



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 05:33 am BST

PDB ID : 4PBA  
Title : The 5-Hydroxymethylcytosine-Specific Restriction Enzyme AbaSI in a Complex with Substrate-like DNA  
Authors : Horton, J.R.; Cheng, X.  
Deposited on : 2014-04-11  
Resolution : 3.30 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

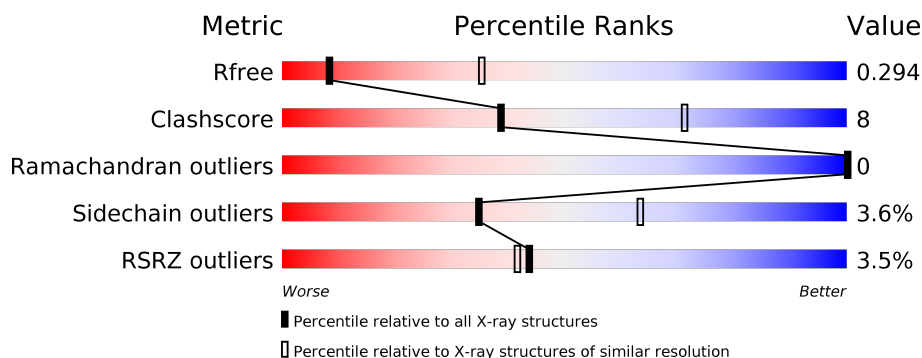
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	321	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	321	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>• •</div> </div> </div>
1	C	321	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	D	321	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
2	E	32	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
2	F	32	<div> <div>9%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11655 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 Uncharacterized protein AbaSI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	313	Total	C	N	O	S	0	0	0
			2592	1653	445	488	6			
1	A	314	Total	C	N	O	S	0	0	0
			2601	1658	446	491	6			
1	C	314	Total	C	N	O	S	0	0	0
			2601	1659	447	489	6			
1	D	313	Total	C	N	O	S	0	0	0
			2592	1653	445	488	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	CYS	engineered mutation	UNP B0VN39
B	309	SER	CYS	engineered mutation	UNP B0VN39
B	321	SER	CYS	engineered mutation	UNP B0VN39
A	2	SER	CYS	engineered mutation	UNP B0VN39
A	309	SER	CYS	engineered mutation	UNP B0VN39
A	321	SER	CYS	engineered mutation	UNP B0VN39
C	2	SER	CYS	engineered mutation	UNP B0VN39
C	309	SER	CYS	engineered mutation	UNP B0VN39
C	321	SER	CYS	engineered mutation	UNP B0VN39
D	2	SER	CYS	engineered mutation	UNP B0VN39
D	309	SER	CYS	engineered mutation	UNP B0VN39
D	321	SER	CYS	engineered mutation	UNP B0VN39

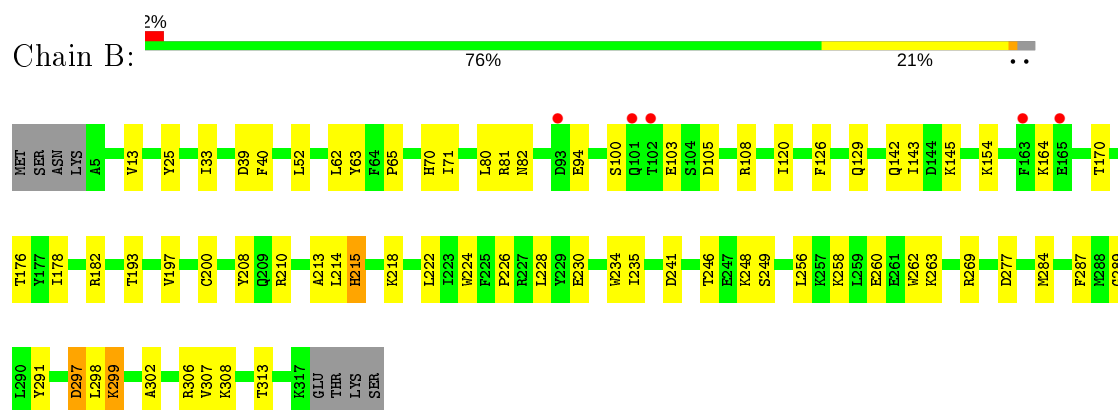
- Molecule 2 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	31	Total	C	N	O	P	0	0	0
			636	306	115	185	30			
2	F	31	Total	C	N	O	P	0	0	0
			633	305	113	185	30			

