



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:12 PM BST

PDB ID : 2WY3  
Title : Structure of the HCMV UL16-MICB complex elucidates select binding of a viral immunoevasin to diverse NKG2D ligands  
Authors : Mueller, S.; Zocher, G.; Steinle, A.; Stehle, T.  
Deposited on : 2009-11-11  
Resolution : 1.80 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
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) : 2.13.1

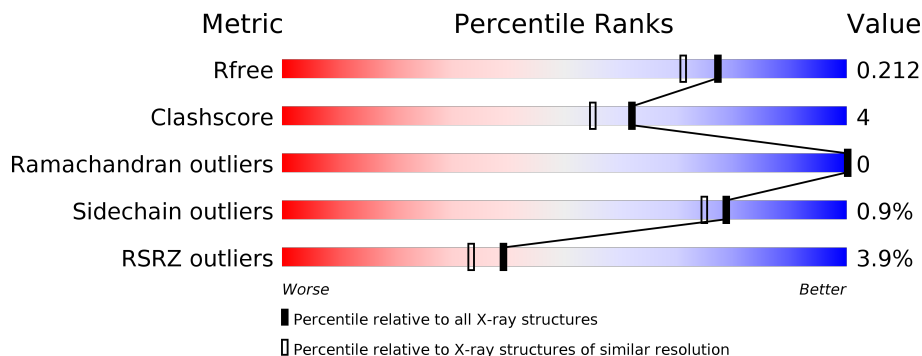
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	319	 3% 50% 6% 41%
1	C	319	 4% 46% 6% 44%
2	B	158	 3% 80% 6% 11%
2	D	158	 78% 6% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	C	1177	-	-	X	-
5	NAG	B	1202[A]	X	-	-	-
5	NAG	D	1202[B]	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5980 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 MHC CLASS I POLYPEPTIDE-RELATED SEQUENCE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1453	897	266	285	5	0	8	0
1	C	167	1382	852	258	267	5	0	3	0

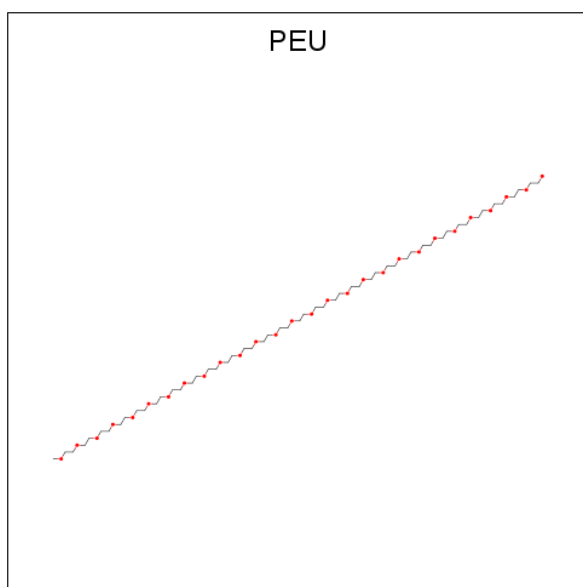
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLU	LYS	conflict	UNP Q29980
A	113	ASN	ASP	conflict	UNP Q29980
C	57	GLU	LYS	conflict	UNP Q29980
C	113	ASN	ASP	conflict	UNP Q29980

- Molecule 2 is a protein called UNCHARACTERIZED PROTEIN UL16.

