



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:07 am BST

PDB ID : 3M9E  
Title : Thyroid hormone beta DNA binding domain homodimer with inverted palindrome TRE  
Authors : Chen, Y.  
Deposited on : 2010-03-22  
Resolution : 2.41 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

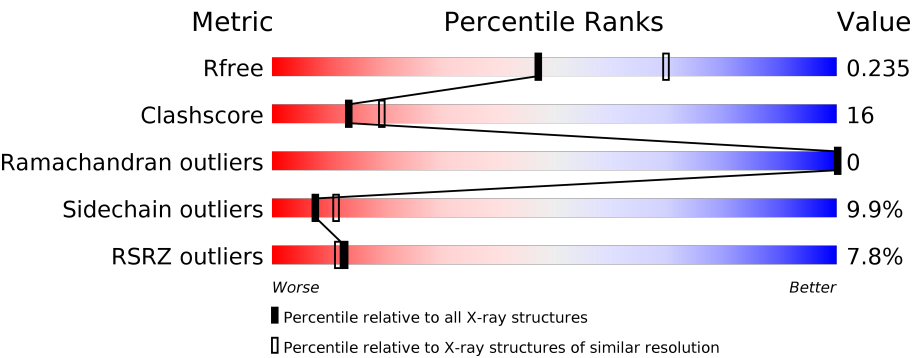
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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.




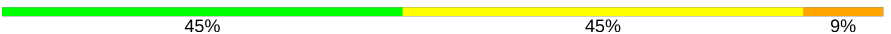
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	105	<div><div>8%</div><div>54%</div><div>30%</div><div>10%</div><div></div></div>
1	B	105	<div><div>16%</div><div>59%</div><div>32%</div><div>6%</div><div></div></div>
1	E	105	<div><div>9%</div><div>68%</div><div>22%</div><div>8%</div><div></div></div>
1	F	105	<div><div>4%</div><div>60%</div><div>29%</div><div>8%</div><div></div></div>
2	C	22	<div><div>45%</div><div>50%</div><div>5%</div></div>
2	D	22	<div><div>59%</div><div>36%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	22	 55% 45%
2	H	22	 45% 45% 9%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5309 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 Thyroid hormone receptor beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			827	511	156	149	11			
1	B	99	Total	C	N	O	S	0	1	0
			815	505	153	146	11			
1	E	102	Total	C	N	O	S	0	1	0
			847	523	162	151	11			
1	F	97	Total	C	N	O	S	0	0	0
			792	490	151	140	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	-	EXPRESSION TAG	UNP P18113
A	102	SER	-	EXPRESSION TAG	UNP P18113
B	101	GLY	-	EXPRESSION TAG	UNP P18113
B	102	SER	-	EXPRESSION TAG	UNP P18113
E	101	GLY	-	EXPRESSION TAG	UNP P18113
E	102	SER	-	EXPRESSION TAG	UNP P18113
F	101	GLY	-	EXPRESSION TAG	UNP P18113
F	102	SER	-	EXPRESSION TAG	UNP P18113

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*CP\*AP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			447	215	82	129	21			
2	D	22	Total	C	N	O	P	0	0	0
			447	215	82	129	21			
2	G	22	Total	C	N	O	P	0	0	0
			447	215	82	129	21			
2	H	22	Total	C	N	O	P	0	0	0
			447	215	82	129	21			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0