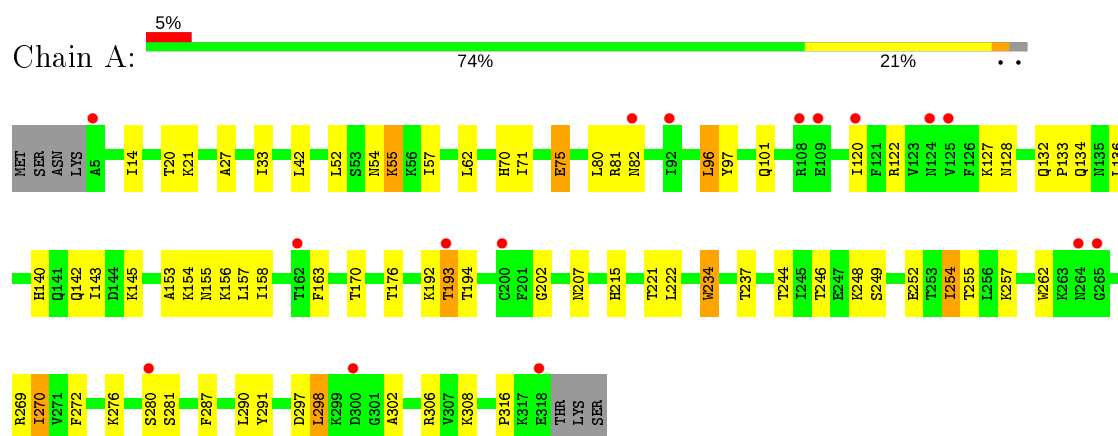
### 3 Residue-property plots [i](#)

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.

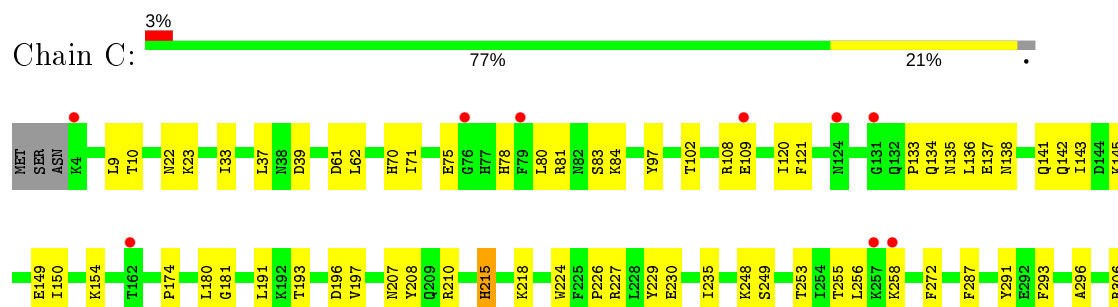
- Molecule 1: Uncharacterized protein AbaSI

