



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 05:19 AM EST

PDB ID : 5CTH  
Title : The 3.7 Å resolution structure of a eukaryotic SWEET transporter  
Authors : Feng, L.; Tao, Y.; Perry, K.  
Deposited on : 2015-07-24  
Resolution : 3.69 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  
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) : 2.36

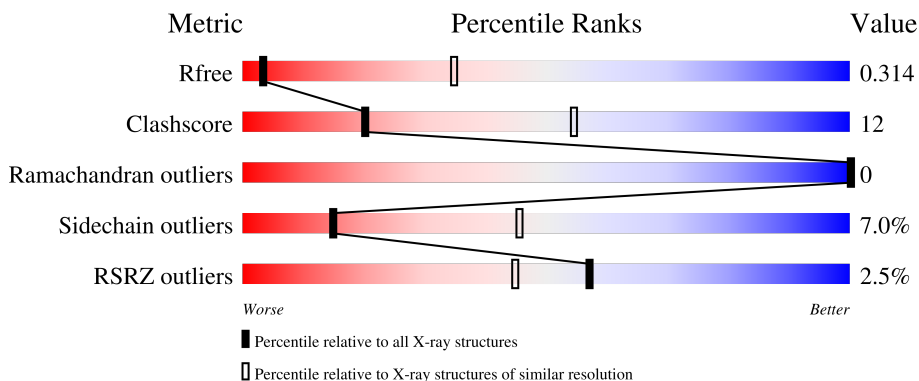
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.69 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	224	69% 24% • 5%
1	B	224	62% 31% • •
1	C	224	68% 25% • 5%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PE5	A	301	-	-	-	X
2	PE5	A	302	-	-	-	X
2	PE5	B	302	-	-	-	X
2	PE5	C	301	-	-	-	X
2	PE5	C	302	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5013 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 Bidirectional sugar transporter SWEET2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1631	C 1096	N 254	O 269	S 12	0	0	0
1	B	215	Total 1643	C 1106	N 251	O 274	S 12	0	0	0
1	C	213	Total 1586	C 1064	N 243	O 267	S 12	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

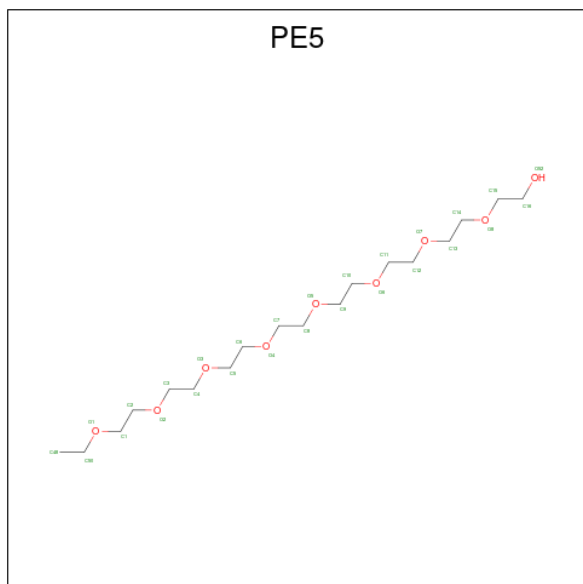
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	SER	-	expression tag	UNP Q5N8J1
A	217	ASN	-	expression tag	UNP Q5N8J1
A	218	SER	-	expression tag	UNP Q5N8J1
A	219	LEU	-	expression tag	UNP Q5N8J1
A	220	GLU	-	expression tag	UNP Q5N8J1
A	221	VAL	-	expression tag	UNP Q5N8J1
A	222	LEU	-	expression tag	UNP Q5N8J1
A	223	PHE	-	expression tag	UNP Q5N8J1
A	224	GLN	-	expression tag	UNP Q5N8J1
B	216	SER	-	expression tag	UNP Q5N8J1
B	217	ASN	-	expression tag	UNP Q5N8J1
B	218	SER	-	expression tag	UNP Q5N8J1
B	219	LEU	-	expression tag	UNP Q5N8J1
B	220	GLU	-	expression tag	UNP Q5N8J1
B	221	VAL	-	expression tag	UNP Q5N8J1
B	222	LEU	-	expression tag	UNP Q5N8J1
B	223	PHE	-	expression tag	UNP Q5N8J1
B	224	GLN	-	expression tag	UNP Q5N8J1
C	216	SER	-	expression tag	UNP Q5N8J1
C	217	ASN	-	expression tag	UNP Q5N8J1
C	218	SER	-	expression tag	UNP Q5N8J1
C	219	LEU	-	expression tag	UNP Q5N8J1
C	220	GLU	-	expression tag	UNP Q5N8J1

