



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:01 AM UTC

PDB ID : 3EBC / pdb\_00003ebc  
Title : Structure of N141A HincII with Cognate DNA  
Authors : Little, E.J.; Babic, A.C.; Horton, N.C.  
Deposited on : 2008-08-27  
Resolution : 2.55 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

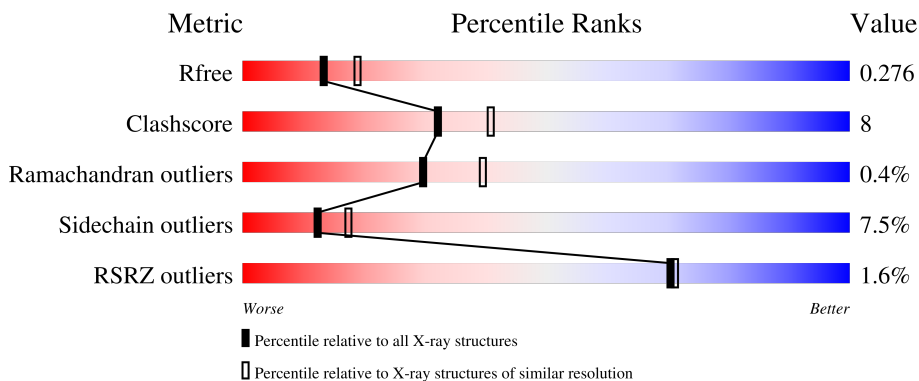
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
2	E	14	
3	F	14	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4759 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 protein called Type-2 restriction enzyme HincII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1934	1262	306	360	6	0	0	0
1	B	244	1956	1278	310	362	6	0	0	0

