



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:45 AM UTC

PDB ID : 6LWL / pdb_00006lwl
Title : Crystal structure of human NEIL1(R242) bound to duplex DNA containing 2'-fluoro-2'-deoxy-5,6-dihydrouridine
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

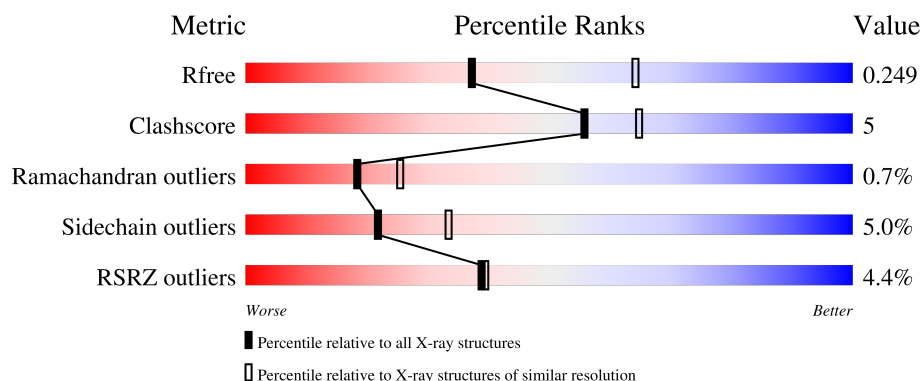
1 Overall quality at a glance

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 ≥ 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	% 79% 11% • 8%
1	D	295	3% 79% 9% • 10%
1	G	295	8% 69% 9% • 21%
2	B	13	85% 8% 8%
2	E	13	77% 8% 15%

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Mol	Chain	Length	Quality of chain
2	H	13	 85% 8% 8%
3	C	13	 92% 8%
3	F	13	 46% 38% 15%
3	I	13	 54% 31% 15%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7719 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
1	A	270	Total	C	N	O	S	0	0	0
			2142	1365	390	377	10			
1	D	266	Total	C	N	O	S	0	0	0
			2107	1346	385	366	10			
1	G	233	Total	C	N	O	S	0	0	0
			1667	1033	318	308	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	variant	UNP Q96FI4
D	242	ARG	LYS	variant	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*(FDU)P*GP*TP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	F	N	O	P	0	0
			258	124	1	43	78	12		
2	E	13	Total	C	F	N	O	P	0	0
			258	124	1	43	78	12		
2	H	13	Total	C	F	N	O	P	0	0
			258	124	1	43	78	12		

- 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
3	C	13	Total	C	N	O	P	0	0	0
			267	127	53	75	12			

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	114	Total	O	0	0
			114	114		
5	B	14	Total	O	0	0
			14	14		
5	C	7	Total	O	0	0
			7	7		
5	D	69	Total	O	0	0
			69	69		
5	E	9	Total	O	0	0
			9	9		
5	F	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		
5	I	2	Total	O	0	0
			2	2		

- Molecule 1: Endonuclease 8-like 1



Chain B: 



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

Chain E: 



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

Chain H: 



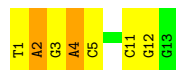
- Molecule 3: DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*G)-3')

Chain C: 



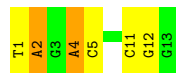
- Molecule 3: DNA (5'-D(*TP*AP*GP*AP*CP*CP*TP*GP*GP*AP*CP*GP*G)-3')

Chain F: 



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

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.77Å 108.65Å 170.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.08 – 2.55 36.08 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.08-2.55) 99.8 (36.08-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.253 0.211 , 0.249	Depositor DCC
R_{free} test set	2310 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7719	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, EW3

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	1.13	4/2201 (0.2%)	1.33	5/2977 (0.2%)
1	D	1.11	2/2165 (0.1%)	1.32	1/2927 (0.0%)
1	G	1.05	0/1701	1.33	0/2277
2	B	0.45	0/264	0.81	0/402
2	E	0.48	0/264	1.01	1/402 (0.2%)
2	H	0.38	0/264	0.75	0/402
3	C	0.54	0/300	0.94	1/462 (0.2%)
3	F	0.51	0/300	0.97	3/462 (0.6%)
3	I	0.40	0/300	0.91	2/462 (0.4%)
All	All	1.00	6/7759 (0.1%)	1.24	13/10773 (0.1%)

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	D	0	2
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	GLU	CD-OE1	11.51	1.47	1.25
1	D	92	GLU	CD-OE2	11.22	1.46	1.25
1	D	92	GLU	CD-OE1	10.81	1.45	1.25
1	A	92	GLU	CD-OE2	9.90	1.44	1.25
1	A	230	HIS	CE1-NE2	6.41	1.39	1.32

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DG	O5'-P-OP1	-8.58	83.26	109.00
3	F	4	DA	C4'-C3'-O3'	7.96	121.94	110.00
1	A	67	GLN	CB-CA-C	7.87	120.97	109.48
3	I	4	DA	C4'-C3'-O3'	6.90	120.35	110.00
3	F	2	DA	C2'-C3'-O3'	-5.88	102.68	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	PRO	Peptide
1	A	67	GLN	Peptide,Mainchain
1	D	105	PRO	Peptide
1	D	67	GLN	Peptide

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	2142	0	2110	24	0
1	D	2107	0	2078	18	0
1	G	1667	0	1478	18	0
2	B	258	0	137	8	0
2	E	258	0	137	3	0
2	H	258	0	137	2	0
3	C	267	0	147	0	0
3	F	267	0	147	3	0
3	I	267	0	147	3	0
4	D	6	0	8	1	0
5	A	114	0	0	3	0
5	B	14	0	0	0	0
5	C	7	0	0	0	0
5	D	69	0	0	1	0
5	E	9	0	0	0	0
5	F	5	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7719	0	6526	66	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 5.