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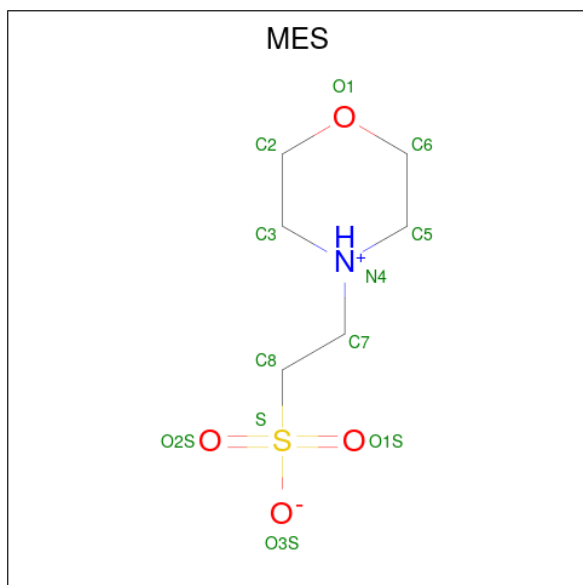
Chain	Residue	Modelled	Actual	Comment	Reference
C	221	VAL	-	expression tag	UNP Q5N8J1
C	222	LEU	-	expression tag	UNP Q5N8J1
C	223	PHE	-	expression tag	UNP Q5N8J1
C	224	GLN	-	expression tag	UNP Q5N8J1

- Molecule 2 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>9</sub>).



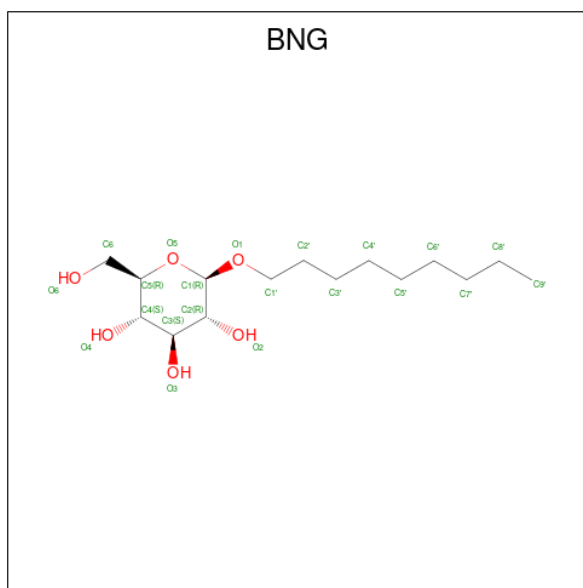
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	16	8		
2	A	1	Total	C	O	0	0
			24	16	8		
2	B	1	Total	C	O	0	0
			24	16	8		
2	C	1	Total	C	O	0	0
			24	16	8		
2	C	1	Total	C	O	0	0
			24	16	8		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0

- Molecule 4 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula:  $C_{15}H_{30}O_6$ ).