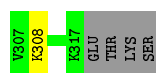


- Molecule 1: Uncharacterized protein AbaSI

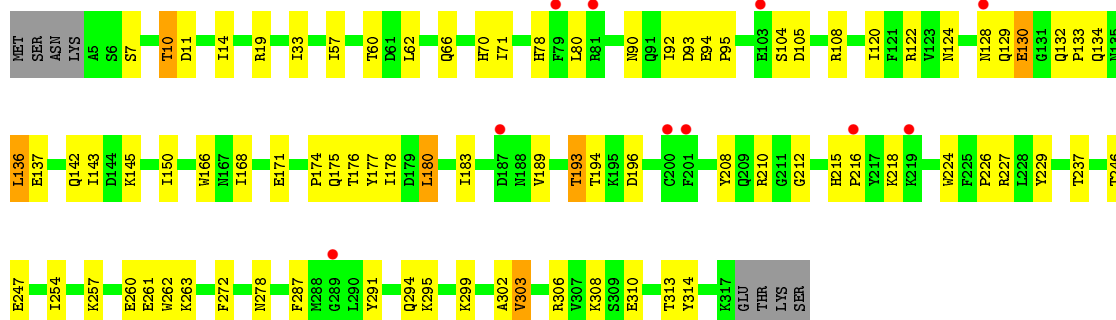


- Molecule 1: Uncharacterized protein AbaSI

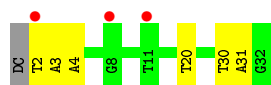
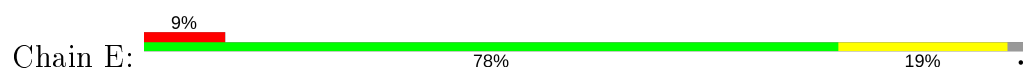




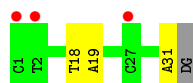
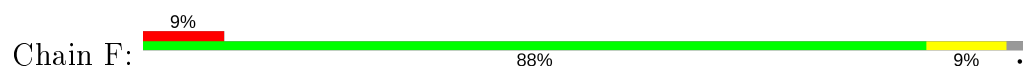
- Molecule 1: Uncharacterized protein AbaSI



- Molecule 2: DNA (32-MER)



- Molecule 2: DNA (32-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.67Å 147.13Å 103.48Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	35.09 – 3.30 35.09 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.09-3.30) 89.2 (35.09-3.30)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, $R_{free}$	0.240 , 0.293 0.243 , 0.294	Depositor DCC
$R_{free}$ test set	1188 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 28.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% 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: 5HC

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	0.22	0/2655	0.41	0/3583
1	B	0.23	0/2646	0.41	0/3571
1	C	0.23	0/2655	0.42	0/3582
1	D	0.24	0/2646	0.42	0/3571
2	E	0.51	0/689	0.92	0/1060
2	F	0.50	0/685	0.92	0/1053
All	All	0.28	0/11976	0.51	0/16420

There are no bond length outliers.

There are no bond angle outliers.