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P17743
A	0	ALA	-	expression tag	UNP P17743
A	130	THR	ARG	conflict	UNP P17743
A	141	ALA	ASN	engineered mutation	UNP P17743
A	173	TRP	SER	conflict	UNP P17743
A	259	ARG	-	expression tag	UNP P17743
A	260	SER	-	expression tag	UNP P17743
A	261	ARG	-	expression tag	UNP P17743
A	262	GLU	-	expression tag	UNP P17743
A	263	LEU	-	expression tag	UNP P17743
A	264	VAL	-	expression tag	UNP P17743
A	265	ASP	-	expression tag	UNP P17743
A	266	PRO	-	expression tag	UNP P17743
A	267	ASN	-	expression tag	UNP P17743
A	268	SER	-	expression tag	UNP P17743
A	269	VAL	-	expression tag	UNP P17743
A	270	GLN	-	expression tag	UNP P17743
A	271	ALA	-	expression tag	UNP P17743
A	272	ARG	-	expression tag	UNP P17743
A	273	LEU	-	expression tag	UNP P17743
A	274	GLN	-	expression tag	UNP P17743
A	275	ASP	-	expression tag	UNP P17743
A	276	VAL	-	expression tag	UNP P17743
A	277	ASP	-	expression tag	UNP P17743
A	278	GLY	-	expression tag	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
A	279	THR	-	expression tag	UNP P17743
A	280	ILE	-	expression tag	UNP P17743
A	281	ASP	-	expression tag	UNP P17743
A	282	THR	-	expression tag	UNP P17743
A	283	ARG	-	expression tag	UNP P17743
A	284	SER	-	expression tag	UNP P17743
A	285	LYS	-	expression tag	UNP P17743
A	286	LEU	-	expression tag	UNP P17743
A	287	ALA	-	expression tag	UNP P17743
A	288	ALA	-	expression tag	UNP P17743
A	289	ALA	-	expression tag	UNP P17743
A	290	GLN	-	expression tag	UNP P17743
A	291	LEU	-	expression tag	UNP P17743
A	292	TYR	-	expression tag	UNP P17743
A	293	THR	-	expression tag	UNP P17743
A	294	ARG	-	expression tag	UNP P17743
A	295	ALA	-	expression tag	UNP P17743
A	296	SER	-	expression tag	UNP P17743
A	297	GLN	-	expression tag	UNP P17743
A	298	PRO	-	expression tag	UNP P17743
A	299	GLU	-	expression tag	UNP P17743
A	300	LEU	-	expression tag	UNP P17743
A	301	ALA	-	expression tag	UNP P17743
A	302	PRO	-	expression tag	UNP P17743
A	303	GLU	-	expression tag	UNP P17743
A	304	ASP	-	expression tag	UNP P17743
A	305	PRO	-	expression tag	UNP P17743
A	306	GLU	-	expression tag	UNP P17743
A	307	ASP	-	expression tag	UNP P17743
A	308	LEU	-	expression tag	UNP P17743
A	309	GLU	-	expression tag	UNP P17743
A	310	HIS	-	expression tag	UNP P17743
A	311	HIS	-	expression tag	UNP P17743
A	312	HIS	-	expression tag	UNP P17743
A	313	HIS	-	expression tag	UNP P17743
A	314	HIS	-	expression tag	UNP P17743
A	315	HIS	-	expression tag	UNP P17743
B	-1	MET	-	expression tag	UNP P17743
B	0	ALA	-	expression tag	UNP P17743
B	130	THR	ARG	conflict	UNP P17743
B	141	ALA	ASN	engineered mutation	UNP P17743
B	173	TRP	SER	conflict	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	259	ARG	-	expression tag	UNP P17743
B	260	SER	-	expression tag	UNP P17743
B	261	ARG	-	expression tag	UNP P17743
B	262	GLU	-	expression tag	UNP P17743
B	263	LEU	-	expression tag	UNP P17743
B	264	VAL	-	expression tag	UNP P17743
B	265	ASP	-	expression tag	UNP P17743
B	266	PRO	-	expression tag	UNP P17743
B	267	ASN	-	expression tag	UNP P17743
B	268	SER	-	expression tag	UNP P17743
B	269	VAL	-	expression tag	UNP P17743
B	270	GLN	-	expression tag	UNP P17743
B	271	ALA	-	expression tag	UNP P17743
B	272	ARG	-	expression tag	UNP P17743
B	273	LEU	-	expression tag	UNP P17743
B	274	GLN	-	expression tag	UNP P17743
B	275	ASP	-	expression tag	UNP P17743
B	276	VAL	-	expression tag	UNP P17743
B	277	ASP	-	expression tag	UNP P17743
B	278	GLY	-	expression tag	UNP P17743
B	279	THR	-	expression tag	UNP P17743
B	280	ILE	-	expression tag	UNP P17743
B	281	ASP	-	expression tag	UNP P17743
B	282	THR	-	expression tag	UNP P17743
B	283	ARG	-	expression tag	UNP P17743
B	284	SER	-	expression tag	UNP P17743
B	285	LYS	-	expression tag	UNP P17743
B	286	LEU	-	expression tag	UNP P17743
B	287	ALA	-	expression tag	UNP P17743
B	288	ALA	-	expression tag	UNP P17743
B	289	ALA	-	expression tag	UNP P17743
B	290	GLN	-	expression tag	UNP P17743
B	291	LEU	-	expression tag	UNP P17743
B	292	TYR	-	expression tag	UNP P17743
B	293	THR	-	expression tag	UNP P17743
B	294	ARG	-	expression tag	UNP P17743
B	295	ALA	-	expression tag	UNP P17743
B	296	SER	-	expression tag	UNP P17743
B	297	GLN	-	expression tag	UNP P17743
B	298	PRO	-	expression tag	UNP P17743
B	299	GLU	-	expression tag	UNP P17743
B	300	LEU	-	expression tag	UNP P17743

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	ALA	-	expression tag	UNP P17743
B	302	PRO	-	expression tag	UNP P17743
B	303	GLU	-	expression tag	UNP P17743
B	304	ASP	-	expression tag	UNP P17743
B	305	PRO	-	expression tag	UNP P17743
B	306	GLU	-	expression tag	UNP P17743
B	307	ASP	-	expression tag	UNP P17743
B	308	LEU	-	expression tag	UNP P17743
B	309	GLU	-	expression tag	UNP P17743
B	310	HIS	-	expression tag	UNP P17743
B	311	HIS	-	expression tag	UNP P17743
B	312	HIS	-	expression tag	UNP P17743
B	313	HIS	-	expression tag	UNP P17743
B	314	HIS	-	expression tag	UNP P17743
B	315	HIS	-	expression tag	UNP P17743

- Molecule 2 is a DNA chain called 5'-D(\*DGP\*DCP\*DCP\*DGP\*DGP\*DTP\*DCP\*DGP\*DAP\*DCP\*DGP\*DGP\*DGP\*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	14	286	135	57	81	13	0	0	0

- Molecule 3 is a DNA chain called 5'-D(\*DGP\*DCP\*DCP\*DCP\*DGP\*DTP\*DCP\*DGP\*DAP\*DCP\*DCP\*DGP\*DGP\*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	14	281	133	53	82	13	0	0	0