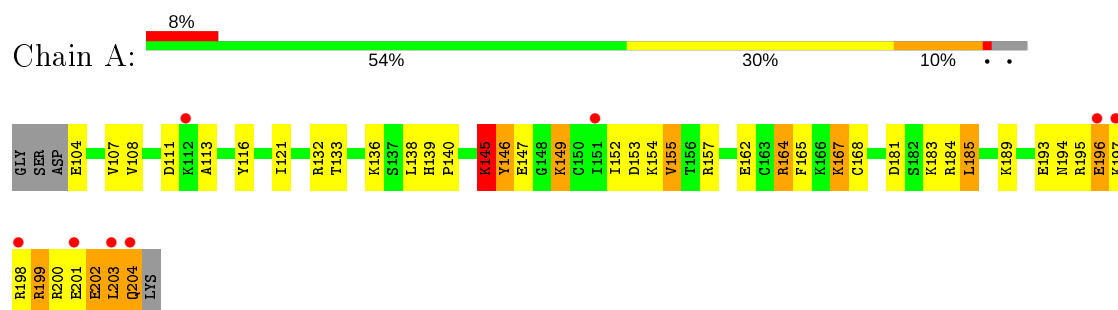
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total 28	O 28	0	0
4	B	48	Total 48	O 48	0	0
4	C	20	Total 20	O 20	0	0
4	D	16	Total 16	O 16	0	0
4	E	43	Total 43	O 43	0	0
4	F	43	Total 43	O 43	0	0
4	G	17	Total 17	O 17	0	0
4	H	17	Total 17	O 17	0	0

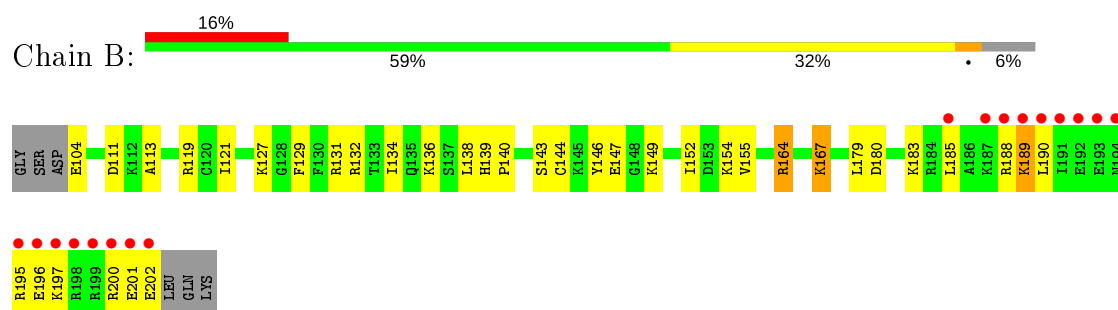
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

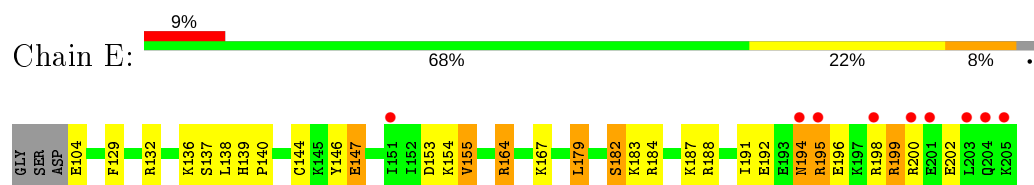
- Molecule 1: Thyroid hormone receptor beta



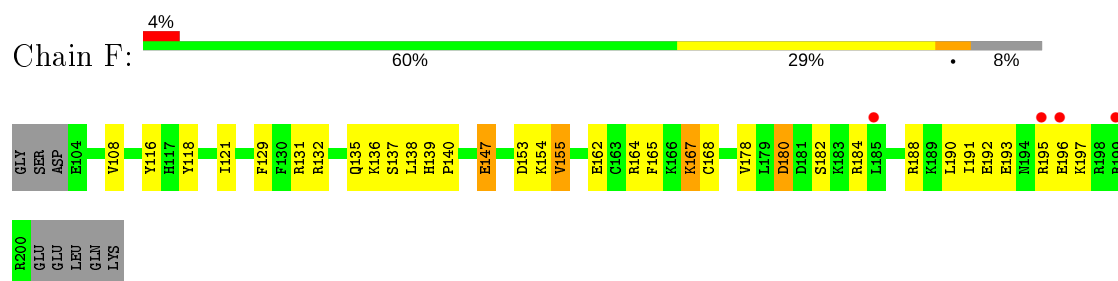
- Molecule 1: Thyroid hormone receptor beta



- Molecule 1: Thyroid hormone receptor beta

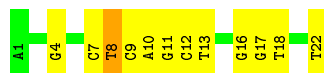


- Molecule 1: Thyroid hormone receptor beta



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*CP\*AP\*AP\*T)-3')