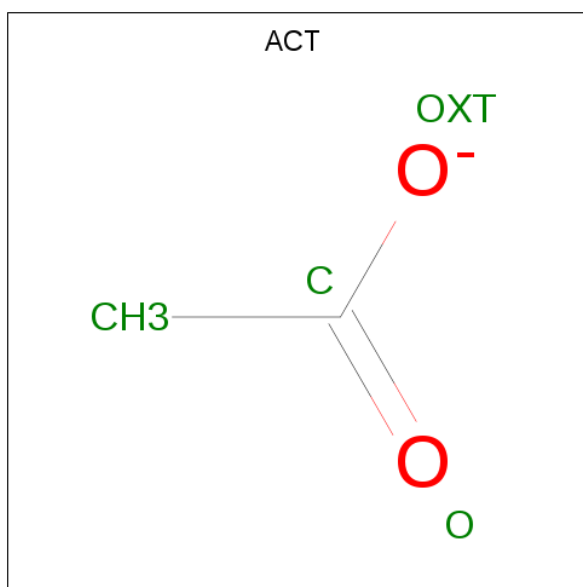
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	137	1135	711	192	221	11	0	6	0
2	D	133	1114	693	191	217	13	0	8	0

- Molecule 3 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-HEPTACOSAOXADOCTACONTAN-82-OL (three-letter code: PEU) (formula: C<sub>55</sub>H<sub>112</sub>O<sub>28</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			17	11	6		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



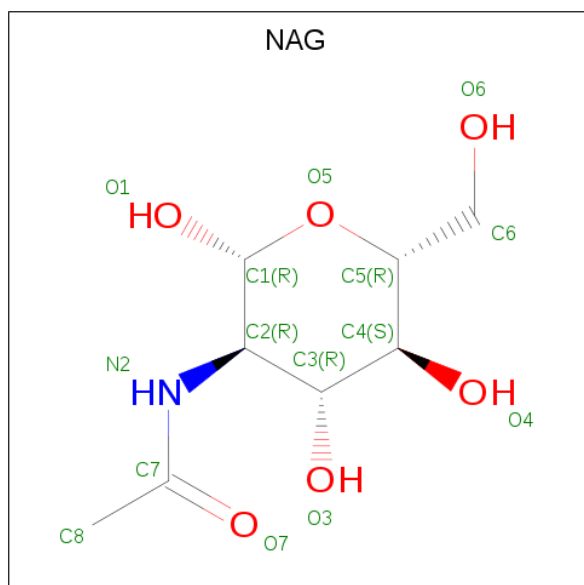
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	1
			28	16	2	10		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	1
			28	16	2	10		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	170	Total	O	0	0
			170	170		
6	B	173	Total	O	0	0
			173	173		
6	C	119	Total	O	0	0
			119	119		
6	D	177	Total	O	0	0
			177	177		





Chain D:  78% 6% 16%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.12Å 104.17Å 146.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 1.80 49.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.09-1.80) 98.7 (49.09-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 1.79Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.177 , 0.213 0.176 , 0.212	Depositor DCC
$R_{free}$ test set	4114 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: PEU, NAG, ACT

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	0.31	0/1494	0.47	0/2012
1	C	0.29	0/1408	0.45	0/1897
2	B	0.37	0/1161	0.60	0/1582
2	D	0.38	0/1132	0.62	0/1539
All	All	0.34	0/5195	0.53	0/7030

