



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:36 pm BST

PDB ID : 5XJG  
Title : Crystal structure of Vac8p bound to Nvj1p  
Authors : Jeong, H.; Park, J.; Jun, Y.; Lee, C.  
Deposited on : 2017-05-01  
Resolution : 2.40 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  
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) : 2.11

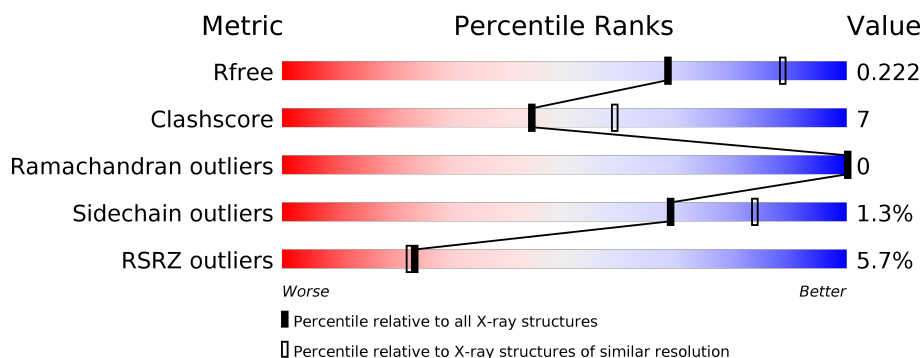
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	C	506	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> <div></div> </div>
2	B	93	<div> <div></div> <div> <div>29%</div> <div>68%</div> </div> <div></div> </div>
2	D	93	<div> <div></div> <div> <div>30%</div> <div>68%</div> </div> <div></div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8212 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.

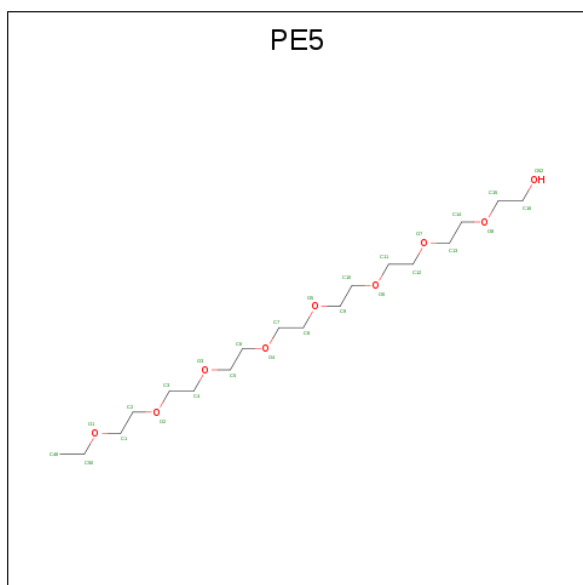
- Molecule 1 is a protein called Vacuolar protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3747	2354	648	729	16			
1	C	489	Total	C	N	O	S	0	0	0
			3747	2354	648	729	16			

- Molecule 2 is a protein called Nucleus-vacuole junction protein 1.

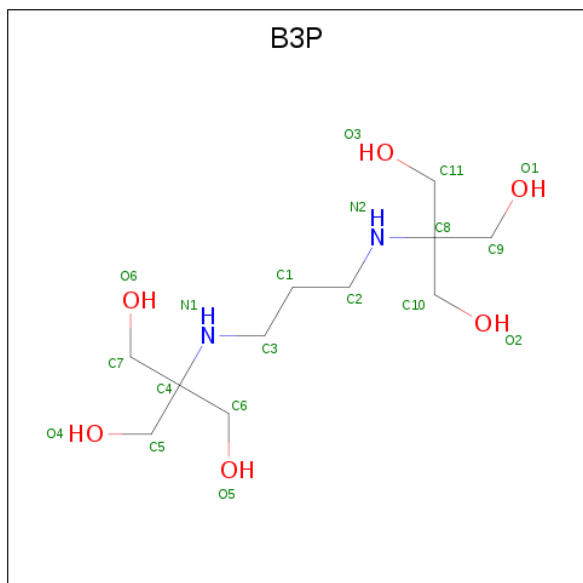
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	0	0	0
			242	152	42	48			
2	D	30	Total	C	N	O	0	0	0
			242	152	42	48			

- Molecule 3 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula:  $C_{18}H_{38}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	11	6		
3	C	1	Total	C	O	0	0
			17	11	6		