Chain C: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*CP\*AP\*AP\*T)-3')

Chain D: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*CP\*AP\*AP\*T)-3')

Chain G: 



- Molecule 2: DNA (5'-D(\*AP\*TP\*TP\*GP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*CP\*AP\*AP\*T)-3')

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.74Å 83.47Å 75.74Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	42.18 – 2.41 42.18 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (42.18-2.41) 98.4 (42.18-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.179 , 0.231 0.186 , 0.235	Depositor DCC
$R_{free}$ test set	1770 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	1.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.63% 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

### 5.1 Standard geometry

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

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	0.40	0/837	0.63	1/1112 (0.1%)
1	B	0.36	0/828	0.57	0/1100
1	E	0.45	0/857	0.61	0/1137
1	F	0.53	0/802	0.62	0/1065
2	C	0.64	0/501	1.49	6/772 (0.8%)
2	D	0.67	0/501	1.40	3/772 (0.4%)
2	G	0.65	0/501	1.42	4/772 (0.5%)
2	H	0.69	0/501	1.41	5/772 (0.6%)
All	All	0.53	0/5328	1.03	19/7502 (0.3%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	18	DT	O4'-C1'-N1	-10.93	100.35	108.00
2	C	16	DG	O4'-C1'-N9	8.57	114.00	108.00
2	C	10	DA	O4'-C1'-N9	-8.43	102.10	108.00
2	G	18	DT	O4'-C1'-N1	-8.07	102.35	108.00
2	G	13	DT	O4'-C1'-N1	-8.02	102.39	108.00
2	H	6	DC	O4'-C1'-N1	7.70	113.39	108.00
2	H	18	DT	O4'-C1'-N1	-7.44	102.79	108.00
2	D	11	DG	O4'-C4'-C3'	-6.74	101.80	104.50
2	C	22	DT	O4'-C4'-C3'	-6.68	101.83	104.50
2	H	7	DC	O4'-C4'-C3'	-6.59	101.86	104.50
1	A	145	LYS	CB-CA-C	-5.94	98.52	110.40
2	C	8	DT	O4'-C1'-N1	-5.52	104.13	108.00
2	G	2	DT	O4'-C1'-N1	-5.46	104.18	108.00
2	H	8	DT	O4'-C1'-N1	-5.18	104.37	108.00
2	G	3	DT	N3-C4-O4	5.17	123.00	119.90
2	H	2	DT	P-O3'-C3'	5.17	125.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	11	DG	C4'-C3'-C2'	-5.10	98.51	103.10
2	D	3	DT	O4'-C1'-N1	-5.09	104.44	108.00
2	C	13	DT	O4'-C1'-N1	-5.06	104.46	108.00

There are no chirality outliers.

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	A	827	0	836	40	0
1	B	815	0	828	39	0
1	E	847	0	861	29	0
1	F	792	0	805	28	0
2	C	447	0	247	8	0
2	D	447	0	247	7	0
2	G	447	0	247	5	0
2	H	447	0	247	6	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	28	0	0	2	0
4	B	48	0	0	4	0
4	C	20	0	0	0	0
4	D	16	0	0	0	0
4	E	43	0	0	4	0
4	F	43	0	0	4	0
4	G	17	0	0	0	0
4	H	17	0	0	1	0
All	All	5309	0	4318	150	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 16.