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	2601	0	2596	42	0
1	B	2592	0	2590	40	0
1	C	2601	0	2603	40	0
1	D	2592	0	2590	50	0
2	E	636	0	355	4	0
2	F	633	0	355	3	0
All	All	11655	0	11089	171	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 (171) 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:70:HIS:HB2	1:B:120:ILE:HG12	1.69	0.74
1:C:135:ASN:O	1:C:138:ASN:ND2	2.22	0.72
1:D:134:GLN:OE1	1:D:142:GLN:NE2	2.24	0.71
1:A:70:HIS:HB2	1:A:120:ILE:HG12	1.74	0.69
1:C:70:HIS:HB2	1:C:120:ILE:HG12	1.74	0.69
1:D:70:HIS:HB2	1:D:120:ILE:HG12	1.77	0.65
1:D:294:GLN:HB3	1:D:303:VAL:HG12	1.79	0.64
1:C:39:ASP:OD2	1:C:154:LYS:NZ	2.30	0.63
1:D:218:LYS:NZ	1:D:314:TYR:OH	2.31	0.63
1:A:170:THR:HB	1:A:176:THR:HG21	1.79	0.63
1:A:96:LEU:HD21	1:A:122:ARG:HE	1.63	0.63
1:A:192:LYS:HG3	1:A:193:THR:HG22	1.79	0.63
1:B:62:LEU:HD23	1:B:71:ILE:HD12	1.81	0.62
1:A:62:LEU:HD23	1:A:71:ILE:HD12	1.82	0.62
1:C:80:LEU:HD12	1:C:81:ARG:H	1.65	0.60
1:D:227:ARG:NH1	1:D:229:TYR:OH	2.35	0.59
1:B:256:LEU:HB2	1:B:298:LEU:HD11	1.85	0.58
1:C:62:LEU:HD23	1:C:71:ILE:HD12	1.85	0.58
1:A:254:ILE:HA	1:A:257:LYS:HG2	1.85	0.58
1:C:207:ASN:HB2	2:E:20:DT:H4'	1.85	0.58
1:B:170:THR:HB	1:B:176:THR:HG21	1.84	0.58
1:C:227:ARG:NH1	1:C:229:TYR:OH	2.37	0.58
1:D:183:ILE:HG23	1:D:189:VAL:HG11	1.86	0.56
1:B:100:SER:OG	1:B:103:GLU:OE2	2.23	0.56
1:D:33:ILE:HG12	1:D:143:ILE:HG23	1.89	0.55
1:A:62:LEU:HB3	1:A:71:ILE:HB	1.89	0.55
1:A:193:THR:OG1	1:A:194:THR:N	2.39	0.55
1:B:234:TRP:HH2	1:B:258:LYS:HE3	1.72	0.55
1:D:193:THR:OG1	1:D:194:THR:N	2.40	0.55
1:A:33:ILE:HG12	1:A:143:ILE:HG23	1.89	0.54
1:B:230:GLU:HG3	1:B:235:ILE:HG12	1.88	0.54
1:D:208:TYR:CZ	1:D:210:ARG:HB3	2.43	0.54
1:C:208:TYR:CZ	1:C:210:ARG:HB3	2.43	0.53
1:C:293:PHE:HZ	1:C:296:ALA:HB2	1.74	0.53
1:B:62:LEU:HB3	1:B:71:ILE:HB	1.91	0.53
1:D:62:LEU:HD23	1:D:71:ILE:HD12	1.89	0.53
1:A:222:LEU:HB3	1:A:269:ARG:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:OD2	1:B:154:LYS:NZ	2.39	0.52
1:C:142:GLN:HA	1:C:145:LYS:HE3	1.92	0.52
1:C:180:LEU:N	1:C:181:GLY:HA2	2.24	0.52
1:D:308:LYS:HG2	1:D:310:GLU:H	1.75	0.51
1:A:127:LYS:HG3	1:A:128:ASN:H	1.76	0.51
1:A:248:LYS:HG2	1:A:249:SER:H	1.76	0.51
1:D:124:ASN:OD1	1:D:128:ASN:ND2	2.44	0.51
1:B:33:ILE:HG12	1:B:143:ILE:HG23	1.92	0.51
1:D:261:GLU:OE1	1:D:261:GLU:N	2.43	0.51
1:A:127:LYS:HB3	1:A:134:GLN:HG3	1.92	0.50
1:B:105:ASP:OD1	1:B:108:ARG:NH1	2.41	0.50
1:C:23:LYS:NZ	1:C:61:ASP:OD2	2.39	0.50
1:A:276:LYS:HE3	1:A:281:SER:HB2	1.93	0.50
1:C:255:THR:HA	1:C:258:LYS:HE3	1.94	0.50
1:A:202:GLY:HA2	1:A:316:PRO:HA	1.94	0.50
1:A:75:GLU:O	1:A:97:TYR:OH	2.28	0.50
1:D:71:ILE:HD11	1:D:150:ILE:HD11	1.93	0.49
1:B:287:PHE:CZ	1:B:289:GLY:HA2	2.47	0.49
1:B:260:GLU:HA	1:B:263:LYS:HE2	1.93	0.49