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	11	2	6		

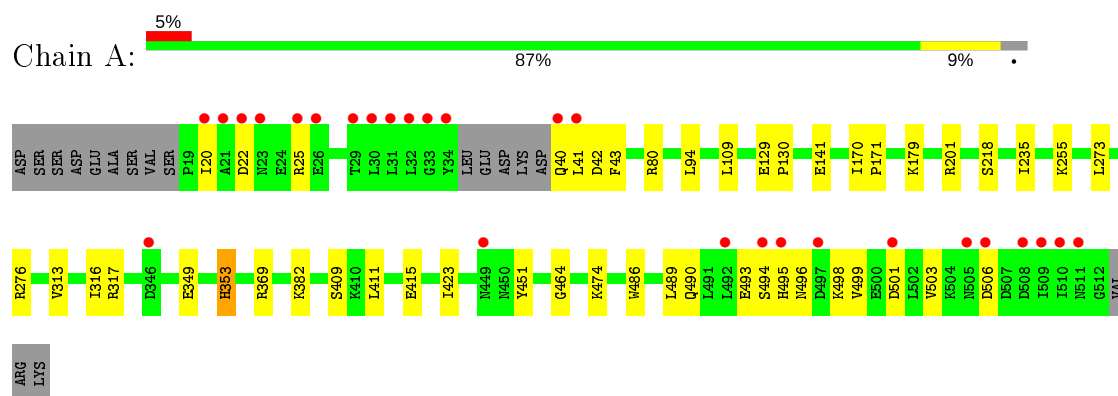
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	78	Total	O	0	0
			78	78		
5	B	7	Total	O	0	0
			7	7		
5	C	88	Total	O	0	0
			88	88		
5	D	8	Total	O	0	0
			8	8		

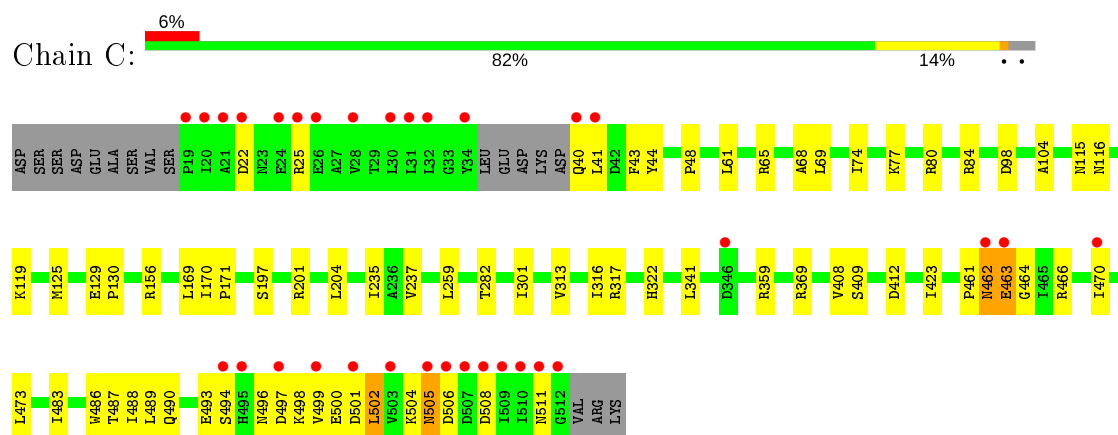
### 3 Residue-property plots [i](#)

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.

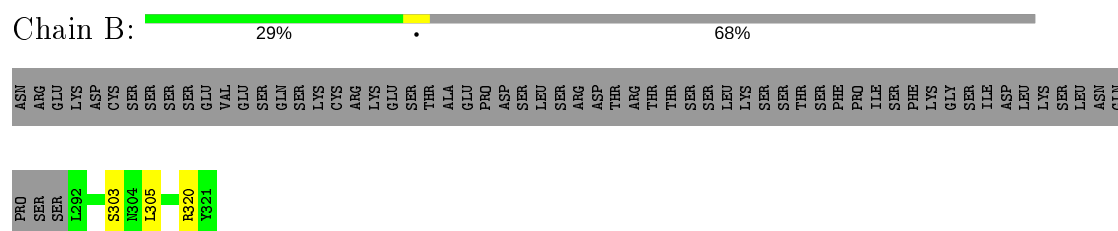
#### • Molecule 1: Vacuolar protein 8



#### • Molecule 1: Vacuolar protein 8



#### • Molecule 2: Nucleus-vacuole junction protein 1



#### • Molecule 2: Nucleus-vacuole junction protein 1

Chain D: 