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	123	123	123	0	0

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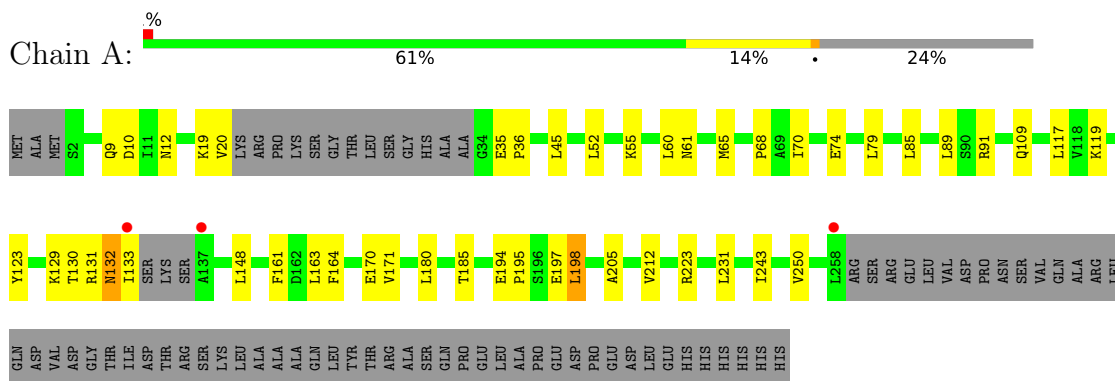
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	133	Total 133	O 133	0	0
5	E	23	Total 23	O 23	0	0
5	F	22	Total 22	O 22	0	0

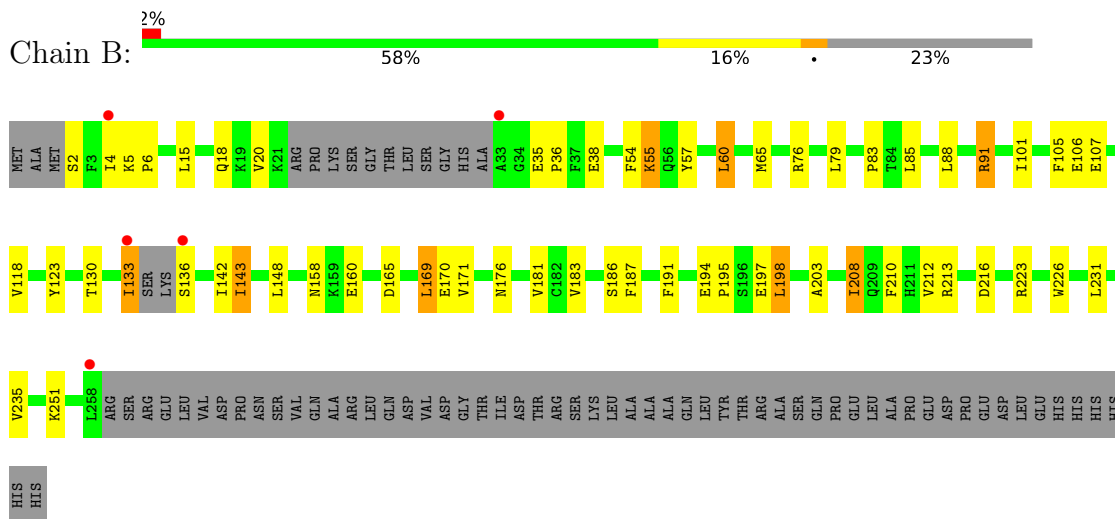
### 3 Residue-property plots [i](#)

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 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.

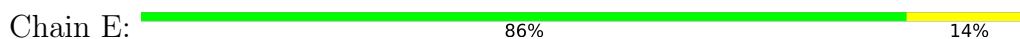
- Molecule 1: Type-2 restriction enzyme HincII