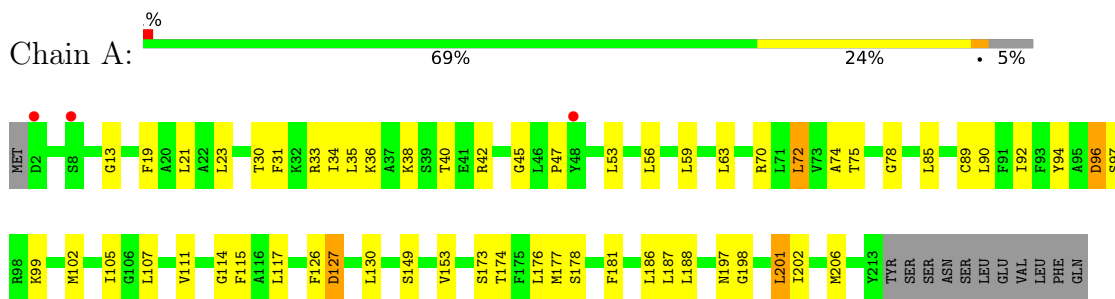


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	21	15	6	0	0

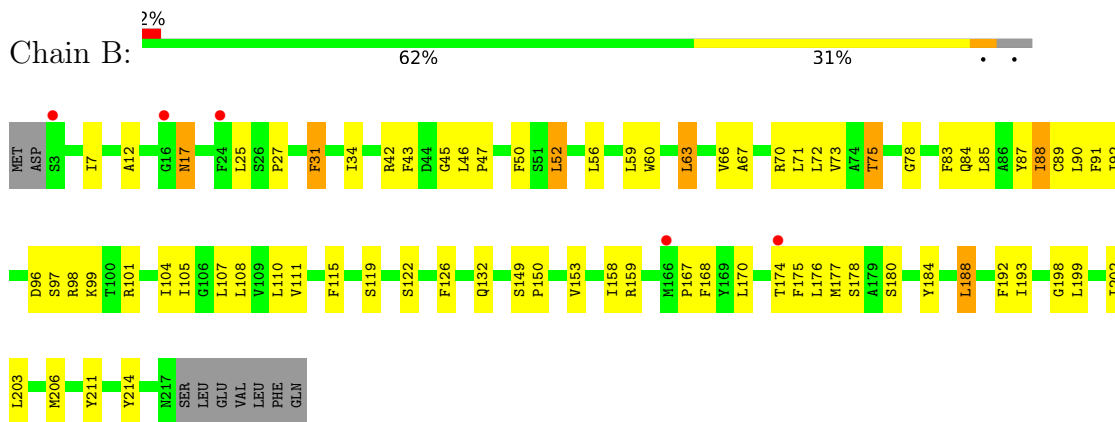
### 3 Residue-property plots [i](#)

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.

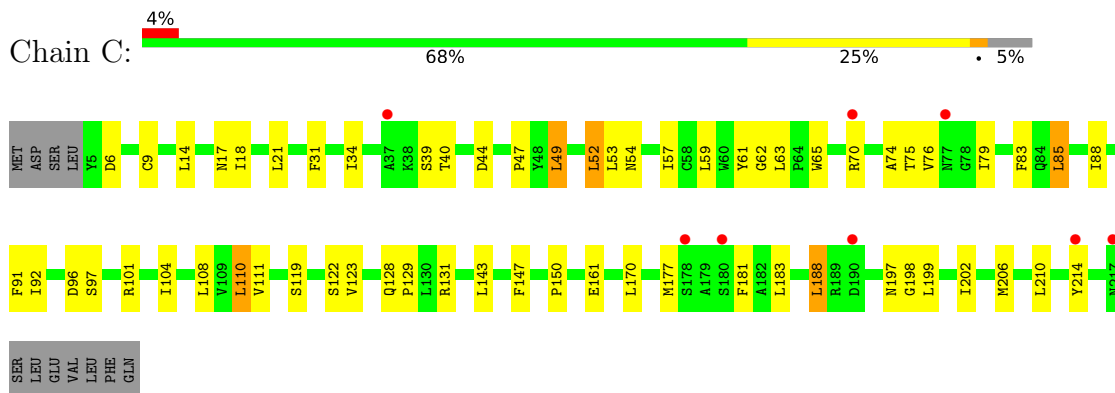
- Molecule 1: Bidirectional sugar transporter SWEET2b



- Molecule 1: Bidirectional sugar transporter SWEET2b



- Molecule 1: Bidirectional sugar transporter SWEET2b



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.98Å 95.49Å 150.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 3.69 49.40 – 3.69	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.55-3.69) 91.4 (49.40-3.69)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 3.67Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.256 , 0.307 0.261 , 0.314	Depositor DCC
$R_{free}$ test set	1334 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.2	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 99.8	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	0.84	EDS
Total number of atoms	5013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, BNG, PE5

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	0.36	0/1672	0.59	0/2269
1	B	0.40	0/1687	0.59	0/2297
1	C	0.35	0/1626	0.59	0/2216
All	All	0.37	0/4985	0.59	0/6782

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	1631	0	1680	43	0
1	B	1643	0	1656	50	0
1	C	1586	0	1575	34	0
2	A	48	0	56	1	0
2	B	24	0	28	1	0
2	C	48	0	56	4	0
3	A	12	0	12	1	0
4	B	21	0	30	3	0
All	All	5013	0	5093	126	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 12.