30%

68%

ASN	ARG	GLU	LYS	ASP	CYS	SER	SER	SER	SER	GLU	VAL	GLU	SER	GLN	SER	LYS	CYS	ARG	LYS	GLU	SER	THR	ALA	GLU	PRO	ASP	SER	SER	LEU	SER	ARG	ASP	THR	ARG	THR	THR	SER	SER	LEU	LYS	SER	SER	THR	SER	PHE	PRO	ILE	SER	PHE	LYS	GLY	ILE	ASP	LEU	LYS	SER	LEU	ASN	GLN
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PRO	SER	SER	L292	S303	V309	Y321
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.08Å 115.63Å 84.13Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	29.59 – 2.40 31.88 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.59-2.40) 99.7 (31.88-2.39)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.190 , 0.222 0.192 , 0.222	Depositor DCC
$R_{free}$ test set	2032 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: PE5, B3P

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	0.25	0/3794	0.43	0/5149
1	C	0.26	0/3794	0.46	0/5149
2	B	0.24	0/247	0.42	0/336
2	D	0.24	0/247	0.40	0/336
All	All	0.26	0/8082	0.44	0/10970

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	3747	0	3832	49	0
1	C	3747	0	3832	72	0
2	B	242	0	233	4	0
2	D	242	0	233	2	0
3	A	17	0	20	0	0
3	C	17	0	20	1	0
4	A	19	0	26	1	0
5	A	78	0	0	2	0
5	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	88	0	0	3	0
5	D	8	0	0	0	0
All	All	8212	0	8196	107	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 7.