1:D:92:ILE:HG23	1:D:93:ASP:H	1.77	0.49
1:B:277:ASP:HB2	1:B:284:MET:HG3	1.94	0.49
1:C:121:PHE:CZ	1:C:149:GLU:HG2	2.48	0.49
1:B:164:LYS:NZ	1:B:182:ARG:HH22	2.10	0.49
1:B:52:LEU:HD22	1:B:94:GLU:HB3	1.95	0.49
1:D:57:ILE:HD12	1:D:104:SER:HB2	1.94	0.48
2:F:18:DT:H4'	2:F:19:DA:OP1	2.13	0.48
1:D:224:TRP:CE2	1:D:226:PRO:HB3	2.48	0.48
1:C:62:LEU:HB3	1:C:71:ILE:HB	1.94	0.48
1:D:178:ILE:HA	1:D:313:THR:HG21	1.96	0.48
1:C:134:GLN:HG2	1:C:138:ASN:ND2	2.29	0.47
1:C:9:LEU:HD23	1:D:136:LEU:HG	1.95	0.47
1:D:19:ARG:NH2	1:D:278:ASN:OD1	2.46	0.47
1:A:234:TRP:HB2	1:A:248:LYS:O	2.13	0.47
1:C:224:TRP:CZ2	1:C:226:PRO:HB3	2.50	0.47
1:D:208:TYR:OH	1:D:212:GLY:O	2.30	0.47
1:D:260:GLU:HA	1:D:263:LYS:HG2	1.97	0.47
1:A:207:ASN:HB2	2:F:31:DA:H5'	1.96	0.47
1:A:55:LYS:HZ1	1:A:101:GLN:HG2	1.80	0.47
1:A:297:ASP:OD1	1:A:298:LEU:N	2.46	0.47
1:D:132:GLN:HA	1:D:133:PRO:HD3	1.78	0.47
1:B:200:CYS:O	1:B:313:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:HG21	1:A:136:LEU:HD11	1.96	0.46
1:C:230:GLU:HG3	1:C:235:ILE:HG12	1.97	0.46
1:D:254:ILE:HA	1:D:257:LYS:HG2	1.98	0.46
1:D:105:ASP:OD2	1:D:108:ARG:NH2	2.48	0.46
1:D:66:GLN:HE22	1:D:166:TRP:HB2	1.80	0.46
1:C:248:LYS:HG2	1:C:249:SER:H	1.81	0.46
1:C:224:TRP:CE2	1:C:226:PRO:HB3	2.50	0.46
1:B:248:LYS:HG2	1:B:249:SER:H	1.81	0.46
1:A:142:GLN:HA	1:A:145:LYS:HE3	1.97	0.46
1:A:55:LYS:HG2	1:A:55:LYS:O	2.16	0.46
1:C:22:ASN:O	1:C:80:LEU:HD13	2.16	0.46
1:D:62:LEU:HB3	1:D:71:ILE:HB	1.98	0.46
1:C:133:PRO:HB2	1:D:7:SER:HB3	1.96	0.46
1:B:291:TYR:CE2	1:B:306:ARG:HB2	2.51	0.45
1:C:80:LEU:HD12	1:C:81:ARG:N	2.31	0.45
2:E:3:DA:H2"	2:E:4:DA:C8	2.52	0.45
1:C:71:ILE:HD11	1:C:150:ILE:HD11	1.98	0.45
1:D:175:GLN:O	1:D:178:ILE:HG12	2.16	0.45
1:D:176:THR:O	1:D:180:LEU:HG	2.15	0.45
1:A:81:ARG:HA	1:A:82:ASN:HA	1.69	0.45
1:D:215:HIS:HD2	1:D:216:PRO:HD2	1.81	0.45
1:C:33:ILE:HD13	1:C:71:ILE:HD13	1.99	0.45
1:A:132:GLN:HA	1:A:133:PRO:HD3	1.78	0.45
1:B:224:TRP:CE2	1:B:226:PRO:HB3	2.52	0.45
1:A:237:THR:OG1	1:A:246:THR:OG1	2.28	0.45
1:B:178:ILE:HA	1:B:313:THR:HG21	1.99	0.45
1:A:33:ILE:HD13	1:A:71:ILE:HD13	1.99	0.44
1:A:215:HIS:ND1	1:A:221:THR:OG1	2.48	0.44
1:A:252:GLU:O	1:A:255:THR:OG1	2.26	0.44
1:A:54:ASN:O	1:A:55:LYS:HB3	2.16	0.44
1:B:291:TYR:HA	1:B:306:ARG:HA	2.00	0.44
1:C:174:PRO:HG3	1:C:196:ASP:HB3	1.99	0.44
1:D:237:THR:OG1	1:D:246:THR:OG1	2.24	0.44
1:C:272:PHE:CE2	1:C:287:PHE:HB2	2.53	0.44
1:A:270:ILE:HD11	1:A:272:PHE:CE1	2.52	0.44
1:A:42:LEU:HD11	1:A:154:LYS:HD2	1.99	0.44
2:E:30:DT:H2"	2:E:31:DA:C8	2.53	0.44
1:B:25:TYR:CE2	1:A:14:ILE:HG13	2.53	0.44
1:D:129:GLN:O	1:D:130:GLU:HB2	2.18	0.44
2:E:2:DT:H2"	2:E:3:DA:C8	2.53	0.43
1:D:262:TRP:CE3	1:D:302:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLN:HA	1:B:145:LYS:HE3	2.00	0.43