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 [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	1453	0	1401	11	0
1	C	1382	0	1314	15	0
2	B	1135	0	1106	9	0
2	D	1114	0	1073	11	0
3	A	19	0	24	0	0
3	C	17	0	23	0	0
3	D	13	0	16	4	0
4	A	4	0	3	1	0
4	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	3	2	0
5	B	98	0	91	0	0
5	D	98	0	91	2	0
6	A	170	0	0	2	0
6	B	173	0	0	2	0
6	C	119	0	0	1	0
6	D	177	0	0	2	0
All	All	5980	0	5148	46	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 (46) 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)
2:D:29:LEU:HB2	2:D:143[B]:CYS:SG	2.09	0.92
1:C:23:LEU:HD23	1:C:38:ARG:HD2	1.63	0.79
2:D:53[B]:THR:HG22	2:D:153:ARG:HB3	1.70	0.71
2:B:29:LEU:HB2	2:B:143[B]:CYS:SG	2.34	0.67
1:A:108:ARG:HH21	1:A:157:TYR:HE1	1.44	0.66
1:C:156[B]:HIS:CE1	2:D:114:LEU:HD11	2.34	0.61
2:D:100:ARG:NH1	3:D:1160:PEU:HAF2	2.18	0.59
2:B:120:PRO:HD2	6:B:2007:HOH:O	2.03	0.59
2:B:144:GLU:O	2:B:147:THR:HG22	2.04	0.58
1:A:61[B]:THR:HG23	6:A:2073:HOH:O	2.03	0.57
1:C:154:LYS:NZ	4:C:1177:ACT:H2	2.22	0.55
1:C:1:GLU:N	1:C:2:PRO:HD2	2.23	0.54
2:D:29:LEU:CB	2:D:143[B]:CYS:SG	2.92	0.53
1:C:146:TRP:O	1:C:147:LYS:HB2	2.10	0.53
1:A:6:ARG:HG3	1:A:95[B]:VAL:HG22	1.91	0.52
1:C:154:LYS:HE2	6:D:2114:HOH:O	2.10	0.51
2:B:114:LEU:HD12	2:B:114:LEU:O	2.11	0.51
1:A:35:ARG:HD3	1:A:46:GLN:OE1	2.12	0.49
1:C:101:ASP:O	1:C:102:SER:HB2	2.12	0.49
2:D:50:PRO:HG2	2:D:53[B]:THR:CG2	2.42	0.49
1:C:132:SER:O	1:C:136:GLN:HG2	2.13	0.48
4:C:1177:ACT:H1	6:D:2113:HOH:O	2.14	0.48
2:D:103[B]:SER:HB2	3:D:1160:PEU:HAJ1	1.95	0.48
1:C:108:ARG:HD3	1:C:160:MET:HE1	1.95	0.48
1:C:134:ARG:HG3	6:C:2102:HOH:O	2.14	0.47
1:C:69:ASN:HD22	1:C:69:ASN:C	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH1	4:A:1177:ACT:H3	2.29	0.47
2:B:114:LEU:HD12	2:B:114:LEU:C	2.36	0.46
1:A:108:ARG:NH2	1:A:157:TYR:HE1	2.10	0.46
2:D:103[A]:SER:OG	3:D:1160:PEU:HAL1	2.16	0.46
1:C:34:LEU:HD23	1:C:34:LEU:C	2.36	0.46
1:A:69:ASN:C	1:A:69:ASN:HD22	2.20	0.45
1:C:153:THR:O	1:C:157:TYR:HD2	2.00	0.45
2:D:70:THR:CG2	5:D:1202[B]:NAG:H62	2.47	0.45
1:C:160:MET:HB3	1:C:160:MET:HE3	1.71	0.44
2:B:29:LEU:CD2	2:B:40:LEU:HB2	2.47	0.44
2:D:103[A]:SER:HB3	3:D:1160:PEU:HAJ1	1.98	0.44
2:B:29:LEU:CB	2:B:143[B]:CYS:SG	3.05	0.43
2:D:70:THR:HG21	5:D:1202[B]:NAG:H62	2.00	0.43
1:C:23:LEU:CD2	1:C:38:ARG:HD2	2.41	0.42
2:B:28:ASP:C	2:B:29:LEU:HD22	2.40	0.42
1:A:101:ASP:O	1:A:102:SER:HB2	2.19	0.41
1:A:136[B]:GLN:NE2	6:A:2146:HOH:O	2.54	0.40
2:B:38[B]:CYS:HB2	6:B:2148:HOH:O	2.21	0.40
1:A:124:THR:O	1:A:125[A]:GLN:HB2	2.21	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	177/319 (56%)	175 (99%)	2 (1%)	0	100	100
1	C	164/319 (51%)	158 (96%)	6 (4%)	0	100	100
2	B	142/158 (90%)	138 (97%)	4 (3%)	0	100	100
2	D	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
All	All	622/954 (65%)	608 (98%)	14 (2%)	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	160/282 (57%)	158 (99%)	2 (1%)	69	62
1	C	149/282 (53%)	148 (99%)	1 (1%)	84	81
2	B	134/143 (94%)	133 (99%)	1 (1%)	84	81
2	D	131/143 (92%)	130 (99%)	1 (1%)	81	78
All	All	574/850 (68%)	569 (99%)	5 (1%)	78	75