All (107) 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:41:LEU:CB	1:C:41:LEU:HD11	1.69	1.22
1:A:41:LEU:HB3	1:C:41:LEU:CD1	1.81	1.10
1:A:41:LEU:HB3	1:C:41:LEU:HD11	1.12	1.09
1:A:40:GLN:O	1:C:41:LEU:HD13	1.52	1.08
1:C:462:ASN:O	1:C:463:GLU:HG3	1.54	1.07
1:A:41:LEU:O	1:C:41:LEU:CD1	2.09	1.01
1:C:41:LEU:HG	1:C:41:LEU:O	1.58	0.99
1:C:462:ASN:C	1:C:463:GLU:HG3	1.83	0.98
1:A:41:LEU:O	1:C:41:LEU:HD12	1.62	0.97
1:A:41:LEU:CG	1:C:41:LEU:HD11	1.98	0.93
1:A:317:ARG:HD2	1:A:353:HIS:HB3	1.58	0.83
1:C:462:ASN:O	1:C:463:GLU:CG	2.30	0.78
1:C:489:LEU:HD23	1:C:493:GLU:HG3	1.65	0.76
1:C:501:ASP:O	1:C:504:LYS:HG2	1.87	0.73
1:C:423:ILE:HD13	1:C:464:GLY:HA2	1.69	0.73
1:A:41:LEU:HD11	1:C:74:ILE:HA	1.71	0.73
1:A:353:HIS:HD1	2:B:305:LEU:HD11	1.56	0.70
1:A:349:GLU:HG2	1:A:353:HIS:NE2	2.06	0.70
1:C:461:PRO:HB2	1:C:462:ASN:ND2	2.07	0.69
1:A:94:LEU:HD11	1:A:109:LEU:HD22	1.74	0.69
1:A:41:LEU:CB	1:C:41:LEU:CD1	2.52	0.68
1:C:462:ASN:C	1:C:463:GLU:CG	2.60	0.67
1:A:41:LEU:HB2	1:C:77:LYS:HB3	1.77	0.66
1:A:349:GLU:O	1:A:353:HIS:HD2	1.79	0.66
1:C:505:ASN:ND2	1:C:505:ASN:O	2.30	0.65
1:A:141:GLU:OE2	2:B:320:ARG:NH2	2.29	0.65
1:C:496:ASN:O	1:C:500:GLU:HG3	1.97	0.65
1:A:349:GLU:O	1:A:353:HIS:CD2	2.51	0.64
1:A:382:LYS:NZ	5:A:701:HOH:O	2.30	0.64
1:A:496:ASN:HB3	1:A:499:VAL:HG22	1.80	0.62
1:C:505:ASN:ND2	1:C:505:ASN:C	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:HIS:ND1	2:B:305:LEU:HD11	2.14	0.62
1:C:41:LEU:CG	1:C:41:LEU:O	2.40	0.62
1:C:505:ASN:HD22	1:C:505:ASN:C	2.04	0.61
1:A:42:ASP:OD2	1:A:80:ARG:NH1	2.32	0.61
1:A:41:LEU:HG	1:C:41:LEU:HD11	1.83	0.59
1:C:408:VAL:O	5:C:701:HOH:O	2.16	0.59
1:C:498:LYS:O	1:C:502:LEU:HD12	2.03	0.59
1:C:505:ASN:ND2	1:C:508:ASP:H	2.02	0.58
1:A:170:ILE:HB	1:A:171:PRO:HD3	1.87	0.56
1:C:84:ARG:HG3	1:C:125:MET:HE1	1.86	0.56
1:C:170:ILE:HB	1:C:171:PRO:HD3	1.88	0.56
1:A:41:LEU:HB2	1:C:77:LYS:CB	2.35	0.56
1:A:129:GLU:HB3	1:A:130:PRO:HD3	1.88	0.55
1:C:237:VAL:HG21	2:D:309:VAL:HG22	1.87	0.55
1:C:129:GLU:HB3	1:C:130:PRO:HD3	1.89	0.54
1:C:505:ASN:HD21	1:C:508:ASP:H	1.56	0.54
1:A:41:LEU:CD1	1:C:74:ILE:HA	2.38	0.53
1:A:498:LYS:HD2	1:A:501:ASP:HB2	1.91	0.52
1:A:41:LEU:C	1:C:41:LEU:CD1	2.78	0.52
1:A:218:SER:OG	1:A:255:LYS:NZ	2.39	0.52
1:A:22:ASP:HA	1:A:25:ARG:HB3	1.91	0.52
1:C:41:LEU:HD12	1:C:43:PHE:HE2	1.74	0.51
1:C:462:ASN:O	1:C:463:GLU:CB	2.58	0.50
1:C:501:ASP:HA	1:C:504:LYS:HD2	1.93	0.50
1:C:466:ARG:O	1:C:470:ILE:HG12	2.12	0.49
1:C:483:ILE:O	1:C:487:THR:HG22	2.13	0.49
1:C:412:ASP:OD2	5:C:701:HOH:O	2.20	0.48
1:A:317:ARG:NH1	2:B:303:SER:O	2.38	0.48
1:C:282:THR:HG23	1:C:322:HIS:CD2	2.49	0.48
1:C:473:LEU:HD22	1:C:511:ASN:ND2	2.30	0.47
1:A:451:TYR:OH	1:A:494:SER:CB	2.62	0.47
1:A:486:TRP:O	1:A:490:GLN:HG2	2.15	0.47
1:C:461:PRO:C	1:C:462:ASN:ND2	2.69	0.47
1:C:68:ALA:HB1	1:C:104:ALA:HB3	1.97	0.46
1:C:44:TYR:HB2	1:C:80:ARG:NH2	2.30	0.46
4:A:602:B3P:H31	4:A:602:B3P:H62	1.53	0.46
1:C:488:ILE:HD13	5:C:735:HOH:O	2.15	0.46
1:C:486:TRP:O	1:C:490:GLN:HG2	2.16	0.46
1:A:423:ILE:HD13	1:A:464:GLY:HA2	1.97	0.46
1:C:84:ARG:HA	1:C:125:MET:HE1	1.97	0.45
1:C:496:ASN:OD1	1:C:499:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:O	1:A:415:GLU:HG2	2.18	0.44
1:C:301:ILE:HG12	1:C:341:LEU:HD11	1.99	0.44
1:A:273:LEU:HD12	1:A:276:ARG:HD3	1.99	0.44
1:A:41:LEU:HB3	1:C:41:LEU:HD13	1.89	0.44
1:A:474:LYS:O	1:A:474:LYS:HG3	2.17	0.44
1:C:461:PRO:HB2	1:C:462:ASN:HD21	1.78	0.43
1:A:499:VAL:O	1:A:503:VAL:HG23	2.17	0.43
1:C:505:ASN:HD21	1:C:508:ASP:N	2.17	0.43
1:A:489:LEU:O	1:A:493:GLU:HB2	2.18	0.43
1:C:369:ARG:HD2	1:C:409:SER:OG	2.19	0.43
1:C:506:ASP:OD1	1:C:506:ASP:N	2.52	0.43
1:C:61:LEU:HD11	1:C:98:ASP:HB2	2.00	0.43
1:C:116:ASN:OD1	1:C:156:ARG:NH1	2.52	0.43
1:A:313:VAL:HA	1:A:316:ILE:HG22	2.01	0.42
1:A:317:ARG:HD2	1:A:353:HIS:CB	2.40	0.42
1:C:259:LEU:HA	1:C:259:LEU:HD23	1.87	0.42
1:A:369:ARG:HD2	1:A:409:SER:OG	2.19	0.42
1:C:22:ASP:HA	1:C:25:ARG:HB3	2.00	0.42
1:C:313:VAL:HA	1:C:316:ILE:HG22	2.01	0.42
1:A:179:LYS:HD2	1:A:179:LYS:HA	1.86	0.42
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.92	0.42
3:C:601:PE5:H102	3:C:601:PE5:H81	1.78	0.42
1:C:65:ARG:O	1:C:69:LEU:HD12	2.20	0.42
1:C:473:LEU:HD22	1:C:511:ASN:HD22	1.85	0.42
1:C:201:ARG:HD2	1:C:235:ILE:HA	2.02	0.41
1:A:201:ARG:HD2	1:A:235:ILE:HA	2.01	0.41
1:A:317:ARG:HD2	1:A:353:HIS:HD1	1.85	0.41
1:A:43:PHE:CE2	1:C:48:PRO:HB3	2.56	0.41
1:C:197:SER:O	1:C:201:ARG:HG3	2.20	0.41
1:C:504:LYS:O	1:C:504:LYS:CG	2.69	0.41
1:C:317:ARG:NH1	2:D:303:SER:O	2.37	0.41
1:C:115:ASN:O	1:C:119:LYS:HG3	2.21	0.41
1:C:423:ILE:HD13	1:C:464:GLY:CA	2.47	0.40
1:A:495:HIS:HE1	5:A:768:HOH:O	2.03	0.40
1:A:496:ASN:HB3	1:A:499:VAL:CG2	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	485/506 (96%)	474 (98%)	11 (2%)	0	100	100
1	C	485/506 (96%)	476 (98%)	9 (2%)	0	100	100
2	B	28/93 (30%)	28 (100%)	0	0	100	100
2	D	28/93 (30%)	28 (100%)	0	0	100	100
All	All	1026/1198 (86%)	1006 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/434 (96%)	415 (99%)	3 (1%)	84	92
1	C	418/434 (96%)	409 (98%)	9 (2%)	52	71
2	B	28/89 (32%)	28 (100%)	0	100	100
2	D	28/89 (32%)	28 (100%)	0	100	100
All	All	892/1046 (85%)	880 (99%)	12 (1%)	69	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	353	HIS