- Molecule 1: Type-2 restriction enzyme HincII



- Molecule 2: 5'-D>(\*DGP\*DCP\*DCP\*DGP\*DGP\*DTP\*DCP\*DGP\*DAP\*DCP\*DGP\*DGP\*DG\*GP\*DC)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.55Å 91.57Å 70.59Å 90.00° 107.46° 90.00°	Depositor
Resolution (Å)	43.56 – 2.55 43.56 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.56-2.55) 96.0 (43.56-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.279 0.190 , 0.276	Depositor DCC
$R_{free}$ test set	858 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.043 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	A	0.59	0/1978	0.87	1/2680 (0.0%)
1	B	0.57	0/2000	0.90	0/2709
2	E	0.42	0/321	1.18	0/495
3	F	0.44	0/314	1.31	4/482 (0.8%)
All	All	0.56	0/4613	0.95	5/6366 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	DG	C5'-C4'-C3'	-6.93	104.51	114.90
3	F	9	DA	O4'-C1'-N9	6.64	118.36	108.40
3	F	7	DC	O4'-C1'-N1	5.96	117.34	108.40
1	A	55	LYS	N-CA-C	-5.56	103.04	110.55
3	F	11	DC	C4'-C3'-O3'	-5.29	102.06	110.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1934	0	1843	23	0
1	B	1956	0	1879	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	286	0	154	1	0
3	F	281	0	157	4	0
4	A	1	0	0	0	0
5	A	123	0	0	2	0
5	B	133	0	0	5	0
5	E	23	0	0	0	0
5	F	22	0	0	0	0
All	All	4759	0	4033	65	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 8.

All (65) 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:B:54:PHE:O	1:B:55:LYS:HB2	1.52	1.05
1:B:133:ILE:C	1:B:136:SER:N	2.20	0.99
1:B:130:THR:HG22	1:B:171:VAL:HB	1.73	0.71
1:A:70:ILE:HG13	1:A:79:LEU:HD21	1.76	0.68
1:A:161:PHE:O	1:A:223:ARG:HD2	1.95	0.67
1:A:52:LEU:O	1:A:117:LEU:HA	1.95	0.66
1:B:198:LEU:HG	1:B:208:ILE:HD12	1.82	0.61
1:A:195:PRO:HA	1:A:198:LEU:HD22	1.82	0.61
1:A:85:LEU:HG	1:A:89:LEU:HD12	1.84	0.58
1:B:208:ILE:HD11	1:B:210:PHE:CE2	2.39	0.58
1:B:54:PHE:O	1:B:55:LYS:CB	2.37	0.58
3:F:1:DG:H2''	3:F:2:DC:C6	2.40	0.57
1:A:61:ASN:O	1:A:65:MET:HG3	2.04	0.57
1:B:142:ILE:HG22	1:B:143:ILE:HG13	1.86	0.57
1:B:83:PRO:HG2	1:B:158:ASN:OD1	2.05	0.56
1:A:12:ASN:HD22	1:A:185:THR:HB	1.72	0.54
1:B:142:ILE:HB	1:B:208:ILE:HG12	1.89	0.54
1:B:210:PHE:HB3	5:B:425:HOH:O	2.09	0.53
1:A:250:VAL:HG13	1:B:235:VAL:HG13	1.90	0.53
1:A:123:TYR:O	1:A:164:PHE:HA	2.09	0.53
1:B:208:ILE:HD11	1:B:210:PHE:HE2	1.75	0.52
1:A:12:ASN:ND2	1:A:185:THR:HB	2.25	0.52
1:B:198:LEU:HG	1:B:208:ILE:CD1	2.39	0.51
1:B:76:ARG:O	1:B:79:LEU:HB2	2.10	0.51
1:B:191:PHE:CG	1:B:223:ARG:HD2	2.45	0.50
1:B:4:ILE:HD11	1:B:187:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:SER:N	5:B:405:HOH:O	2.46	0.49
1:B:165:ASP:OD1	1:B:223:ARG:NH2	2.47	0.48
1:A:129:LYS:O	1:A:170:GLU:HA	2.14	0.48
1:B:85:LEU:HD21	1:B:123:TYR:CE1	2.48	0.48
1:B:170:GLU:HB2	1:B:212:VAL:HB	1.96	0.48
1:A:20:VAL:HG11	1:A:36:PRO:HB2	1.96	0.47
1:A:20:VAL:HG23	1:A:180:LEU:HB2	1.97	0.47
3:F:8:DG:H2''	3:F:9:DA:O5'	2.14	0.47
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.80	0.47
1:B:5:LYS:HB3	1:B:6:PRO:HD3	1.96	0.46
1:B:213:ARG:NH1	5:B:499:HOH:O	2.48	0.45
1:A:65:MET:O	1:A:68:PRO:HD3	2.17	0.45
1:B:65:MET:HG2	1:B:101:ILE:CD1	2.46	0.45
1:A:85:LEU:HD21	1:A:123:TYR:CE1	2.52	0.45
1:A:119:LYS:NZ	5:A:334:HOH:O	2.49	0.45
1:A:170:GLU:HB2	1:A:212:VAL:HB	2.00	0.44
1:A:74:GLU:HG3	5:A:411:HOH:O	2.18	0.44
1:B:194:GLU:HG3	1:B:197:GLU:HG2	1.97	0.44
1:B:15:LEU:HA	1:B:18:GLN:HE21	1.83	0.44
1:A:194:GLU:HG3	1:A:197:GLU:HG2	2.00	0.43
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.33	0.43
3:F:10:DC:H2''	3:F:11:DC:H5'	2.01	0.43
1:B:65:MET:HG2	1:B:101:ILE:HD12	2.01	0.43
1:B:169:LEU:HD23	1:B:186:SER:O	2.19	0.42
1:A:19:LYS:HA	1:A:180:LEU:O	2.19	0.42
1:A:132:ASN:O	1:A:133:ILE:HG23	2.20	0.41
1:A:205:ALA:HA	1:B:203:ALA:O	2.20	0.41
1:B:158:ASN:HB2	1:B:160:GLU:HG3	2.03	0.41
2:E:1:DG:H2''	2:E:2:DC:O5'	2.20	0.41
1:B:35:GLU:N	1:B:36:PRO:CD	2.84	0.41
1:B:60:LEU:HB3	1:B:105:PHE:HD1	1.85	0.41
1:B:197:GLU:HB2	5:B:450:HOH:O	2.19	0.41
1:B:91:ARG:NH1	1:B:106:GLU:O	2.53	0.41
1:A:130:THR:HG22	1:A:171:VAL:HB	2.03	0.41
3:F:5:DG:H2''	3:F:6:DT:O5'	2.20	0.41
1:B:38:GLU:HB2	5:B:502:HOH:O	2.21	0.41
1:B:57:TYR:CE1	1:B:107:GLU:HB2	2.55	0.41
1:B:101:ILE:HG22	1:B:101:ILE:O	2.21	0.40
1:B:195:PRO:HG3	1:B:226:TRP:CE2	2.56	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	
1	A	235/317 (74%)	222 (94%)	12 (5%)	1 (0%)	30	39
1	B	238/317 (75%)	223 (94%)	14 (6%)	1 (0%)	30	39
All	All	473/634 (75%)	445 (94%)	26 (6%)	2 (0%)	30	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	LYS
1	A	132	ASN