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	141	ASN
2	B	111	GLN
1	C	69	ASN
2	D	111	GLN

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

Mol	Chain	Res	Type
1	A	69	ASN
1	C	69	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 ligands 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
5	NAG	D	1201	2	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
5	NAG	B	1201	2	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
5	NAG	B	1202[A]	2	14,14,15	0.47	0	17,19,21	1.62	2 (11%)
5	NAG	D	1202[B]	2	14,14,15	0.48	0	17,19,21	1.68	3 (17%)
3	PEU	D	1160	-	12,12,82	0.54	0	11,11,81	0.88	0
5	NAG	B	1206	2	14,14,15	0.56	0	17,19,21	0.79	0
5	NAG	D	1202[A]	2	14,14,15	0.55	0	17,19,21	0.75	0
3	PEU	A	1176	-	18,18,82	0.57	0	17,17,81	0.72	0
5	NAG	B	1205	2	14,14,15	0.58	0	17,19,21	0.97	1 (5%)
5	NAG	D	1206	2	14,14,15	0.56	0	17,19,21	1.18	2 (11%)
3	PEU	C	1176	-	16,16,82	0.55	0	15,15,81	0.72	0
5	NAG	B	1204	2	14,14,15	0.48	0	17,19,21	1.05	1 (5%)
5	NAG	B	1203	2	14,14,15	0.58	0	17,19,21	0.64	0
4	ACT	C	1177	-	1,3,3	1.33	0	0,3,3	0.00	-
4	ACT	B	1164	-	1,3,3	1.29	0	0,3,3	0.00	-
4	ACT	A	1177	-	1,3,3	1.34	0	0,3,3	0.00	-
5	NAG	D	1204	2	14,14,15	0.45	0	17,19,21	0.98	2 (11%)
5	NAG	D	1203	2	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
5	NAG	B	1202[B]	2	14,14,15	0.53	0	17,19,21	0.70	0
5	NAG	D	1205	2	14,14,15	0.65	0	17,19,21	1.00	1 (5%)

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
5	NAG	D	1201	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1201	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1202[B]	2	1/1/5/7	0/6/23/26	0/1/1/1
3	PEU	D	1160	-	-	6/10/10/80	-
5	NAG	B	1206	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1202[A]	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1205	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1206	2	-	0/6/23/26	0/1/1/1
3	PEU	C	1176	-	-	1/14/14/80	-
5	NAG	B	1203	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1202[B]	2	-	2/6/23/26	0/1/1/1
5	NAG	D	1205	2	-	0/6/23/26	0/1/1/1
5	NAG	B	1204	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1204	2	-	0/6/23/26	0/1/1/1
5	NAG	D	1203	2	-	0/6/23/26	0/1/1/1
3	PEU	A	1176	-	-	2/16/16/80	-
5	NAG	B	1202[A]	2	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1202[B]	NAG	C1-O5-C5	4.67	118.52	112.19
5	B	1202[A]	NAG	C1-O5-C5	4.15	117.82	112.19
5	D	1202[B]	NAG	O5-C1-C2	3.55	116.89	111.29
5	D	1206	NAG	C1-O5-C5	3.48	116.91	112.19
5	B	1202[A]	NAG	O5-C1-C2	3.45	116.73	111.29
5	B	1201	NAG	C1-O5-C5	3.17	116.49	112.19
5	B	1204	NAG	C1-O5-C5	3.00	116.26	112.19
5	B	1205	NAG	C1-O5-C5	2.90	116.12	112.19
5	D	1205	NAG	C1-O5-C5	2.63	115.75	112.19
5	D	1206	NAG	C2-N2-C7	-2.53	119.29	122.90
5	D	1201	NAG	C1-O5-C5	2.29	115.29	112.19
5	D	1203	NAG	O5-C5-C6	2.21	110.67	107.20
5	D	1204	NAG	C1-O5-C5	2.18	115.14	112.19
5	D	1204	NAG	O5-C1-C2	-2.13	107.92	111.29
5	D	1202[B]	NAG	C2-N2-C7	-2.08	119.95	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1202[A]	NAG	C1