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Mol	Chain	Res	Type
1	A	506	ASP
1	C	40	GLN
1	C	204	LEU
1	C	359	ARG
1	C	462	ASN
1	C	463	GLU
1	C	494	SER
1	C	497	ASP
1	C	502	LEU
1	C	505	ASN

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

Mol	Chain	Res	Type
1	C	462	ASN
1	C	505	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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
3	PE5	C	601	-	16,16,26	0.85	0	15,15,25	0.25	0
3	PE5	A	601	-	16,16,26	0.85	0	15,15,25	0.23	0
4	B3P	A	602	-	18,18,18	0.93	0	21,23,23	1.22	1 (4%)

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
3	PE5	C	601	-	-	7/14/14/24	-
3	PE5	A	601	-	-	7/14/14/24	-
4	B3P	A	602	-	-	16/28/28/28	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	B3P	C2-N2-C8	-4.13	110.22	116.08

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	B3P	C5-C4-N1-C3
4	A	602	B3P	C6-C4-N1-C3
4	A	602	B3P	C7-C4-N1-C3
4	A	602	B3P	N1-C4-C5-O4
4	A	602	B3P	C6-C4-C5-O4
4	A	602	B3P	C7-C4-C5-O4
4	A	602	B3P	O2-C10-C8-N2
4	A	602	B3P	O2-C10-C8-C9
4	A	602	B3P	O2-C10-C8-C11
3	C	601	PE5	O3-C5-C6-O4
4	A	602	B3P	C3-C1-C2-N2
3	A	601	PE5	O6-C10-C9-O5
3	C	601	PE5	O1-C1-C2-O2
3	A	601	PE5	O3-C5-C6-O4
3	A	601	PE5	O2-C3-C4-O3
4	A	602	B3P	C2-C1-C3-N1

