2	7.11	1.33	1.25
1	C	12	DA	P-O5'	6.97	1.66	1.59
2	B	98	GLU	CD-OE1	6.97	1.33	1.25
1	C	5	DG	N7-C5	-6.94	1.35	1.39
2	B	14	GLU	CD-OE1	6.93	1.33	1.25
2	B	2	GLU	CD-OE1	6.93	1.33	1.25
2	A	51	GLU	CD-OE1	6.68	1.32	1.25
2	B	69	GLU	CD-OE1	6.66	1.32	1.25
2	A	14	GLU	CD-OE2	6.61	1.32	1.25
1	C	11	DT	N1-C6	-6.56	1.33	1.38
1	D	7	DT	C5-C6	-6.53	1.29	1.34
1	C	11	DT	C2-N3	-6.38	1.32	1.37
1	D	7	DT	C5-C7	6.37	1.53	1.50
2	B	51	GLU	CD-OE1	6.33	1.32	1.25
2	B	111	GLU	CD-OE1	-6.32	1.18	1.25
1	D	3	DT	C4-C5	-6.24	1.39	1.45
2	B	11	GLU	CD-OE1	6.22	1.32	1.25
1	C	5	DG	C5-C6	-6.16	1.36	1.42
2	A	167	GLU	CD-OE1	6.01	1.32	1.25
2	B	160	GLU	CD-OE1	5.96	1.32	1.25
2	A	69	GLU	CD-OE2	5.89	1.32	1.25
2	A	77	GLU	CD-OE2	5.89	1.32	1.25
1	C	7	DT	C5-C7	5.86	1.53	1.50
2	B	182	GLU	CD-OE2	-5.84	1.19	1.25
1	D	11	DT	C2-N3	-5.82	1.33	1.37
2	A	6	GLU	CD-OE1	-5.80	1.19	1.25
1	C	12	DA	C5-C6	-5.79	1.35	1.41
1	D	5	DG	C2-N3	-5.67	1.28	1.32
1	C	9	DC	C3'-O3'	-5.58	1.36	1.44
1	C	3	DT	C4-C5	-5.58	1.40	1.45
2	A	163	GLU	CD-OE2	5.54	1.31	1.25
2	B	161	GLU	CD-OE1	5.44	1.31	1.25
1	D	3	DT	C3'-O3'	-5.34	1.37	1.44
2	A	4	GLU	CD-OE2	5.26	1.31	1.25
2	A	182	GLU	CD-OE2	-5.23	1.19	1.25
2	A	98	GLU	CD-OE1	5.21	1.31	1.25
2	A	163	GLU	CD-OE1	-5.20	1.20	1.25
1	C	5	DG	C5-C4	-5.20	1.34	1.38
1	D	6	DA	C5'-C4'	5.16	1.57	1.51
1	C	2	DA	C6-N1	-5.07	1.32	1.35
2	B	77	GLU	CD-OE1	5.04	1.31	1.25
2	A	11	GLU	CD-OE1	5.01	1.31	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	DG	P-O5'-C5'	-16.25	94.90	120.90
2	B	19	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	C	8	DC	C2-N1-C1'	9.75	129.53	118.80
1	C	2	DA	O4'-C1'-N9	-9.69	101.22	108.00
1	D	4	DG	P-O3'-C3'	9.48	131.07	119.70
2	B	137	ASP	CB-CG-OD2	9.47	126.82	118.30
2	B	19	ASP	CB-CG-OD1	9.42	126.78	118.30
1	C	8	DC	C6-N1-C1'	-9.40	109.52	120.80
1	D	1	DT	C4-C5-C7	-8.96	113.63	119.00
1	C	8	DC	P-O3'-C3'	8.67	130.11	119.70
1	C	12	DA	O4'-C1'-N9	8.63	114.04	108.00
1	C	5	DG	C2-N3-C4	-8.62	107.59	111.90
2	B	137	ASP	CB-CG-OD1	-8.57	110.59	118.30
1	D	6	DA	N1-C6-N6	8.42	123.65	118.60
1	C	5	DG	P-O3'-C3'	8.37	129.75	119.70
1	C	5	DG	O4'-C1'-N9	-8.08	102.35	108.00
1	C	9	DC	O4'-C1'-N1	-8.01	102.39	108.00
1	D	6	DA	C5-C6-N6	-7.97	117.32	123.70
1	D	1	DT	C6-N1-C1'	-7.96	108.45	120.40
1	D	10	DA	O4'-C1'-C2'	-7.93	99.55	105.90
1	D	3	DT	O4'-C1'-C2'	-7.88	99.60	105.90
1	D	11	DT	C2-N1-C1'	-7.87	105.61	118.20
2	A	198	MET	N-CA-CB	7.71	124.47	110.60
1	D	6	DA	O4'-C1'-C2'	-7.61	99.81	105.90
1	D	1	DT	C6-C5-C7	7.52	127.41	122.90
1	C	8	DC	N3-C4-C5	7.47	124.89	121.90
1	D	11	DT	C6-N1-C1'	7.43	131.55	120.40
2	A	2	GLU	CB-CA-C	-7.38	95.65	110.40
1	D	7	DT	P-O5'-C5'	-7.33	109.17	120.90
1	D	10	DA	O4'-C1'-N9	-7.31	102.89	108.00
1	C	12	DA	N1-C6-N6	7.30	122.98	118.60
1	D	9	DC	O4'-C1'-N1	-7.27	102.91	108.00