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Mol	Chain	Res	Type	Atom
5	D	1202[B]	NAG	C1

All (11) torsion outliers are listed below:

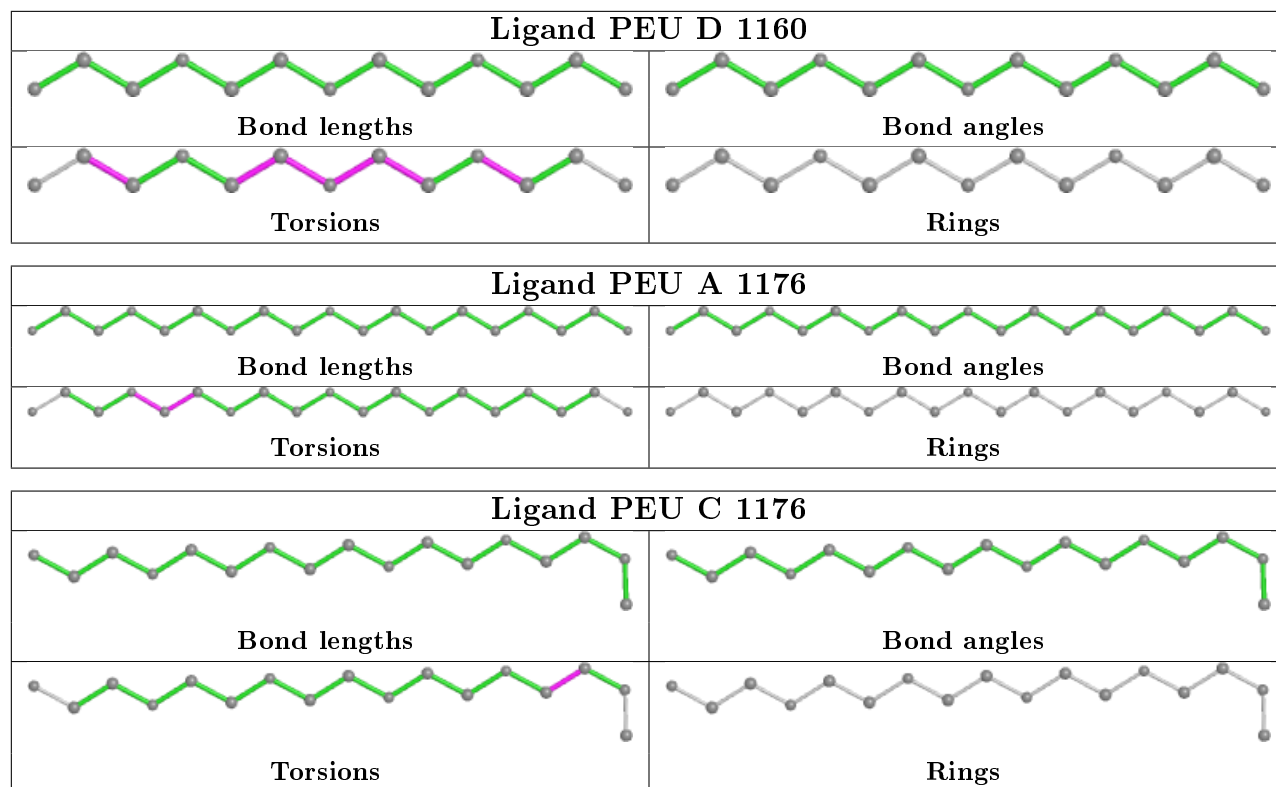
Mol	Chain	Res	Type	Atoms
3	C	1176	PEU	OAB-CAC-CAD-OAE
3	D	1160	PEU	OAH-CAI-CAJ-OAK
3	D	1160	PEU	OAK-CAL-CAM-OAN
3	A	1176	PEU	OAN-CAO-CAP-OAQ
3	D	1160	PEU	CAJ-CAI-OAH-CAG
3	D	1160	PEU	CAF-CAG-OAH-CAI
5	B	1202[B]	NAG	C8-C7-N2-C2
3	D	1160	PEU	CAC-CAD-OAE-CAF
3	A	1176	PEU	CAO-CAP-OAQ-CAR
5	B	1202[B]	NAG	O7-C7-N2-C2
3	D	1160	PEU	OAE-CAF-CAG-OAH