All (150) 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:F:188:ARG:HB3	4:F:216:HOH:O	1.68	0.92
1:F:136:LYS:HE3	1:F:138:LEU:HD11	1.62	0.82
1:E:139:HIS:CG	1:E:140:PRO:HD3	2.14	0.81
1:E:137:SER:HA	4:E:217:HOH:O	1.82	0.79
1:B:185:LEU:HD13	1:B:188:ARG:HD2	1.68	0.74
1:A:202:GLU:O	1:A:202:GLU:HG2	1.88	0.72
1:E:139:HIS:CD2	4:E:217:HOH:O	2.44	0.70
1:B:139:HIS:CG	1:B:140:PRO:HD3	2.27	0.69
1:A:204:GLN:C	1:B:202:GLU:HG2	2.14	0.68
1:B:136:LYS:HE3	1:B:138:LEU:HD11	1.74	0.68
1:E:144:CYS:SG	1:E:146:TYR:O	2.52	0.68
1:A:136:LYS:HE3	1:A:138:LEU:HD11	1.76	0.68
1:A:194:ASN:HB3	1:A:198:ARG:NH1	2.08	0.67
1:B:152[B]:ILE:HG23	1:B:167:LYS:HE3	1.77	0.66
1:A:116:TYR:CZ	1:A:121:ILE:HD11	2.32	0.65
1:F:129:PHE:CE2	1:F:164:ARG:HG2	2.32	0.65
1:E:188:ARG:O	1:E:192:GLU:HG2	1.98	0.64
1:B:139:HIS:CD2	1:B:140:PRO:HD3	2.34	0.63
1:F:167:LYS:HE2	4:F:219:HOH:O	1.99	0.63
1:F:184:ARG:HG2	1:F:188:ARG:HE	1.63	0.63
2:C:12:DC:C6	2:C:12:DC:H5'	2.35	0.62
1:E:191:ILE:O	1:E:195:ARG:HG2	2.00	0.62
1:A:146:TYR:N	1:A:146:TYR:CD2	2.69	0.60
1:A:202:GLU:HA	1:B:201:GLU:HG3	1.84	0.60
1:A:107:VAL:HG22	1:A:121:ILE:O	2.01	0.60
1:E:199:ARG:HG2	1:E:199:ARG:O	2.01	0.60
1:B:129:PHE:CE2	1:B:164:ARG:HG2	2.38	0.59
1:B:201:GLU:HA	1:B:202:GLU:C	2.22	0.59
1:E:153:ASP:OD1	1:E:155:VAL:HG13	2.03	0.58
1:B:196:GLU:O	1:B:200:ARG:HG3	2.04	0.58
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.68	0.57
1:E:132:ARG:NH2	2:H:4:DG:N7	2.52	0.57
1:B:134:ILE:HG23	1:E:182:SER:HB2	1.85	0.57
1:B:144:CYS:SG	1:B:146:TYR:O	2.63	0.57
1:A:116:TYR:CE1	1:A:121:ILE:CD1	2.89	0.56
1:F:132:ARG:NH2	2:G:4:DG:N7	2.53	0.56
1:E:136:LYS:HE3	1:E:138:LEU:HD11	1.86	0.56
1:A:116:TYR:CE1	1:A:121:ILE:HD11	2.40	0.56
1:A:194:ASN:HB3	1:A:198:ARG:HH12	1.69	0.56
2:C:12:DC:H5'	2:C:12:DC:H6	1.69	0.56
1:B:127:LYS:HE3	4:B:8:HOH:O	2.07	0.55
1:A:181:ASP:O	1:A:185:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:HIS:ND1	1:E:140:PRO:HD3	2.22	0.54
1:F:184:ARG:HD3	1:F:188:ARG:HH21	1.72	0.54
1:A:196:GLU:O	1:A:200:ARG:HG2	2.09	0.53
1:B:152[B]:ILE:HD12	1:B:164:ARG:HA	1.90	0.53
1:F:116:TYR:CZ	1:F:121:ILE:HD11	2.43	0.53
1:A:165:PHE:O	1:A:168:CYS:HB2	2.10	0.52
2:G:9:DC:H2''	2:G:10:DA:C8	2.44	0.52
1:A:132:ARG:NH2	2:D:4:DG:N7	2.57	0.52
1:B:132:ARG:NH2	2:C:4:DG:N7	2.57	0.52
1:A:162:GLU:HG2	4:A:213:HOH:O	2.09	0.52
1:F:184:ARG:O	1:F:188:ARG:HG3	2.10	0.52
