



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 06:19 PM JST

PDB ID : 6LWB  
Title : Crystal structure of human NEIL1(P2G, E3Q, R242) bound to duplex DNA containing 5-hydroxyuracil (5-OHU)  
Authors : Liu, M.H.; Zhang, J.; Zhu, C.X.; Zhang, X.X.; Gao, Y.Q.; Yi, C.Q.  
Deposited on : 2020-02-07  
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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

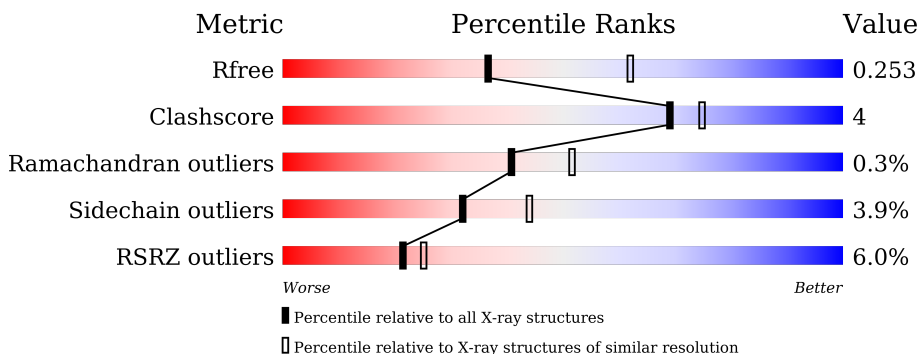
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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.



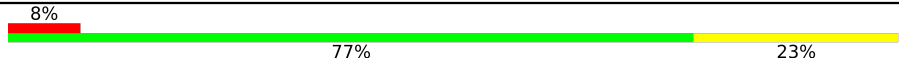
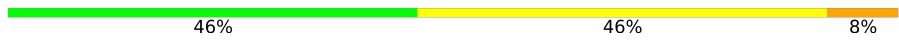

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	295	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      80%      9%      10%</p>
1	D	295	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      79%      9%      12%</p>
1	G	295	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11%      71%      6% •      23%</p>
2	B	13	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">8%      92%      8%</p>
2	E	13	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">8%      85%      15%</p>
2	H	13	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">23%      85%      8%      8%</p>

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Mol	Chain	Length	Quality of chain
3	C	13	 8% 77% 23%
3	F	13	 46% 46% 8%
3	I	13	 69% 31%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7570 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	Total 2106	C 1345	N 385	O 366	S 10	0	0	0
1	D	261	Total 2055	C 1312	N 378	O 355	S 10	0	0	0
1	G	228	Total 1574	C 975	N 301	O 290	S 8	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	PRO	engineered mutation	UNP Q96FI4
A	3	GLN	GLU	engineered mutation	UNP Q96FI4
A	242	ARG	LYS	variant	UNP Q96FI4
D	2	GLY	PRO	engineered mutation	UNP Q96FI4
D	3	GLN	GLU	engineered mutation	UNP Q96FI4
D	242	ARG	LYS	variant	UNP Q96FI4
G	2	GLY	PRO	engineered mutation	UNP Q96FI4
G	3	GLN	GLU	engineered mutation	UNP Q96FI4
G	242	ARG	LYS	variant	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*(OHU)P\*GP\*TP\*CP\*TP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	Total 258	C 124	N 43	O 79	P 12	0	0	0
2	E	13	Total 258	C 124	N 43	O 79	P 12	0	0	0
2	H	13	Total 258	C 124	N 43	O 79	P 12	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*

CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	267	127	53	75	12	0	0	0
3	F	13	267	127	53	75	12	0	0	0
3	I	13	267	127	53	75	12	0	0	0