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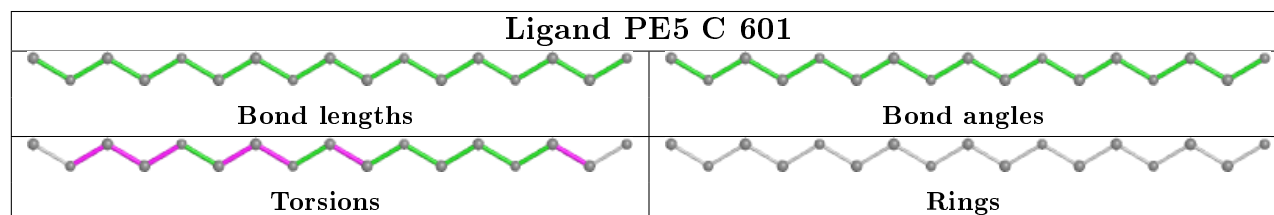
Mol	Chain	Res	Type	Atoms
4	A	602	B3P	C1-C3-N1-C4
3	A	601	PE5	C3-C4-O3-C5
3	A	601	PE5	C1-C2-O2-C3
3	A	601	PE5	C6-C5-O3-C4
3	C	601	PE5	C10-C9-O5-C8
4	A	602	B3P	N2-C8-C9-O1
4	A	602	B3P	C5-C4-C6-O5
4	A	602	B3P	O3-C11-C8-C10
3	C	601	PE5	C9-C10-O6-C11
3	C	601	PE5	O4-C7-C8-O5
3	C	601	PE5	C8-C7-O4-C6
3	A	601	PE5	O1-C1-C2-O2
4	A	602	B3P	C10-C8-C9-O1
3	C	601	PE5	O6-C10-C9-O5

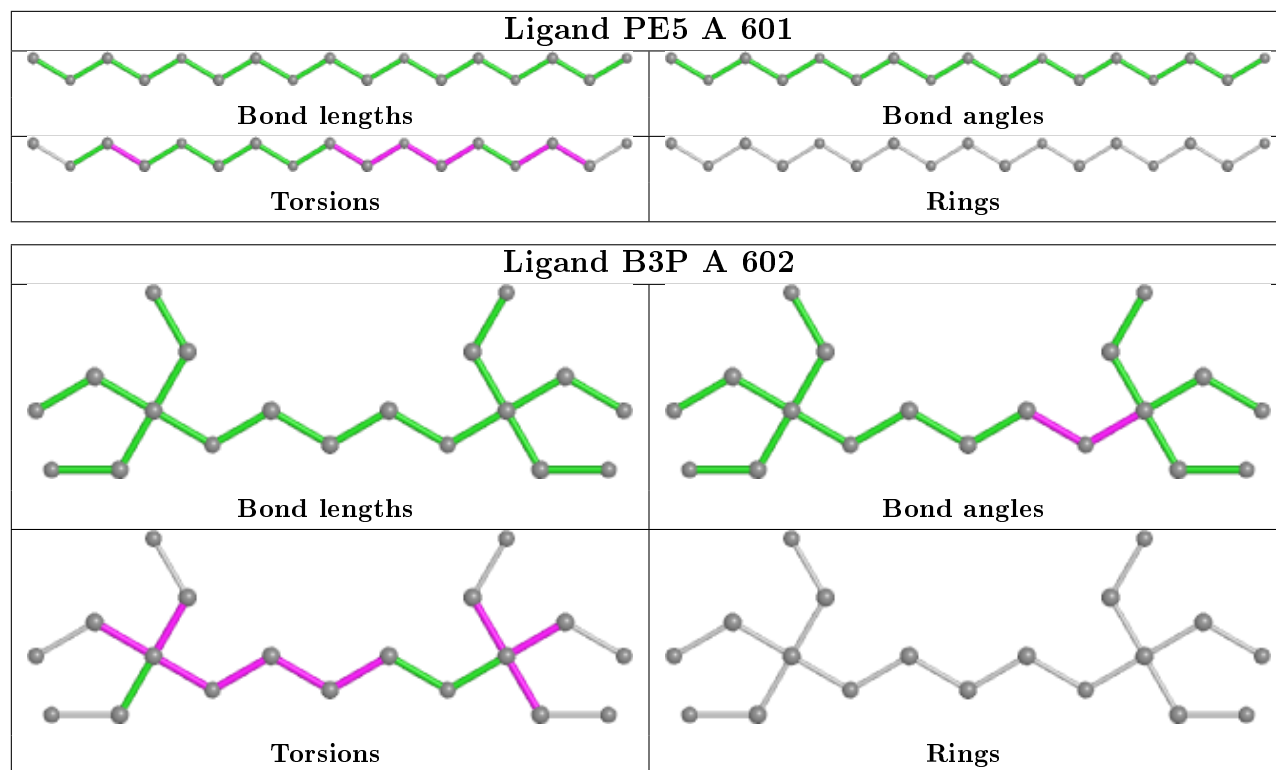
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	PE5	1	0
4	A	602	B3P	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	489/506 (96%)	-0.09	27 (5%) 25 24	28, 41, 83, 119	0
1	C	489/506 (96%)	-0.01	32 (6%) 18 17	29, 41, 87, 123	0
2	B	30/93 (32%)	-0.37	0 100 100	35, 41, 59, 61	0
2	D	30/93 (32%)	-0.27	0 100 100	35, 42, 63, 68	0
All	All	1038/1198 (86%)	-0.06	59 (5%) 23 22	28, 41, 86, 123	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	512	GLY	8.7
1	C	510	ILE	8.0
1	A	30	LEU	6.3
1	C	495	HIS	5.9
1	C	41	LEU	5.8
1	A	21	ALA	5.7
1	C	506	ASP	5.5
1	C	494	SER	5.1
1	C	34	TYR	5.1
1	C	497	ASP	5.0
1	A	41	LEU	4.8
1	A	494	SER	4.6
1	C	499	VAL	4.2
1	A	34	TYR	4.1
1	A	40	GLN	3.8
1	C	19	PRO	3.8
1	A	509	ILE	3.8
1	C	40	GLN	3.8
1	C	28	VAL	3.7
1	A	495	HIS	3.7
1	C	508	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	20	ILE	3.6
1	A	29	THR	3.6
1	A	26	GLU	3.6
1	C	25	ARG	3.5
1	A	510	ILE	3.5
1	C	22	ASP	3.5
1	A	505	ASN	3.5
1	A	511	ASN	3.4
1	A	20	ILE	3.3
1	A	25	ARG	3.3
1	C	509	ILE	3.3
1	C	511	ASN	3.2
1	A	492	LEU	3.1
1	C	505	ASN	3.0
1	C	462	ASN	2.8
1	A	33	GLY	2.7
1	C	32	LEU	2.7
1	C	31	LEU	2.7
1	A	497	ASP	2.7
1	A	501	ASP	2.7
1	A	32	LEU	2.7
1	A	506	ASP	2.6
1	C	26	GLU	2.6
1	A	31	LEU	2.5
1	C	503	VAL	2.5
1	C	30	LEU	2.5
1	A	23	ASN	2.5
1	C	470	ILE	2.5
1	C	501	ASP	2.5
1	A	22	ASP	2.4
1	C	507	ASP	2.3
1	C	463	GLU	2.2
1	C	21	ALA	2.2
1	C	24	GLU	2.2
1	A	449	ASN	2.2
1	A	346	ASP	2.2
1	C	346	ASP	2.1
1	A	508	ASP	2.1