All (126) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:HD11	1:B:43:PHE:HB2	1.50	0.91
1:A:126:PHE:HD2	1:A:130:LEU:HD12	1.55	0.72
1:C:150:PRO:HG2	2:C:302:PE5:H81	1.71	0.71
1:C:53:LEU:HD12	1:C:111:VAL:HG22	1.74	0.69
1:A:45:GLY:H	1:A:47:PRO:HD2	1.58	0.69
1:A:34:ILE:HD13	1:A:40:THR:HG22	1.76	0.68
1:A:53:LEU:HD13	1:A:111:VAL:HG13	1.75	0.67
1:A:99:LYS:HD3	1:B:159:ARG:HD2	1.79	0.64
1:B:168:PHE:HB2	1:B:211:TYR:CZ	2.32	0.64
1:A:126:PHE:CD2	1:A:130:LEU:HD12	2.33	0.64
1:A:59:LEU:HD22	1:A:78:GLY:HA2	1.81	0.63
1:A:102:MET:HA	1:A:105:ILE:HG22	1.81	0.62
1:B:31:PHE:HE2	1:B:90:LEU:HB2	1.65	0.62
1:B:72:LEU:O	1:B:75:THR:HG22	2.02	0.60
1:C:49:LEU:HD21	1:C:108:LEU:HA	1.84	0.59
1:A:206:MET:SD	1:C:110:LEU:HG	2.42	0.59
1:B:150:PRO:HG3	2:B:302:PE5:H121	1.84	0.59
1:B:167:PRO:HG2	1:B:170:LEU:HB3	1.85	0.59
1:B:56:LEU:HD23	1:B:115:PHE:CD2	2.38	0.58
1:B:45:GLY:H	1:B:47:PRO:HD2	1.69	0.58
1:B:175:PHE:HD2	1:B:176:LEU:HD22	1.68	0.58
1:A:19:PHE:O	1:A:173:SER:OG	2.21	0.57
1:A:34:ILE:O	1:A:38:LYS:N	2.27	0.57
1:C:91:PHE:CE2	1:C:104:ILE:HG13	2.40	0.56
1:A:181:PHE:HB3	1:A:197:ASN:ND2	2.22	0.55
1:B:73:VAL:HG23	1:B:184:TYR:HE2	1.72	0.55
1:B:92:ILE:HD11	1:B:105:ILE:HA	1.89	0.55
1:B:89:CYS:O	1:B:92:ILE:HG22	2.07	0.54
1:A:92:ILE:HD11	1:A:105:ILE:HB	1.89	0.54
1:B:70:ARG:HH21	1:B:188:LEU:HG	1.72	0.53
1:C:85:LEU:HD23	1:C:88:ILE:HD11	1.91	0.53
1:C:39:SER:H	1:C:40:THR:HA	1.73	0.53
1:C:147:PHE:HE2	1:C:199:LEU:HB3	1.74	0.53
1:C:181:PHE:HB3	1:C:197:ASN:ND2	2.23	0.53
1:A:23:LEU:HD11	2:A:301:PE5:H52A	1.91	0.52
1:C:70:ARG:NH2	1:C:188:LEU:HD23	2.26	0.51
1:B:52:LEU:HD23	1:B:111:VAL:HG11	1.92	0.51
1:B:84:GLN:O	1:B:88:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:O	1:C:101:ARG:HG3	2.10	0.50
1:C:31:PHE:HA	1:C:34:ILE:HG23	1.94	0.50
1:C:147:PHE:CD1	2:C:302:PE5:H82	2.47	0.50
1:B:27:PRO:HG2	1:B:87:TYR:CE1	2.46	0.50
1:B:101:ARG:O	1:B:105:ILE:HG13	2.12	0.49
1:A:56:LEU:HD23	1:A:115:PHE:CD2	2.47	0.49
1:A:96:ASP:O	1:A:97:SER:HB3	2.12	0.49
1:C:54:ASN:O	1:C:57:ILE:HG22	2.13	0.49
1:A:33:ARG:HH22	1:A:42:ARG:HG2	1.76	0.49
1:B:88:ILE:HD13	1:B:108:LEU:HD13	1.94	0.49
1:A:72:LEU:O	1:A:75:THR:OG1	2.19	0.49
1:C:17:ASN:ND2	1:C:75:THR:OG1	2.46	0.49
1:A:126:PHE:HE2	4:B:301:BNG:H2'2	1.78	0.49
1:B:59:LEU:HD22	1:B:78:GLY:HA2	1.94	0.48
1:B:12:ALA:O	1:B:180:SER:OG	2.32	0.48
1:B:88:ILE:HD11	1:B:108:LEU:HB2	1.96	0.47
1:A:174:THR:HA	1:A:177:MET:HG2	1.96	0.46
1:B:192:PHE:CE2	4:B:301:BNG:H1'2	2.50	0.46