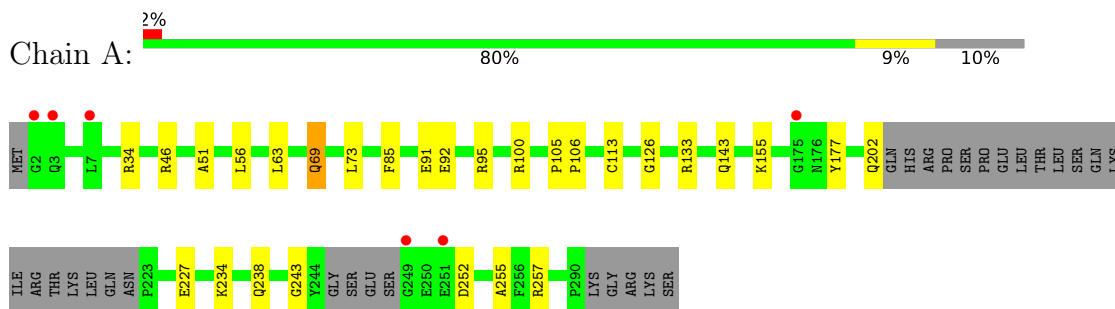
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total 132	O 132	0	0
4	B	16	Total 16	O 16	0	0
4	C	4	Total 4	O 4	0	0
4	D	76	Total 76	O 76	0	0
4	E	11	Total 11	O 11	0	0
4	F	8	Total 8	O 8	0	0
4	G	10	Total 10	O 10	0	0
4	H	1	Total 1	O 1	0	0
4	I	2	Total 2	O 2	0	0

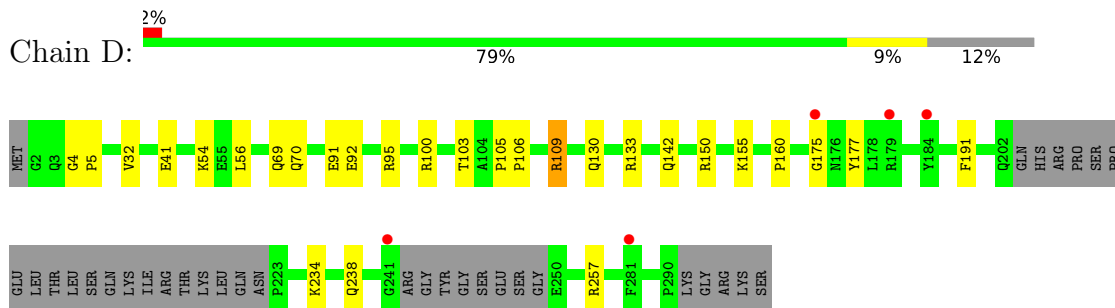
### 3 Residue-property plots [i](#)

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.