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1202[B]	NAG	2	0
3	D	1160	PEU	4	0
4	C	1177	ACT	2	0
4	A	1177	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	173/319 (54%)	0.06	8 (4%) 32 26	18, 28, 64, 117	0
1	C	167/319 (52%)	0.28	12 (7%) 15 12	17, 36, 82, 105	0
2	B	137/158 (86%)	-0.15	4 (2%) 51 46	13, 22, 47, 83	0
2	D	133/158 (84%)	0.01	0 100 100	13, 20, 48, 69	0
All	All	610/954 (63%)	0.06	24 (3%) 39 33	13, 27, 68, 117	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	PHE	6.6
1	C	145	PHE	4.3
1	A	0	MET	4.0
1	C	150	ALA	3.7
1	A	148	GLU	3.7
1	C	146	TRP	2.9
1	C	151	MET	2.8
1	C	79	HIS	2.8
1	C	1	GLU	2.7
1	C	131	GLN	2.7
2	B	27	VAL	2.5
1	C	101	ASP	2.4
1	A	1	GLU	2.4
1	A	147	LYS	2.3
1	C	2	PRO	2.2
1	A	141	ASN	2.2
1	C	99	HIS	2.2
2	B	160	SER	2.2
1	C	144	ASN	2.2
2	B	161	LEU	2.1
2	B	162	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	LYS	2.1
1	C	136	GLN	2.1
1	A	146	TRP	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](#)