1:B:307:VAL:HG22	1:B:308:LYS:HG3	2.00	0.43
1:B:80:LEU:HB3	1:B:82:ASN:O	2.18	0.43
1:B:260:GLU:HA	1:B:263:LYS:HG2	2.00	0.43
1:C:255:THR:HA	1:C:258:LYS:CE	2.49	0.43
1:D:291:TYR:CE2	1:D:306:ARG:HB2	2.54	0.43
1:A:291:TYR:CE2	1:A:306:ARG:HB2	2.54	0.43
1:B:298:LEU:HA	1:B:298:LEU:HD12	1.83	0.43
1:C:215:HIS:CD2	1:C:218:LYS:HB2	2.54	0.43
1:C:33:ILE:HG12	1:C:143:ILE:HG23	2.01	0.43
1:D:189:VAL:HG13	1:D:287:PHE:HB3	2.00	0.43
1:D:295:LYS:HG2	1:D:303:VAL:HB	2.01	0.43
1:B:40:PHE:CE2	1:A:140:HIS:HE1	2.36	0.42
1:C:191:LEU:HD12	1:C:197:VAL:HG22	2.00	0.42
1:D:142:GLN:HA	1:D:145:LYS:HE2	2.01	0.42
1:A:272:PHE:CE2	1:A:287:PHE:HB2	2.53	0.42
1:C:80:LEU:HD21	1:C:83:SER:HB2	2.01	0.42
1:D:272:PHE:CE2	1:D:287:PHE:HB2	2.53	0.42
1:B:126:PHE:HB3	1:B:129:GLN:HB3	2.01	0.42
1:B:208:TYR:CZ	1:B:210:ARG:HB2	2.55	0.42
1:B:297:ASP:OD1	1:B:299:LYS:N	2.52	0.42
1:A:290:LEU:HD23	1:A:308:LYS:HB2	2.01	0.42
1:B:215:HIS:CD2	1:B:218:LYS:HB2	2.54	0.42
1:C:137:GLU:O	1:C:141:GLN:HG2	2.20	0.42
1:B:33:ILE:HD13	1:B:71:ILE:HD13	2.02	0.42
1:C:136:LEU:HG	1:D:10:THR:HG22	2.02	0.42
1:C:108:ARG:NH1	1:C:230:GLU:O	2.53	0.41
1:C:109:GLU:HG2	1:C:229:TYR:CZ	2.55	0.41
1:C:291:TYR:CE2	1:C:306:ARG:HB2	2.55	0.41
1:B:262:TRP:CE3	1:B:302:ALA:HB2	2.55	0.41
1:D:90:ASN:HB3	1:D:94:GLU:OE1	2.19	0.41
1:D:224:TRP:CZ2	1:D:226:PRO:HB3	2.55	0.41
1:A:157:LEU:HB3	1:A:163:PHE:HB2	2.02	0.41
1:A:262:TRP:CE3	1:A:302:ALA:HB2	2.56	0.41
2:F:18:DT:H2''	2:F:19:DA:O5'	2.21	0.41
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.93	0.41
1:D:105:ASP:O	1:D:108:ARG:HG3	2.21	0.41
1:A:153:ALA:O	1:A:156:LYS:HG2	2.20	0.41
1:D:168:ILE:O	1:D:171:GLU:HG2	2.21	0.41
1:A:155:ASN:O	1:A:158:ILE:HG13	2.21	0.41
1:B:63:TYR:CZ	1:B:65:PRO:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HB3	1:D:137:GLU:H	1.57	0.41
1:D:174:PRO:HG3	1:D:196:ASP:HB3	2.03	0.41
1:A:21:LYS:HZ2	1:A:27:ALA:H	1.68	0.41
1:C:75:GLU:O	1:C:97:TYR:OH	2.34	0.41
1:D:177:TYR:O	1:D:313:THR:HG21	2.20	0.41
1:B:208:TYR:CE2	1:B:213:ALA:HB2	2.57	0.40
1:B:222:LEU:HB3	1:B:269:ARG:HG2	2.03	0.40
1:D:11:ASP:O	1:D:14:ILE:HG13	2.22	0.40
1:D:66:GLN:NE2	1:D:166:TRP:HB2	2.36	0.40
1:D:60:THR:HG22	1:D:95:PRO:HB3	2.03	0.40
1:C:253:THR:O	1:C:256:LEU:HG	2.22	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	312/321 (97%)	299 (96%)	13 (4%)	0	100	100
1	B	311/321 (97%)	306 (98%)	5 (2%)	0	100	100
1	C	312/321 (97%)	305 (98%)	7 (2%)	0	100	100
1	D	311/321 (97%)	303 (97%)	8 (3%)	0	100	100
All	All	1246/1284 (97%)	1213 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	289/296 (98%)	275 (95%)	14 (5%)	25	56
1	B	288/296 (97%)	279 (97%)	9 (3%)	40	67
1	C	289/296 (98%)	281 (97%)	8 (3%)	43	70
1	D	288/296 (97%)	277 (96%)	11 (4%)	33	62
All	All	1154/1184 (98%)	1112 (96%)	42 (4%)	35	63