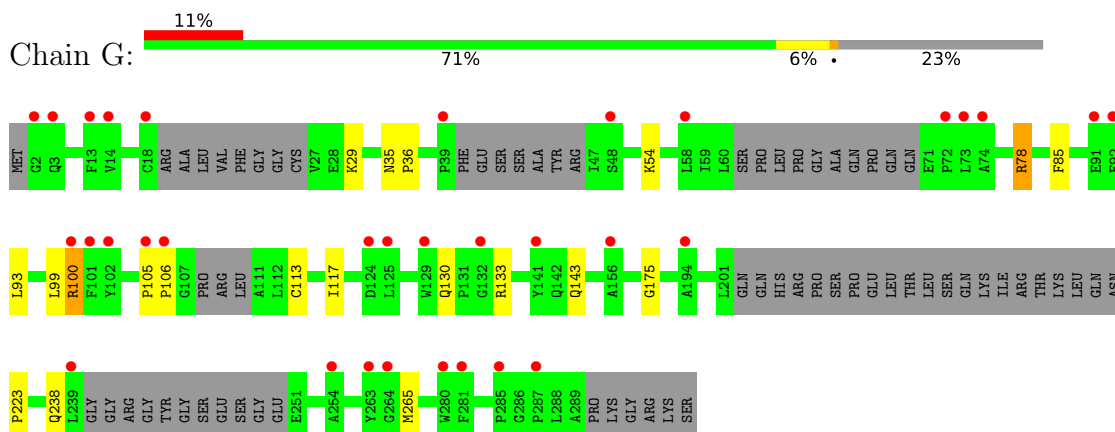
- Molecule 1: Endonuclease 8-like 1



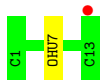
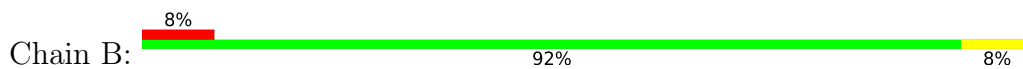
- Molecule 1: Endonuclease 8-like 1



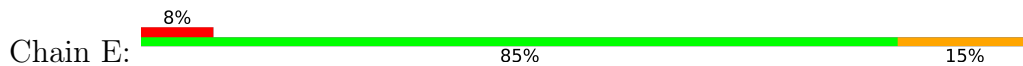
- Molecule 1: Endonuclease 8-like 1



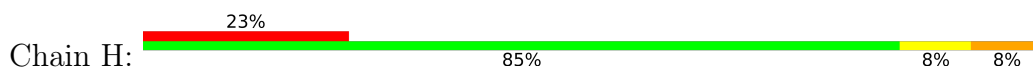
- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*(OHU)P\*GP\*TP\*CP\*TP\*AP\*C)-3')



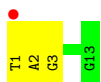
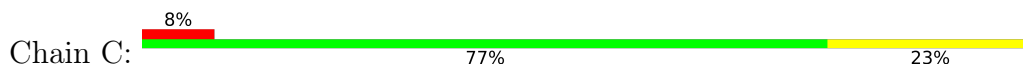
- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*(OHU)P\*GP\*TP\*CP\*TP\*AP\*C)-3')



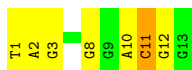
- Molecule 2: DNA (5'-D(\*CP\*GP\*TP\*CP\*CP\*AP\*(OHU)P\*GP\*TP\*CP\*TP\*AP\*C)-3')



- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



- Molecule 3: DNA (5'-D(\*TP\*AP\*GP\*AP\*CP\*CP\*TP\*GP\*GP\*AP\*CP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.81Å 109.24Å 169.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.34 – 2.55 32.32 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.34-2.55) 99.6 (32.32-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.210 , 0.253 0.211 , 0.253	Depositor DCC
$R_{free}$ test set	2275 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtrriage
Anisotropy	0.459	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: OHU

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	0.82	4/2163 (0.2%)	0.89	1/2923 (0.0%)
1	D	0.83	5/2110 (0.2%)	0.88	0/2852
1	G	0.70	0/1607	0.79	0/2148
2	B	0.45	0/264	0.85	0/402
2	E	0.57	0/264	1.31	2/402 (0.5%)
2	H	0.39	0/264	0.81	0/402
3	C	0.55	0/300	0.81	0/462
3	F	0.63	0/300	0.93	2/462 (0.4%)
3	I	0.47	0/300	0.75	0/462
All	All	0.74	9/7572 (0.1%)	0.88	5/10515 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	G	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	GLU	CD-OE1	12.57	1.39	1.25
1	A	92	GLU	CD-OE1	11.07	1.37	1.25
1	A	91	GLU	CG-CD	10.01	1.67	1.51
1	A	92	GLU	CD-OE2	9.26	1.35	1.25
1	D	92	GLU	CD-OE2	7.82	1.34	1.25
1	D	91	GLU	CG-CD	7.26	1.62	1.51
1	A	227	GLU	CD-OE1	6.18	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	150	ARG	NE-CZ	6.07	1.41	1.33
1	D	91	GLU	CD-OE2	5.57	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O5'-P-OP1	-19.59	87.19	110.70
2	E	8	DG	O5'-P-OP2	6.96	119.05	110.70
1	A	133	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	F	8	DG	O5'-P-OP1	-5.13	101.08	105.70
3	F	11	DC	C5'-C4'-C3'	-5.08	104.96	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Mainchain,Peptide
1	A	243	GLY	Peptide
1	G	105	PRO	Peptide