2:H:11:DG:H1'	2:H:12:DC:H5'	1.92	0.51
1:F:191:ILE:O	1:F:195:ARG:HG3	2.11	0.51
1:B:201:GLU:HA	1:B:202:GLU:O	2.11	0.51
1:E:199:ARG:C	1:E:202:GLU:OE1	2.49	0.51
1:A:139:HIS:CG	1:A:140:PRO:HD3	2.46	0.51
1:E:129:PHE:CE2	1:E:164:ARG:HG2	2.46	0.51
1:E:139:HIS:CD2	1:E:140:PRO:HD3	2.45	0.50
1:E:196:GLU:HA	1:E:199:ARG:HD2	1.91	0.50
1:B:131:ARG:NH1	4:B:225:HOH:O	2.44	0.50
1:F:153:ASP:OD1	1:F:155:VAL:HG13	2.12	0.50
1:B:190:LEU:HB2	4:B:214:HOH:O	2.11	0.50
1:E:179:LEU:HD22	2:G:16:DG:H5'	1.93	0.50
1:F:139:HIS:CG	1:F:140:PRO:HD3	2.47	0.49
2:D:7:DC:H2''	2:D:8:DT:H5'	1.94	0.49
2:D:10:DA:H2''	2:D:11:DG:H5'	1.94	0.48
1:E:194:ASN:O	1:E:198:ARG:HB2	2.12	0.48
1:A:202:GLU:HA	1:B:201:GLU:HB2	1.95	0.48
1:A:111:ASP:HB3	1:A:154:LYS:HD2	1.95	0.48
1:B:195:ARG:HD3	2:C:9:DC:OP1	2.12	0.48
1:B:154:LYS:HE3	1:B:154:LYS:HB2	1.76	0.48
1:B:147:GLU:O	1:B:149:LYS:N	2.44	0.48
1:E:195:ARG:O	1:E:199:ARG:HB3	2.13	0.47
1:B:167:LYS:HE2	4:B:211:HOH:O	2.12	0.47
1:E:147:GLU:H	1:E:147:GLU:HG3	1.36	0.47
1:F:193:GLU:HA	1:F:196:GLU:HG2	1.96	0.47
1:A:145:LYS:HB2	1:A:146:TYR:CE2	2.50	0.47
1:A:197:LYS:O	1:A:201:GLU:HB3	2.15	0.47
1:B:189:LYS:HB3	1:B:189:LYS:HE2	1.62	0.47
1:A:184:ARG:HE	2:C:17:DG:P	2.38	0.47
1:E:139:HIS:HD2	4:E:217:HOH:O	1.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:VAL:HG13	1:F:167:LYS:HG2	1.97	0.47
1:B:180:ASP:OD1	1:B:183:LYS:HG3	2.15	0.47
1:E:192:GLU:O	1:E:195:ARG:HB2	2.15	0.47
2:D:10:DA:H1'	2:D:11:DG:H5'	1.96	0.46
1:B:201:GLU:HA	1:B:202:GLU:HB3	1.96	0.46
1:F:162:GLU:HG2	4:F:223:HOH:O	2.15	0.46
1:A:133:THR:HG21	1:A:165:PHE:CD1	2.51	0.46
1:B:201:GLU:HG2	1:B:201:GLU:O	2.16	0.46
2:C:7:DC:H2''	2:C:8:DT:H5'	1.97	0.46
1:A:153:ASP:OD1	1:A:155:VAL:HG13	2.16	0.46
1:A:147:GLU:C	1:A:149:LYS:H	2.18	0.46
1:F:196:GLU:HG3	1:F:197:LYS:N	2.31	0.45
1:F:154:LYS:HB2	1:F:154:LYS:HE3	1.69	0.45
1:B:201:GLU:HA	1:B:202:GLU:CB	2.47	0.45
2:D:7:DC:H2'	2:D:8:DT:C6	2.51	0.45
1:B:119:ARG:NH1	1:B:119:ARG:HG2	2.31	0.45
1:A:116:TYR:CD1	1:A:121:ILE:HD13	2.52	0.45
1:E:154:LYS:HB2	1:E:154:LYS:HE3	1.72	0.45
1:A:113:ALA:CB	1:A:121:ILE:HG22	2.46	0.44
1:A:199:ARG:NE	1:A:199:ARG:HA	2.32	0.44
2:C:7:DC:H2'	2:C:8:DT:H72	1.98	0.44
1:F:118:TYR:CE1	1:F:178:VAL:HG22	2.52	0.44
1:F:190:LEU:HA	1:F:190:LEU:HD23	1.77	0.44
1:E:188:ARG:NE	1:E:188:ARG:HA	2.32	0.44
1:B:201:GLU:CA	1:B:202:GLU:C	2.85	0.44