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ARG
1	B	193	THR
1	B	197	VAL
1	B	214	LEU
1	B	215	HIS
1	B	241	ASP
1	B	246	THR
1	B	297	ASP
1	B	299	LYS
1	A	20	THR
1	A	52	LEU
1	A	55	LYS
1	A	57	ILE
1	A	75	GLU
1	A	80	LEU
1	A	96	LEU
1	A	193	THR
1	A	234	TRP
1	A	244	THR
1	A	254	ILE
1	A	270	ILE
1	A	280	SER
1	A	298	LEU
1	C	10	THR
1	C	37	LEU
1	C	78	HIS
1	C	84	LYS
1	C	102	THR
1	C	193	THR
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	308	LYS
1	D	10	THR
1	D	78	HIS
1	D	80	LEU
1	D	122	ARG
1	D	130	GLU
1	D	136	LEU
1	D	180	LEU
1	D	193	THR
1	D	247	GLU
1	D	299	LYS
1	D	303	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	ASN
1	D	128	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5HC	E	5	2	16,22,23	4.40	11 (68%)	20,31,34	1.37	3 (15%)
2	5HC	F	5	2	16,22,23	4.43	11 (68%)	20,31,34	1.27	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5HC	E	5	2	-	2/6/23/24	0/2/2/2
2	5HC	F	5	2	-	2/6/23/24	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	5HC	O4'-C4'	-8.62	1.25	1.45
2	E	5	5HC	O4'-C4'	-8.46	1.26	1.45
2	F	5	5HC	O4'-C1'	7.95	1.60	1.42
2	E	5	5HC	O4'-C1'	7.93	1.60	1.42
2	E	5	5HC	C2'-C1'	-7.26	1.32	1.52
2	F	5	5HC	C2'-C1'	-7.16	1.32	1.52
2	F	5	5HC	C2-N3	4.96	1.48	1.38
2	F	5	5HC	C4-N3	4.94	1.42	1.35
2	E	5	5HC	C4-N4	4.83	1.46	1.34
2	E	5	5HC	C6-C5	4.83	1.48	1.37
2	F	5	5HC	C4-N4	4.83	1.46	1.34
2	E	5	5HC	C2-N3	4.81	1.47	1.38
2	F	5	5HC	C6-C5	4.74	1.48	1.37
2	E	5	5HC	C4-N3	4.73	1.41	1.35
2	F	5	5HC	O3'-C3'	-3.03	1.36	1.43
2	E	5	5HC	O3'-C3'	-3.02	1.36	1.43
2	F	5	5HC	C5-C4	2.88	1.47	1.42
2	E	5	5HC	C5-C4	2.77	1.47	1.42
2	F	5	5HC	C1'-N1	-2.47	1.42	1.49
2	E	5	5HC	C1'-N1	-2.40	1.42	1.49
2	E	5	5HC	C3'-C4'	2.20	1.59	1.53
2	F	5	5HC	C3'-C4'	2.11	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	5HC	C2-N3-C4	3.73	120.52	116.02
2	F	5	5HC	C2-N3-C4	3.33	120.04	116.02
2	F	5	5HC	N4-C4-N3	2.15	120.07	117.03
2	E	5	5HC	N4-C4-N3	2.12	120.03	117.03
2	E	5	5HC	C2'-C1'-N1	-2.06	109.51	114.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	5	5HC	O4'-C4'-C5'-O5'
2	F	5	5HC	C3'-C4'-C5'-O5'
2	E	5	5HC	O4'-C4'-C5'-O5'
2	E	5	5HC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