## 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	2106	0	2082	11	0
1	D	2055	0	2034	17	0
1	G	1574	0	1320	11	0
2	B	258	0	147	0	0
2	E	258	0	147	2	0
2	H	258	0	147	2	0
3	C	267	0	147	4	0
3	F	267	0	147	4	0
3	I	267	0	147	5	0
4	A	132	0	0	3	0
4	B	16	0	0	0	0
4	C	4	0	0	0	0
4	D	76	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	11	0	0	0	0
4	F	8	0	0	0	0
4	G	10	0	0	1	0
4	H	1	0	0	0	0
4	I	2	0	0	0	0
All	All	7570	0	6318	50	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 4.

All (50) 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:D:109:ARG:HG3	1:D:109:ARG:HH11	1.32	0.95
1:D:109:ARG:N	1:D:109:ARG:HD2	1.92	0.82
1:A:143:GLN:NE2	4:A:301:HOH:O	1.70	0.80
1:G:78:ARG:NH1	1:G:130:GLN:OE1	2.16	0.79
1:D:109:ARG:HG3	1:D:109:ARG:NH1	1.95	0.77
3:I:1:DT:H2'	3:I:2:DA:C8	2.19	0.77
1:A:69:GLN:NE2	1:A:69:GLN:HA	2.07	0.68
1:A:51:ALA:H	1:D:142:GLN:HE22	1.40	0.67
1:D:234:LYS:O	1:D:238:GLN:HG2	2.01	0.59
1:A:73:LEU:C	1:A:73:LEU:HD23	2.26	0.56
3:F:11:DC:H2''	3:F:12:DG:C8	2.41	0.56
1:G:175:GLY:HA3	2:H:8:DG:OP1	2.05	0.55
3:F:10:DA:H2''	3:F:11:DC:H5''	1.89	0.54
3:I:2:DA:H2''	3:I:3:DG:OP2	2.08	0.53
3:C:2:DA:H2''	3:C:3:DG:OP2	2.10	0.52
1:G:29:LYS:CE	1:G:35:ASN:O	2.59	0.51
1:D:41:GLU:O	1:D:70:GLN:NE2	2.43	0.50
1:A:257:ARG:NH1	4:A:304:HOH:O	2.45	0.49
1:D:175:GLY:HA3	2:E:8:DG:OP1	2.11	0.49
1:D:109:ARG:HH11	1:D:109:ARG:CG	2.09	0.49
3:F:2:DA:H2''	3:F:3:DG:OP2	2.12	0.49
3:C:1:DT:C2'	3:C:2:DA:C8	2.97	0.48
1:G:117:ILE:CG2	3:I:8:DG:H5'	2.44	0.48
1:A:46:ARG:HG3	1:A:63:LEU:HD21	1.96	0.48
3:F:1:DT:H2''	3:F:2:DA:OP2	2.14	0.47
1:G:29:LYS:HE3	1:G:35:ASN:O	2.14	0.47
1:G:117:ILE:HG21	3:I:8:DG:H5'	1.96	0.47
1:D:56:LEU:HD23	1:D:56:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:DT:H2''	3:C:2:DA:C8	2.51	0.45
1:D:130:GLN:HE21	1:D:133:ARG:HD2	1.82	0.45
1:G:36:PRO:HD3	4:G:309:HOH:O	2.17	0.45
3:C:1:DT:H2'	3:C:2:DA:C8	2.51	0.45
1:D:106:PRO:HG3	1:G:223:PRO:HG2	1.99	0.44
1:A:126:GLY:HA3	4:A:389:HOH:O	2.17	0.43
1:A:56:LEU:C	1:A:56:LEU:HD23	2.39	0.43
2:E:7:OHU:H6	2:E:7:OHU:C5'	2.49	0.43
3:I:1:DT:H2'	3:I:2:DA:N7	2.32	0.43
1:D:54:LYS:HB2	1:D:133:ARG:NH2	2.34	0.42
1:A:85:PHE:HA	1:A:113:CYS:O	2.19	0.42
1:A:252:ASP:HA	1:A:255:ALA:HB3	2.02	0.42
1:G:54:LYS:HB2	1:G:133:ARG:NH2	2.34	0.42
2:H:7:OHU:C5'	2:H:7:OHU:H6	2.48	0.42
1:G:85:PHE:HA	1:G:113:CYS:O	2.19	0.42
1:D:105:PRO:HA	1:D:106:PRO:HA	1.53	0.41
1:A:234:LYS:O	1:A:238:GLN:HG2	2.19	0.41
1:D:105:PRO:O	1:D:105:PRO:HG2	2.21	0.41
1:G:93:LEU:HD13	1:G:100:ARG:CD	2.50	0.41
1:D:160:PRO:HB3	1:D:191:PHE:HA	2.03	0.40
1:D:130:GLN:NE2	1:D:133:ARG:HD2	2.36	0.40
1:D:4:GLY:N	1:D:5:PRO:CD	2.84	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	259/295 (88%)	247 (95%)	11 (4%)	1 (0%)	34 46
1	D	255/295 (86%)	242 (95%)	13 (5%)	0	100 100
1	G	214/295 (72%)	203 (95%)	10 (5%)	1 (0%)	29 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	728/885 (82%)	692 (95%)	34 (5%)	2 (0%)	41 51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	G	106	PRO