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

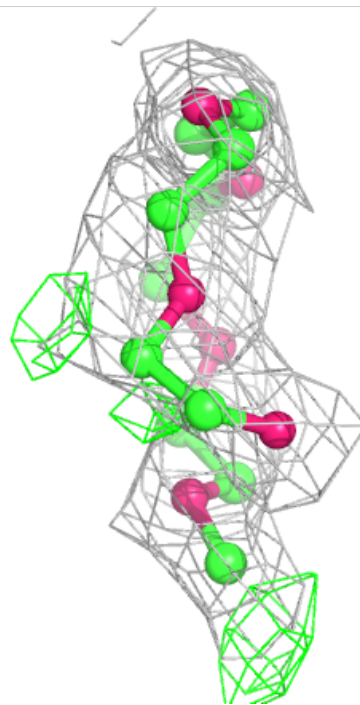
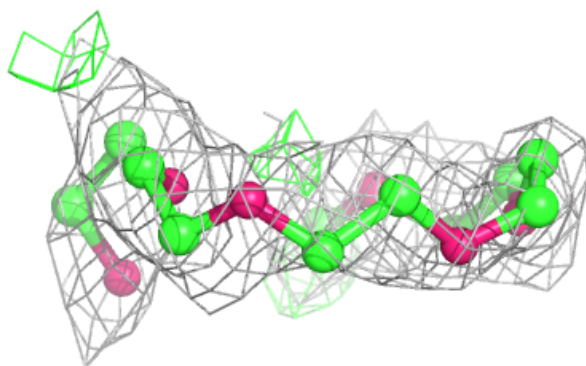
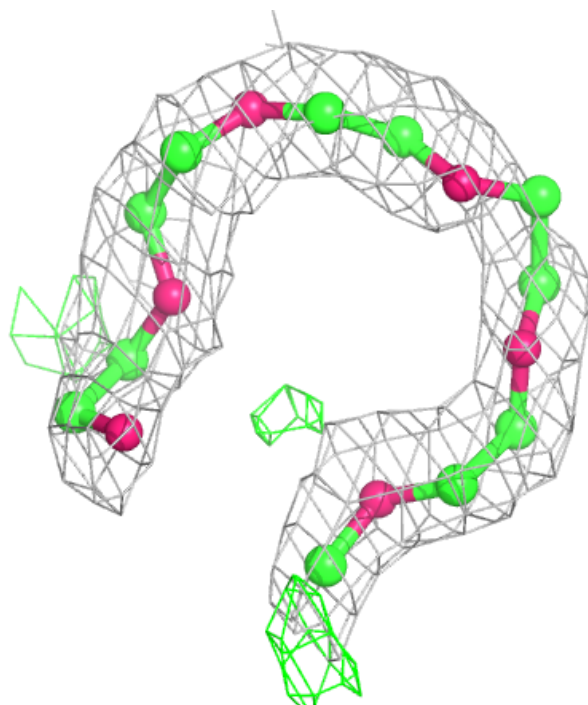
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PE5	A	601	17/27	0.77	0.25	56,67,79,81	0
4	B3P	A	602	19/19	0.83	0.21	60,76,89,106	0
3	PE5	C	601	17/27	0.84	0.21	42,62,72,77	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.