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	314/321 (97%)	0.24	16 (5%) 28 26	44, 120, 193, 231	0
1	B	313/321 (97%)	-0.06	5 (1%) 72 70	35, 80, 154, 206	0
1	C	314/321 (97%)	-0.03	9 (2%) 51 50	28, 82, 148, 227	0
1	D	313/321 (97%)	0.07	10 (3%) 47 46	27, 92, 154, 188	0
2	E	30/32 (93%)	0.39	3 (10%) 7 7	71, 105, 206, 242	0
2	F	30/32 (93%)	0.57	3 (10%) 7 7	66, 118, 211, 253	0
All	All	1314/1348 (97%)	0.07	46 (3%) 44 42	27, 93, 172, 253	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	GLU	9.3
1	A	5	ALA	6.3
1	D	187	ASP	4.7
1	A	162	THR	4.4
2	F	1	DC	4.4
2	F	2	DT	3.9
1	A	264	ASN	3.8
1	D	128	ASN	3.6
1	C	258	LYS	3.4
1	A	265	GLY	3.4
2	E	8	DG	3.4
2	E	2	DT	3.2
1	A	300	ASP	3.2
1	A	124	ASN	3.1
1	A	200	CYS	3.0
1	D	200	CYS	3.0
1	D	201	PHE	2.9
1	C	76	GLY	2.9
1	B	102	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	27	DC	2.7
1	C	79	PHE	2.7
1	C	124	ASN	2.7
1	B	93	ASP	2.6
1	B	165	GLU	2.6
2	E	11	DT	2.6
1	D	219	LYS	2.6
1	C	162	THR	2.6
1	C	109	GLU	2.5
1	D	103	GLU	2.5
1	A	280	SER	2.5
1	B	163	PHE	2.4
1	A	82	ASN	2.4
1	C	257	LYS	2.3
1	D	216	PRO	2.3
1	A	108	ARG	2.3
1	A	125	VAL	2.2
1	B	101	GLN	2.2
1	A	109	GLU	2.2
1	D	81	ARG	2.1
1	C	4	LYS	2.1
1	D	79	PHE	2.1
1	A	193	THR	2.1
1	A	92	ILE	2.0
1	D	289	GLY	2.0
1	C	131	GLY	2.0
1	A	120	ILE	2.0

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

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
2	5HC	E	5	21/22	0.80	0.17	168,181,189,198	0
2	5HC	F	5	21/22	0.86	0.20	109,115,124,124	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.