1:A:202:ILE:O	1:A:206:MET:HG3	2.16	0.46
1:B:73:VAL:HG21	1:B:193:ILE:HD12	1.98	0.46
1:B:91:PHE:CE2	1:B:104:ILE:HG13	2.51	0.46
1:C:119:SER:O	1:C:122:SER:OG	2.21	0.46
1:B:110:LEU:HA	1:C:206:MET:HE1	1.98	0.46
1:C:198:GLY:O	1:C:202:ILE:HG13	2.15	0.46
1:B:158:ILE:HA	1:B:214:TYR:HE1	1.80	0.46
1:C:150:PRO:HB3	2:C:302:PE5:H121	1.98	0.46
1:C:49:LEU:HA	1:C:52:LEU:HD23	1.98	0.45
1:A:206:MET:HE2	1:A:206:MET:HB3	1.72	0.45
1:A:31:PHE:HA	1:A:34:ILE:HB	1.99	0.45
1:C:14:LEU:O	1:C:18:ILE:HG12	2.17	0.45
1:A:13:GLY:HA3	1:A:72:LEU:HG	1.97	0.45
1:B:17:ASN:HD21	1:B:75:THR:HG23	1.83	0.44
1:A:31:PHE:O	1:A:35:LEU:N	2.42	0.44
1:C:128:GLN:HG3	1:C:129:PRO:HA	2.00	0.44
1:A:127:ASP:OD2	1:A:127:ASP:N	2.51	0.43
1:B:67:ALA:HA	1:B:132:GLN:HE21	1.82	0.43
1:B:149:SER:O	1:B:153:VAL:HG13	2.17	0.43
1:C:70:ARG:HE	1:C:70:ARG:HB3	1.58	0.43
1:B:119:SER:O	1:B:122:SER:OG	2.18	0.43
1:A:59:LEU:O	1:A:63:LEU:HD13	2.19	0.43
1:B:70:ARG:NH2	1:B:188:LEU:HG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HG3	1:B:99:LYS:N	2.34	0.43
1:A:198:GLY:HA2	1:A:201:LEU:HD23	2.01	0.43
1:B:92:ILE:HD11	1:B:105:ILE:HG12	1.99	0.43
1:B:7:ILE:HD13	1:B:7:ILE:HA	1.86	0.43
1:A:13:GLY:C	1:A:72:LEU:HG	2.39	0.42
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.88	0.42
1:C:21:LEU:HD21	1:C:79:ILE:HD12	2.01	0.42
1:A:114:GLY:O	1:A:117:LEU:HB3	2.19	0.42
1:B:88:ILE:O	1:B:92:ILE:HB	2.18	0.42
1:C:44:ASP:O	1:C:47:PRO:HD2	2.19	0.42
1:B:198:GLY:O	1:B:202:ILE:HG13	2.19	0.42
1:A:89:CYS:O	1:A:92:ILE:HG22	2.20	0.42
1:C:161:GLU:HA	1:C:214:TYR:CE1	2.55	0.42
1:A:30:THR:O	1:A:34:ILE:N	2.52	0.42
1:B:177:MET:HG3	1:B:178:SER:N	2.34	0.42
1:A:70:ARG:CZ	1:A:188:LEU:HD23	2.50	0.42
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.88	0.42
1:B:202:ILE:O	1:B:206:MET:HG3	2.20	0.41
1:B:206:MET:HB3	1:B:206:MET:HE2	1.80	0.41
1:B:63:LEU:HD12	1:B:63:LEU:HA	1.90	0.41
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.77	0.41
1:B:158:ILE:HA	1:B:214:TYR:CE1	2.56	0.41
1:C:96:ASP:O	1:C:97:SER:HB3	2.20	0.41
1:A:35:LEU:HD13	1:A:94:TYR:HE2	1.86	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.76	0.41
4:B:301:BNG:H5'2	4:B:301:BNG:H8'1	1.71	0.41
1:A:59:LEU:HD13	1:A:74:ALA:O	2.20	0.41
1:B:60:TRP:O	1:B:66:VAL:HG11	2.21	0.41
1:C:54:ASN:HD21	1:C:143:LEU:HD23	1.86	0.41
1:C:123:VAL:HA	1:C:131:ARG:HD2	2.03	0.41
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.79	0.41
1:C:177:MET:CE	2:C:302:PE5:H21	2.51	0.41