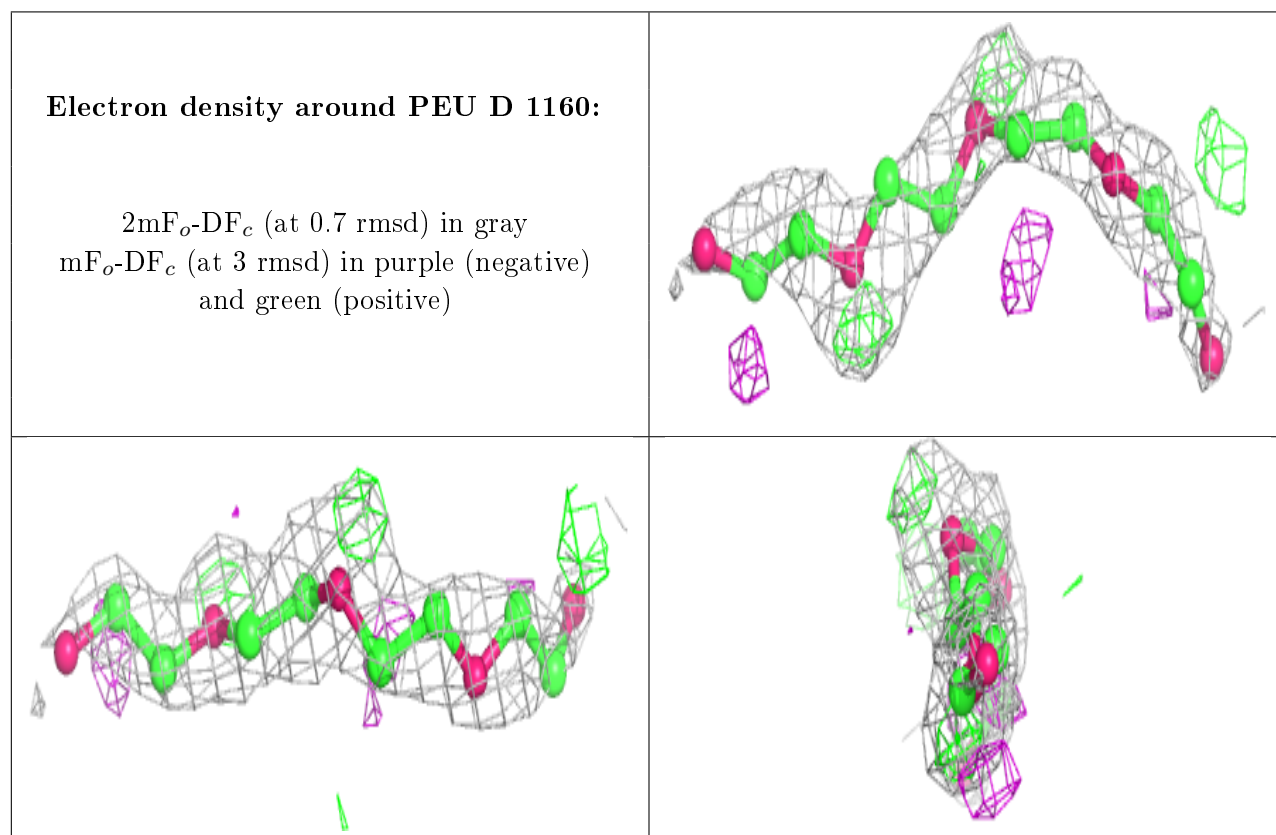
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