### 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	
1	A	198/280 (71%)	185 (93%)	13 (7%)	15	21
1	B	201/280 (72%)	184 (92%)	17 (8%)	10	13
All	All	399/560 (71%)	369 (92%)	30 (8%)	12	17

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	10	ASP
1	A	35	GLU
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	91	ARG
1	A	109	GLN
1	A	131	ARG
1	A	148	LEU
1	A	163	LEU
1	A	198	LEU
1	A	231	LEU
1	A	243	ILE
1	B	20	VAL
1	B	60	LEU
1	B	88	LEU
1	B	91	ARG
1	B	118	VAL
1	B	133	ILE
1	B	143	ILE
1	B	148	LEU
1	B	169	LEU
1	B	176	ASN
1	B	181	VAL
1	B	183	VAL
1	B	198	LEU
1	B	208	ILE
1	B	216	ASP
1	B	231	LEU
1	B	251	LYS

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	12	ASN
1	A	81	ASN
1	A	132	ASN
1	A	237	GLN
1	B	121	GLN
1	B	176	ASN

### 5.3.3 RNA

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 1 ligands modelled in this entry, 1 is 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	241/317 (76%)	-0.18	3 (1%) 76 77	10, 24, 42, 48	0
1	B	244/317 (76%)	-0.01	5 (2%) 65 65	10, 28, 47, 52	0
2	E	14/14 (100%)	-0.28	0 100 100	11, 27, 35, 38	0
3	F	14/14 (100%)	-0.38	0 100 100	11, 29, 37, 41	0
All	All	513/662 (77%)	-0.11	8 (1%) 70 71	10, 26, 45, 52	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	SER	3.9
1	B	133	ILE	3.8
1	B	258	LEU	3.4
1	B	33	ALA	3.3
1	B	4	ILE	2.9
1	A	133	ILE	2.8
1	A	137	ALA	2.2
1	A	258	LEU	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MN	A	316	1/1	0.85	0.09	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.