1	D	6	DA	O4'-C1'-N9	-7.24	102.94	108.00
2	A	107	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	5	DG	P-O3'-C3'	7.15	128.28	119.70
1	D	3	DT	N1-C2-N3	-6.94	110.44	114.60
1	D	3	DT	P-O3'-C3'	6.78	127.83	119.70
1	D	11	DT	C6-C5-C7	-6.64	118.92	122.90
1	C	6	DA	P-O3'-C3'	6.60	127.62	119.70
1	D	6	DA	O4'-C4'-C3'	-6.58	101.87	104.50
2	B	76	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	12	DA	C5-N7-C8	-6.36	100.72	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	DG	OP1-P-OP2	6.36	129.14	119.60
2	B	196	ASP	CB-CG-OD1	-6.34	112.59	118.30
2	A	94	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	10	DA	O4'-C1'-N9	6.30	112.41	108.00
1	C	11	DT	C2-N1-C1'	-6.30	108.13	118.20
2	A	122	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	D	11	DT	N3-C2-O2	-6.21	118.57	122.30
2	B	75	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	C	11	DT	C6-C5-C7	-6.13	119.22	122.90
1	C	8	DC	O4'-C1'-C2'	-6.03	101.08	105.90
2	B	94	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	3	DT	C2-N3-C4	5.99	130.79	127.20
1	D	1	DT	C5-C4-O4	-5.94	120.74	124.90
1	C	10	DA	OP1-P-OP2	5.92	128.49	119.60
1	C	12	DA	C4-C5-N7	5.89	113.65	110.70
1	D	6	DA	N9-C4-C5	-5.88	103.45	105.80
1	C	3	DT	O4'-C1'-N1	5.87	112.11	108.00
2	B	155	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	A	137	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	D	10	DA	C4-N9-C1'	5.82	136.78	126.30
1	D	5	DG	C8-N9-C1'	5.81	134.56	127.00
1	C	11	DT	C6-N1-C1'	5.81	129.12	120.40
2	A	196	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	C	11	DT	C4-C5-C6	5.76	121.46	118.00
1	D	7	DT	N1-C2-O2	5.70	127.66	123.10
2	B	196	ASP	CB-CG-OD2	5.68	123.41	118.30
1	C	12	DA	C5-C6-N6	-5.68	119.16	123.70
1	D	1	DT	C2-N1-C1'	5.67	127.27	118.20
2	A	19	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	6	DA	P-O3'-C3'	5.60	126.42	119.70
1	C	11	DT	O4'-C1'-C2'	-5.59	101.42	105.90
1	C	1	DT	O4'-C1'-N1	-5.59	104.08	108.00
1	D	11	DT	C4-C5-C7	5.57	122.34	119.00
2	B	129	LEU	CB-CA-C	5.56	120.77	110.20
1	D	11	DT	N1-C2-O2	5.55	127.54	123.10
1	D	1	DT	O4'-C1'-C2'	-5.46	101.53	105.90
1	C	10	DA	C8-N9-C4	5.45	107.98	105.80
2	B	201	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	4	DG	C6-N1-C2	-5.43	121.84	125.10
2	A	107	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	5	DG	C4-N9-C1'	-5.42	119.46	126.50
2	B	155	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	3	DT	C6-N1-C1'	5.32	128.38	120.40
1	D	10	DA	C8-N9-C1'	-5.31	118.14	127.70
1	C	4	DG	OP1-P-O3'	-5.30	93.55	105.20
2	B	6	GLU	N-CA-CB	-5.26	101.14	110.60
1	D	5	DG	O4'-C1'-N9	-5.25	104.33	108.00
2	B	208	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	7	DT	N3-C2-O2	-5.15	119.21	122.30
1	C	12	DA	C6-C5-N7	-5.14	128.70	132.30