2:H:15:DA:H2''	2:H:16:DG:H5'	2.00	0.44
1:A:152:ILE:HB	1:A:167:LYS:HE3	2.00	0.44
2:H:9:DC:H2''	2:H:10:DA:C8	2.53	0.44
1:F:180:ASP:OD1	1:F:180:ASP:N	2.50	0.43
1:E:199:ARG:NH2	4:E:207:HOH:O	2.36	0.43
2:G:7:DC:H2'	2:G:8:DT:H72	2.00	0.43
2:H:7:DC:H2''	2:H:8:DT:H5'	2.00	0.43
1:A:204:GLN:O	1:B:202:GLU:HG2	2.18	0.43
1:E:104:GLU:HA	1:E:104:GLU:OE1	2.17	0.43
1:F:147:GLU:H	1:F:147:GLU:HG3	1.51	0.43
1:A:157:ARG:HB2	1:A:164:ARG:HD3	2.01	0.42
1:F:192:GLU:HG2	1:F:195:ARG:HH21	1.84	0.42
1:A:116:TYR:CE1	1:A:121:ILE:HD13	2.55	0.42
1:F:165:PHE:O	1:F:168:CYS:HB2	2.19	0.42
2:D:11:DG:H1'	2:D:12:DC:C6	2.53	0.42
1:E:182:SER:OG	1:E:183:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HB2	1:B:136:LYS:HE2	2.02	0.42
2:C:11:DG:O5'	2:C:11:DG:H2'	2.20	0.42
1:F:131:ARG:NE	4:F:229:HOH:O	2.34	0.42
1:F:139:HIS:N	1:F:140:PRO:CD	2.83	0.42
1:E:132:ARG:HD2	4:H:140:HOH:O	2.20	0.42
1:E:187:LYS:HE2	1:E:188:ARG:HH21	1.85	0.42
1:F:131:ARG:O	1:F:135:GLN:HB2	2.20	0.42
1:B:111:ASP:HB3	1:B:154:LYS:HD2	2.01	0.41
1:B:152[B]:ILE:CD1	1:B:164:ARG:HA	2.49	0.41
2:D:21:DA:H2''	2:D:22:DT:O5'	2.20	0.41
2:H:15:DA:H2'	2:H:16:DG:C8	2.56	0.41
1:A:195:ARG:O	1:A:199:ARG:HD2	2.21	0.41
1:B:152[B]:ILE:HG23	1:B:167:LYS:CE	2.49	0.41
1:F:193:GLU:HB3	1:F:197:LYS:NZ	2.35	0.41
1:A:189:LYS:HE3	1:A:193:GLU:OE2	2.21	0.41
1:A:203:LEU:O	1:A:204:GLN:HB3	2.19	0.41
1:B:147:GLU:H	1:B:147:GLU:HG3	1.65	0.41
1:F:136:LYS:O	1:F:137:SER:HB3	2.21	0.41
1:B:113:ALA:CB	1:B:121:ILE:HG22	2.51	0.41
1:B:196:GLU:HG3	1:B:197:LYS:N	2.36	0.41
1:A:147:GLU:C	1:A:149:LYS:N	2.75	0.40
1:A:167:LYS:HE2	4:A:224:HOH:O	2.21	0.40
1:A:183:LYS:HE2	1:A:183:LYS:HB2	1.85	0.40
1:A:108:VAL:HG13	1:A:167:LYS:HG2	2.02	0.40
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.86	0.40
2:G:7:DC:H2'	2:G:8:DT:C7	2.52	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	99/105 (94%)	97 (98%)	2 (2%)	0	100	100
1	B	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
1	E	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
1	F	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
All	All	393/420 (94%)	384 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
1	A	92/95 (97%)	79 (86%)	13 (14%)	3	4
1	B	91/95 (96%)	84 (92%)	7 (8%)	13	20
1	E	94/95 (99%)	83 (88%)	11 (12%)	5	7
1	F	88/95 (93%)	83 (94%)	5 (6%)	20	33
All	All	365/380 (96%)	329 (90%)	36 (10%)	8	11