### 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	219/247 (89%)	212 (97%)	7 (3%)	39 53
1	D	213/247 (86%)	204 (96%)	9 (4%)	30 40
1	G	132/247 (53%)	126 (96%)	6 (4%)	27 37
All	All	564/741 (76%)	542 (96%)	22 (4%)	32 44

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	69	GLN
1	A	95	ARG
1	A	100	ARG
1	A	155	LYS
1	A	177	TYR
1	A	202	GLN
1	D	32	VAL
1	D	69	GLN
1	D	95	ARG
1	D	100	ARG
1	D	103	THR
1	D	109	ARG
1	D	155	LYS

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Mol	Chain	Res	Type
1	D	177	TYR
1	D	257	ARG
1	G	78	ARG
1	G	99	LEU
1	G	100	ARG
1	G	143	GLN
1	G	238	GLN
1	G	265	MET

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	69	GLN
1	A	130	GLN
1	A	139	GLN
1	A	238	GLN
1	D	130	GLN
1	D	142	GLN
1	D	238	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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	OHU	E	7	2	16,21,22	1.32	1 (6%)	23,30,33	1.75	4 (17%)
2	OHU	H	7	2	16,21,22	1.32	1 (6%)	23,30,33	1.64	2 (8%)
2	OHU	B	7	2	16,21,22	1.23	2 (12%)	23,30,33	1.89	7 (30%)