The worst 5 of 66 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:A:81:MET:HE3	2:B:8:DG:C8	2.01	0.93
1:G:76:VAL:HG23	1:G:127:GLY:HA2	1.60	0.83
1:A:242:ARG:HG3	1:A:247:GLU:O	1.87	0.74
1:G:2:PRO:N	2:H:7:EW3:F2	2.11	0.74
1:A:143:GLN:OE1	5:A:301:HOH:O	2.07	0.71

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	266/295 (90%)	253 (95%)	9 (3%)	4 (2%)	8	10
1	D	260/295 (88%)	248 (95%)	11 (4%)	1 (0%)	30	39
1	G	217/295 (74%)	207 (95%)	10 (5%)	0	100	100
All	All	743/885 (84%)	708 (95%)	30 (4%)	5 (1%)	18	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	106	PRO
1	A	68	PRO
1	A	244	TYR

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Mol	Chain	Res	Type
1	A	248	SER
1	A	106	PRO

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	224/248 (90%)	215 (96%)	9 (4%)	28	42
1	D	219/248 (88%)	211 (96%)	8 (4%)	30	45
1	G	153/248 (62%)	140 (92%)	13 (8%)	10	13
All	All	596/744 (80%)	566 (95%)	30 (5%)	22	33

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	197	VAL
1	G	252	ASP
1	G	34	ARG
1	G	274	ARG
1	G	177	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	GLN
1	D	151	ASN
1	G	238	GLN
1	D	238	GLN
1	G	151	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	EW3	B	7	2	18,21,22	1.68	3 (16%)	20,30,33	2.33	7 (35%)
2	EW3	H	7	2	18,21,22	1.13	2 (11%)	20,30,33	2.42	7 (35%)
2	EW3	E	7	2	18,21,22	1.12	1 (5%)	20,30,33	2.32	7 (35%)

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	EW3	B	7	2	-	0/7/38/39	0/2/2/2
2	EW3	H	7	2	-	0/7/38/39	0/2/2/2
2	EW3	E	7	2	-	0/7/38/39	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	EW3	F2-C2'	-5.06	1.30	1.40
2	B	7	EW3	O4'-C1'	2.93	1.48	1.42
2	E	7	EW3	F2-C2'	-2.81	1.34	1.40
2	H	7	EW3	F2-C2'	-2.64	1.35	1.40
2	H	7	EW3	C2-N3	-2.15	1.34	1.38

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	EW3	O4'-C1'-N1	6.38	117.99	109.30
2	E	7	EW3	O4'-C1'-N1	5.55	116.86	109.30
2	B	7	EW3	O4'-C1'-N1	5.50	116.79	109.30
2	H	7	EW3	C5-C4-N3	4.67	121.65	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	7	EW3	C5-C4-N3	4.62	121.60	116.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7	EW3	1	0
2	H	7	EW3	1	0
2	E	7	EW3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
4	GOL	D	301	-	5,5,5	0.20	0	5,5,5	0.45	0

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
4	GOL	D	301	-	-	0/4/4/4	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	GOL	1	0

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, 95th 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 ²)	Q<0.9
1	A	270/295 (91%)	-0.08	4 (1%) 72 73	38, 60, 99, 114	0
1	D	266/295 (90%)	0.22	8 (3%) 52 54	41, 76, 123, 149	0
1	G	233/295 (78%)	1.02	25 (10%) 11 10	78, 118, 143, 155	0
2	B	12/13 (92%)	0.17	0 100 100	61, 93, 142, 167	0
2	E	12/13 (92%)	-0.25	0 100 100	53, 85, 111, 130	0
2	H	12/13 (92%)	0.38	0 100 100	100, 117, 136, 152	0
3	C	13/13 (100%)	-0.05	0 100 100	74, 93, 130, 143	0
3	F	13/13 (100%)	-0.01	0 100 100	56, 82, 125, 138	0
3	I	13/13 (100%)	0.39	0 100 100	95, 124, 143, 145	0
All	All	844/963 (87%)	0.33	37 (4%) 39 39	38, 85, 135, 167	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	157	PHE	3.5
1	G	164	ALA	3.4
1	D	244	TYR	3.3
1	G	170	PHE	3.3
1	G	77	PHE	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	EW3	H	7	20/21	0.82	0.11	99,111,129,132	0
2	EW3	E	7	20/21	0.95	0.11	66,74,114,122	0
2	EW3	B	7	20/21	0.96	0.09	58,67,87,96	0

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, 95th 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
4	GOL	D	301	6/6	0.83	0.24	77,86,93,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.