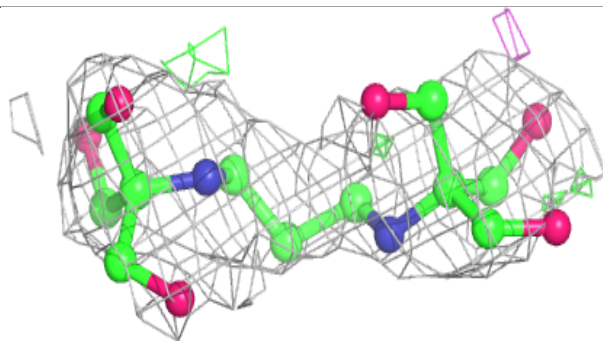
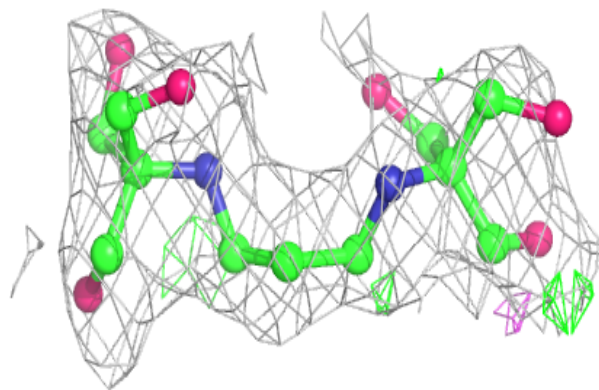
**Electron density around PE5 A 601:**

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

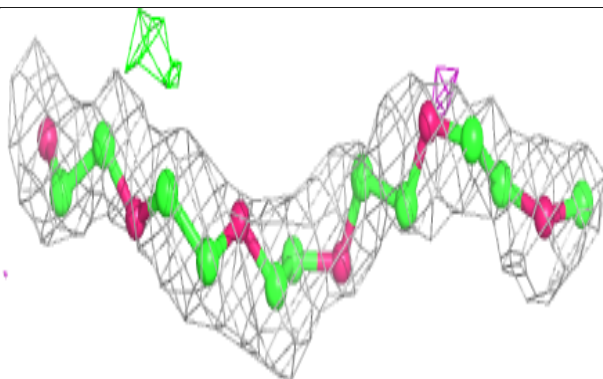
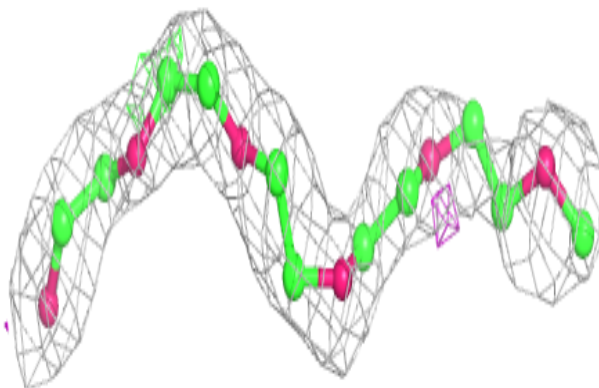


**Electron density around B3P A 602:**

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

**Electron density around PE5 C 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.