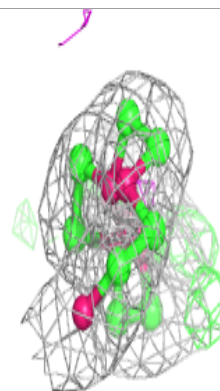
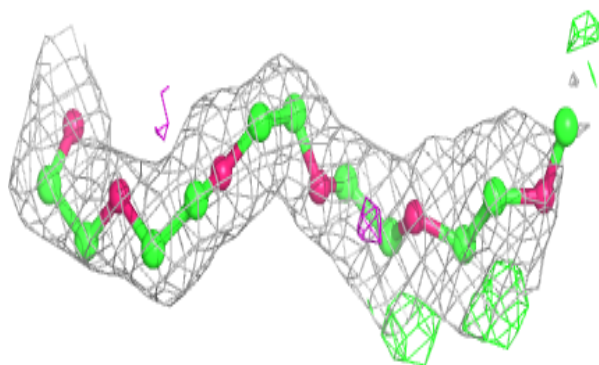
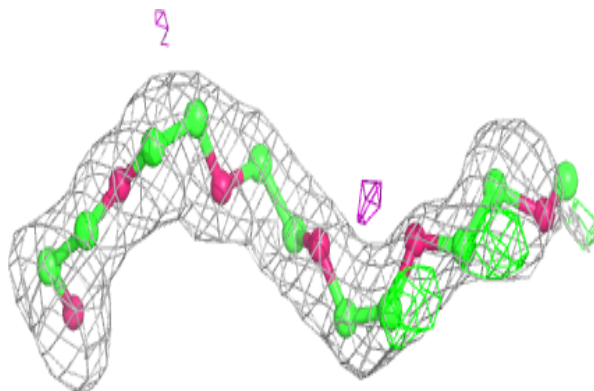
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEU	D	1160	13/83	0.60	0.26	60,70,83,83	0
5	NAG	B	1202[A]	14/15	0.68	0.25	27,37,40,41	14
5	NAG	B	1202[B]	14/15	0.68	0.25	44,50,60,67	14
5	NAG	D	1201	14/15	0.79	0.21	58,67,78,83	0
5	NAG	D	1202[A]	14/15	0.79	0.22	29,37,47,47	14
5	NAG	D	1202[B]	14/15	0.79	0.22	23,38,46,47	14
4	ACT	B	1164	4/4	0.80	0.15	66,69,71,73	0
3	PEU	C	1176	17/83	0.83	0.15	40,45,74,76	0
5	NAG	B	1204	14/15	0.84	0.27	45,61,74,79	0
4	ACT	A	1177	4/4	0.85	0.19	51,57,60,62	0
5	NAG	B	1201	14/15	0.89	0.19	40,57,64,67	0
5	NAG	B	1206	14/15	0.89	0.12	20,28,37,37	0
3	PEU	A	1176	19/83	0.90	0.11	28,39,68,69	0
5	NAG	B	1203	14/15	0.91	0.10	21,38,49,57	0
4	ACT	C	1177	4/4	0.91	0.22	65,67,67,68	0
5	NAG	D	1206	14/15	0.92	0.12	19,28,35,35	0
5	NAG	D	1204	14/15	0.93	0.10	21,33,36,39	0
5	NAG	B	1205	14/15	0.93	0.13	25,33,41,44	0
5	NAG	D	1203	14/15	0.95	0.11	27,40,48,48	0
5	NAG	D	1205	14/15	0.97	0.08	15,22,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

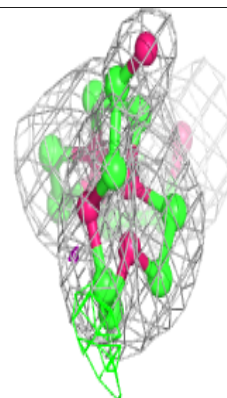
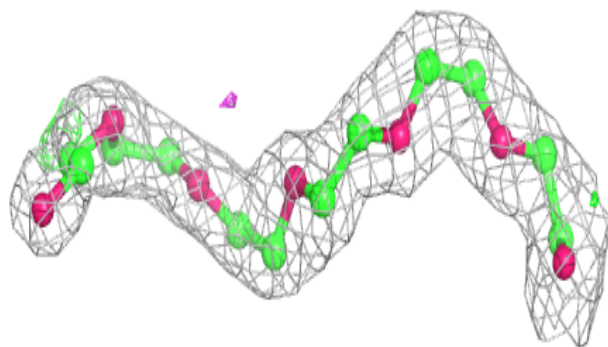
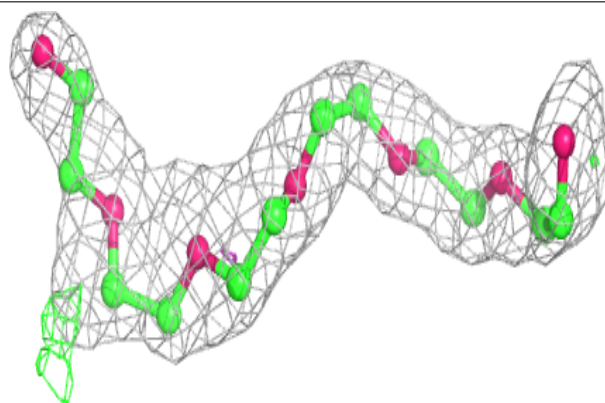


**Electron density around PEU C 1176:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PEU A 1176:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.