1	C	4	DG	N1-C2-N3	-5.14	120.82	123.90
2	B	110	MET	CG-SD-CE	-5.13	91.98	100.20
2	B	70	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	D	1	DT	C5'-C4'-O4'	-5.07	99.67	109.30
2	B	126	LYS	CB-CA-C	5.07	120.53	110.40
2	A	94	ASP	CB-CG-OD2	-5.05	113.76	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	198	MET	CA

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	243	0	137	3	0
1	D	222	0	127	10	0
2	A	1559	0	1520	53	0
2	B	1647	0	1615	34	0
3	A	79	0	0	4	0
3	B	89	0	0	4	0
3	C	24	0	0	0	0
3	D	23	0	0	0	0
All	All	3886	0	3399	90	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 (90) 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:80:LEU:HD21	2:A:93:ILE:HD12	1.64	0.77
2:A:24:GLN:O	2:A:28:GLU:HG3	1.84	0.77
2:A:21:LEU:HD22	2:A:99:PHE:HB3	1.69	0.72
1:D:3:DT:H2'	3:B:231:HOH:O	1.89	0.72
1:D:7:DT:OP2	2:A:153:THR:HG21	1.90	0.72
2:A:153:THR:HG22	2:A:193:LYS:HE2	1.71	0.71
2:B:208:ASP:HB2	3:B:302:HOH:O	1.89	0.71
2:B:97:LYS:HD3	2:B:99:PHE:CZ	2.25	0.71
2:A:187:ASN:HB2	3:A:288:HOH:O	1.90	0.71
2:A:80:LEU:HD21	2:A:93:ILE:CD1	2.21	0.71
2:A:48:ASN:OD1	2:A:50:THR:HG23	1.91	0.70
1:C:11:DT:H2"	1:C:12:DA:H5"	1.73	0.70
2:B:2:GLU:HG3	2:B:182:GLU:HG3	1.74	0.69
2:A:16:LEU:HD23	2:A:22:ILE:HG22	1.75	0.68
2:A:19:ASP:HB3	2:A:22:ILE:HB	1.74	0.68
1:D:3:DT:OP2	2:A:89:LYS:HE3	1.95	0.65
2:A:84:LYS:HA	3:A:272:HOH:O	1.96	0.64
2:A:74:TRP:HE3	2:A:95:VAL:HG12	1.62	0.63
1:D:6:DA:N3	2:A:196:ASP:HB3	2.13	0.62
2:A:110:MET:HG3	2:A:140:ILE:HB	1.82	0.61
2:A:61:LYS:HE2	2:A:114:THR:OG1	2.01	0.60
2:A:87:LYS:NZ	2:B:167:GLU:OE1	2.30	0.58
2:A:8:ILE:HG22	2:A:9:THR:O	2.03	0.58
2:B:62:GLU:OE2	2:B:201:ARG:HD3	2.03	0.58
2:A:99:PHE:O	2:A:105:LEU:HA	2.04	0.57
2:A:80:LEU:CD2	2:A:93:ILE:HD12	2.35	0.57
2:B:59:PRO:HD3	2:B:197:GLY:O	2.05	0.57
2:A:19:ASP:O	2:A:23:GLN:HG3	2.06	0.56
2:A:8:ILE:HG23	2:A:12:ALA:HB3	1.87	0.56
2:B:59:PRO:HG2	2:B:191:ILE:HG23	1.88	0.56
2:B:53:ASN:HA	2:B:152:LEU:O	2.06	0.55
2:B:19:ASP:O	2:B:23:GLN:HG3	2.05	0.55
2:A:74:TRP:CE3	2:A:95:VAL:HG12	2.42	0.54
2:B:61:LYS:NZ	3:B:225:HOH:O	2.31	0.54
1:D:6:DA:H1'	2:A:196:ASP:CB	2.37	0.54
2:A:99:PHE:O	2:A:106:LYS:N	2.41	0.53
2:A:3:VAL:HG13	2:A:177:ILE:HG23	1.91	0.53
2:A:91:GLY:O	2:A:126:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:33:ILE:HG13	2:A:33:ILE:O	2.07	0.53
2:B:48:ASN:HA	2:B:185:ASN:O	2.09	0.53
2:A:99:PHE:HB2	2:A:106:LYS:HB2	1.92	0.52
2:B:9:THR:O	2:B:13:LYS:HG3	2.09	0.52
2:B:69:GLU:CD	2:B:201:ARG:HH22	2.13	0.51
2:B:143:MET:O	2:B:178:GLY:HA2	2.10	0.51
2:B:153:THR:O	2:B:156:VAL:HG13	2.11	0.51
1:D:3:DT:H2"	1:D:4:DG:C8	2.46	0.51
1:D:7:DT:H2"	1:D:8:DC:O5'	2.11	0.50
2:A:167:GLU:OE2	2:B:132:LYS:NZ	2.33	0.50
2:A:167:GLU:OE1	2:B:87:LYS:NZ	2.41	0.50
2:A:143:MET:O	2:A:178:GLY:HA2	2.12	0.50
2:B:75:TYR:CE1	2:B:204:LYS:HD3	2.47	0.50