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	A	145	LYS
1	A	146	TYR
1	A	149	LYS
1	A	155	VAL
1	A	164	ARG
1	A	167	LYS
1	A	185	LEU
1	A	196	GLU
1	A	199	ARG
1	A	202	GLU
1	A	203	LEU
1	A	204	GLN

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Mol	Chain	Res	Type
1	B	104	GLU
1	B	143	SER
1	B	155	VAL
1	B	164	ARG
1	B	167	LYS
1	B	179	LEU
1	B	189	LYS
1	E	147	GLU
1	E	155	VAL
1	E	164	ARG
1	E	167	LYS
1	E	179	LEU
1	E	182	SER
1	E	184	ARG
1	E	194	ASN
1	E	195	ARG
1	E	199	ARG
1	E	200	ARG
1	F	147	GLU
1	F	155	VAL
1	F	167	LYS
1	F	180	ASP
1	F	182	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	139	HIS

### 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

Of 8 ligands modelled in this entry, 8 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 ⓘ

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	101/105 (96%)	0.48	8 (7%) 12 11	34, 53, 138, 179	0
1	B	99/105 (94%)	1.02	17 (17%) 1 1	30, 51, 153, 177	0
1	E	102/105 (97%)	0.49	9 (8%) 10 9	33, 49, 117, 137	0
1	F	97/105 (92%)	0.27	4 (4%) 37 36	33, 51, 116, 147	0
2	C	22/22 (100%)	-0.29	0 100 100	46, 63, 81, 86	0
2	D	22/22 (100%)	-0.28	0 100 100	38, 64, 78, 84	0
2	G	22/22 (100%)	-0.46	0 100 100	42, 65, 74, 79	0
2	H	22/22 (100%)	-0.36	0 100 100	44, 63, 73, 77	0
All	All	487/508 (95%)	0.40	38 (7%) 13 11	30, 54, 127, 179	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	GLU	8.1
1	B	200	ARG	8.0
1	B	199	ARG	7.5
1	B	201	GLU	6.3
1	B	198	ARG	6.2
1	B	191	ILE	5.9
1	B	195	ARG	5.7
1	B	192	GLU	5.5
1	E	203	LEU	5.1
1	B	194	ASN	4.9
1	F	199	ARG	4.9
1	A	204	GLN	4.5
1	B	190	LEU	4.4
1	E	205	LYS	4.2
1	A	201	GLU	4.2
1	F	195	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	204	GLN	3.9
1	E	198	ARG	3.7
1	A	203	LEU	3.6
1	A	196	GLU	3.5
1	B	197	LYS	3.3
1	B	189	LYS	3.2
1	B	185	LEU	3.0
1	B	188	ARG	2.9
1	B	202	GLU	2.8
1	E	201	GLU	2.8
1	E	200	ARG	2.8
1	B	187	LYS	2.7
1	E	195	ARG	2.7
1	F	185	LEU	2.6
1	B	193	GLU	2.5
1	F	196	GLU	2.5
1	A	198	ARG	2.4
1	A	197	LYS	2.4
1	A	112	LYS	2.3
1	A	151	ILE	2.3
1	E	194	ASN	2.2
1	E	151	ILE	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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
3	ZN	F	209	1/1	0.99	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	E	208	1/1	0.99	0.19	40,40,40,40	0
3	ZN	A	209	1/1	0.99	0.17	44,44,44,44	0
3	ZN	A	208	1/1	0.99	0.15	42,42,42,42	0
3	ZN	B	209	1/1	1.00	0.18	40,40,40,40	0
3	ZN	B	208	1/1	1.00	0.20	40,40,40,40	0
3	ZN	F	208	1/1	1.00	0.14	40,40,40,40	0
3	ZN	E	209	1/1	1.00	0.19	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.