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	OHU	E	7	2	-	2/7/21/22	0/2/2/2
2	OHU	H	7	2	-	2/7/21/22	0/2/2/2
2	OHU	B	7	2	-	2/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	7	OHU	C2-N1	3.21	1.43	1.38
2	H	7	OHU	C2-N1	2.93	1.43	1.38
2	B	7	OHU	C2-N1	2.58	1.42	1.38
2	B	7	OHU	O2-C2	2.11	1.26	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	7	OHU	C4-N3-C2	-4.90	121.01	127.35
2	H	7	OHU	C4-N3-C2	-4.54	121.47	127.35
2	B	7	OHU	C4-N3-C2	-4.50	121.53	127.35
2	E	7	OHU	N3-C2-N1	4.46	120.81	114.89
2	H	7	OHU	N3-C2-N1	3.99	120.19	114.89
2	B	7	OHU	N3-C2-N1	3.84	119.98	114.89
2	B	7	OHU	O4'-C1'-N1	-3.19	102.15	107.86
2	B	7	OHU	O2-C2-N1	-2.44	119.54	122.79
2	B	7	OHU	C1'-N1-C2	2.25	122.08	117.64
2	E	7	OHU	O2-C2-N1	-2.20	119.86	122.79
2	E	7	OHU	O4-C4-C5	-2.17	119.16	123.55
2	B	7	OHU	O4-C4-C5	-2.16	119.18	123.55
2	B	7	OHU	O5-C5-C6	-2.12	118.15	121.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	7	OHU	O4'-C4'-C5'-O5'
2	B	7	OHU	O4'-C4'-C5'-O5'
2	H	7	OHU	C3'-C4'-C5'-O5'
2	B	7	OHU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	E	7	OHU	O4'-C4'-C5'-O5'
2	E	7	OHU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	7	OHU	1	0
2	H	7	OHU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	265/295 (89%)	0.18	6 (2%) 60 67	36, 60, 99, 132	0
1	D	261/295 (88%)	0.34	5 (1%) 66 73	39, 72, 126, 140	0
1	G	228/295 (77%)	0.97	33 (14%) 2 3	78, 112, 146, 157	0
2	B	12/13 (92%)	0.59	1 (8%) 11 13	59, 95, 133, 140	0
2	E	12/13 (92%)	0.46	1 (8%) 11 13	66, 92, 109, 127	0
2	H	12/13 (92%)	1.07	3 (25%) 0 0	95, 113, 126, 132	0
3	C	13/13 (100%)	0.15	1 (7%) 13 17	70, 96, 130, 149	0
3	F	13/13 (100%)	0.35	0 100 100	58, 94, 127, 143	0
3	I	13/13 (100%)	0.88	0 100 100	75, 117, 135, 138	0
All	All	829/963 (86%)	0.48	50 (6%) 21 25	36, 83, 135, 157	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	125	LEU	6.6
1	G	287	PRO	5.5
1	G	280	TRP	5.3
1	G	102	TYR	4.7
1	G	13	PHE	4.6
1	G	72	PRO	4.4
1	G	156	ALA	4.3
1	G	194	ALA	4.3
1	G	281	PHE	4.3
1	A	2	GLY	4.2
1	G	100	ARG	3.9
1	G	264	GLY	3.8
1	G	132	GLY	3.8
1	G	74	ALA	3.6
2	E	1	DC	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	73	LEU	3.3
1	G	105	PRO	3.3
2	H	13	DC	3.2
1	G	92	GLU	3.2
1	G	106	PRO	3.1
1	D	241	GLY	3.1
1	A	251	GLU	3.0
2	B	13	DC	3.0
1	G	124	ASP	2.9
1	G	129	TRP	2.9
1	G	18	CYS	2.8
1	A	3	GLN	2.7
1	G	91	GLU	2.7
1	G	58	LEU	2.6
2	H	12	DA	2.5
1	D	184	TYR	2.3
1	G	2	GLY	2.3
1	G	239	LEU	2.3
1	G	3	GLN	2.3
2	H	2	DG	2.2
1	G	101	PHE	2.2
1	G	14	VAL	2.2
1	A	249	GLY	2.2
1	G	263	TYR	2.2
1	A	175	GLY	2.2
1	A	7	LEU	2.2
1	D	179	ARG	2.1
1	D	175	GLY	2.1
1	G	48	SER	2.1
1	G	141	TYR	2.1
3	C	1	DT	2.1
1	G	254	ALA	2.1
1	D	281	PHE	2.1
1	G	285	PRO	2.0
1	G	39	PRO	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( $\text{\AA}^2$ )	Q<0.9
2	OHU	H	7	20/21	0.92	0.18	96,112,127,130	0
2	OHU	E	7	20/21	0.94	0.14	73,84,105,108	0
2	OHU	B	7	20/21	0.97	0.25	59,72,104,107	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.