2:A:32:SER:O	2:A:35:SER:HB2	2.11	0.49
2:A:8:ILE:HG22	2:A:13:LYS:HG3	1.95	0.49
1:D:6:DA:H2	2:A:197:GLY:HA3	1.78	0.48
2:A:4:GLU:O	2:A:4:GLU:HG3	2.12	0.48
2:A:196:ASP:N	2:A:196:ASP:OD1	2.47	0.47
1:C:11:DT:C2'	1:C:12:DA:H5"	2.43	0.47
2:B:97:LYS:HD3	2:B:99:PHE:CE1	2.50	0.46
2:B:128:LEU:HA	2:B:128:LEU:HD12	1.64	0.46
2:A:53:ASN:HA	2:A:152:LEU:O	2.15	0.46
2:A:115:GLY:HA2	3:A:235:HOH:O	2.16	0.45
2:A:14:GLU:OE2	2:A:18:LYS:HE3	2.16	0.45
2:A:136:ILE:HD13	2:A:136:ILE:HG21	1.68	0.45
2:B:94:ASP:N	2:B:111:GLU:OE2	2.37	0.44
1:D:6:DA:H1'	2:A:196:ASP:HB2	2.00	0.44
2:B:131:LEU:HD13	2:B:172:GLN:HB3	2.00	0.44
2:B:69:GLU:OE1	2:B:201:ARG:NH2	2.46	0.43
2:A:48:ASN:ND2	2:A:188:VAL:O	2.43	0.43
2:B:172:GLN:HB3	2:B:172:GLN:HE21	1.49	0.43
2:B:42:SER:OG	2:B:43:LYS:N	2.53	0.42
2:A:35:SER:HB2	2:A:36:PRO:HD3	2.02	0.42
2:B:77:GLU:O	2:B:79:PRO:HD3	2.19	0.42
2:A:143:MET:CE	2:A:176:PHE:HB3	2.50	0.42
2:A:60:ILE:HD13	2:A:60:ILE:HG21	1.73	0.42
2:A:106:LYS:HA	2:A:106:LYS:HD3	1.83	0.41
2:B:132:LYS:HG2	2:B:133:HIS:CD2	2.55	0.41
2:B:144:PRO:HB3	2:B:148:LEU:HD23	2.02	0.41
2:A:82:ILE:HG12	2:A:133:HIS:CD2	2.55	0.41
2:B:76:ARG:HB2	2:B:203:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:65:TYR:O	2:A:69:GLU:HG3	2.19	0.41
1:D:6:DA:H2'	3:A:235:HOH:O	2.20	0.41
1:C:8:DC:N4	2:B:154:ASP:O	2.41	0.41
2:A:168:LEU:HA	2:A:168:LEU:HD23	1.70	0.41
2:A:140:ILE:HG12	2:A:175:ILE:HB	2.02	0.41
2:B:201:ARG:NH1	3:B:228:HOH:O	2.51	0.40
2:A:25:ALA:O	2:A:29:VAL:HG13	2.20	0.40
2:B:3:VAL:HG13	2:B:177:ILE:HG23	2.02	0.40
2:A:67:LEU:HD23	2:A:67:LEU:HA	1.99	0.40
2:B:110:MET:HG3	2:B:140:ILE:HB	2.02	0.40
2:B:172:GLN:HE21	2:B:173:PRO:HD2	1.87	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	196/213 (92%)	187 (95%)	7 (4%)	2 (1%)	19	16
2	B	206/213 (97%)	195 (95%)	10 (5%)	1 (0%)	34	35
All	All	402/426 (94%)	382 (95%)	17 (4%)	3 (1%)	26	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	207	LYS
2	A	102	ASN
2	A	197	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	167/194 (86%)	158 (95%)	9 (5%)	27	31
2	B	179/194 (92%)	168 (94%)	11 (6%)	23	26
All	All	346/388 (89%)	326 (94%)	20 (6%)	25	28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	47	ILE
2	A	57	VAL
2	A	62	GLU
2	A	112	PHE
2	A	126	LYS
2	A	128	LEU
2	A	143	MET
2	A	153	THR
2	A	174	PHE
2	B	42	SER
2	B	62	GLU
2	B	101	GLU
2	B	103	SER
2	B	112	PHE
2	B	126	LYS
2	B	128	LEU
2	B	167	GLU
2	B	174	PHE
2	B	195	SER
2	B	204	LYS

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	125	ASN
2	B	23	GLN

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Mol	Chain	Res	Type
2	B	27	ASN
2	B	125	ASN
2	B	172	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

There are no ligands in this entry.

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.