1:B:174:THR:HA	1:B:177:MET:HG2	2.03	0.41
1:B:122:SER:HA	1:B:126:PHE:HD2	1.86	0.41
1:C:62:GLY:HA3	1:C:74:ALA:HB2	2.03	0.41
1:A:19:PHE:CD1	1:A:176:LEU:HB3	2.56	0.40
1:B:96:ASP:O	1:B:97:SER:OG	2.33	0.40
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.87	0.40
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.84	0.40
1:A:36:LYS:HD2	1:A:36:LYS:N	2.36	0.40
1:B:176:LEU:HD13	1:B:176:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:PHE:HD1	1:C:83:PHE:HA	1.74	0.40
1:A:40:THR:HG1	1:A:96:ASP:H	1.70	0.40
1:A:177:MET:HG3	1:A:178:SER:N	2.35	0.40
3:A:303:MES:H82	3:A:303:MES:H51	1.81	0.40
1:C:17:ASN:CG	1:C:76:VAL:HB	2.41	0.40
1:C:59:LEU:O	1:C:63:LEU:HD13	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/224 (94%)	199 (95%)	11 (5%)	0	100	100
1	B	213/224 (95%)	205 (96%)	8 (4%)	0	100	100
1	C	211/224 (94%)	204 (97%)	7 (3%)	0	100	100
All	All	634/672 (94%)	608 (96%)	26 (4%)	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	171/187 (91%)	162 (95%)	9 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	170/187 (91%)	156 (92%)	14 (8%)	11	41
1	C	159/187 (85%)	147 (92%)	12 (8%)	13	43
All	All	500/561 (89%)	465 (93%)	35 (7%)	15	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	72	LEU
1	A	85	LEU
1	A	96	ASP
1	A	127	ASP
1	A	149	SER
1	A	153	VAL
1	A	186	LEU
1	A	201	LEU
1	B	17	ASN
1	B	31	PHE
1	B	42	ARG
1	B	46	LEU
1	B	50	PHE
1	B	52	LEU
1	B	63	LEU
1	B	71	LEU
1	B	75	THR
1	B	83	PHE
1	B	85	LEU
1	B	88	ILE
1	B	188	LEU
1	B	199	LEU
1	C	6	ASP
1	C	9	CYS
1	C	49	LEU
1	C	52	LEU
1	C	61	TYR
1	C	65	TRP
1	C	85	LEU
1	C	110	LEU
1	C	170	LEU
1	C	183	LEU
1	C	188	LEU

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Mol	Chain	Res	Type
1	C	210	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	ASN
1	B	132	GLN
1	C	197	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](#)

7 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	$\# Z  > 2$
2	PE5	B	302	-	23,23,26	0.82	1 (4%)	22,22,25	0.32	0
2	PE5	C	301	-	23,23,26	0.92	1 (4%)	22,22,25	0.39	0
3	MES	A	303	-	12,12,12	2.19	1 (8%)	14,16,16	2.14	6 (42%)
2	PE5	C	302	-	23,23,26	0.82	0	22,22,25	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PE5	A	301	-	23,23,26	0.89	1 (4%)	22,22,25	0.31	0
4	BNG	B	301	-	21,21,21	1.10	1 (4%)	26,26,26	1.17	3 (11%)
2	PE5	A	302	-	23,23,26	0.90	0	22,22,25	0.40	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
2	PE5	B	302	-	-	16/21/21/24	-
2	PE5	C	301	-	-	13/21/21/24	-
3	MES	A	303	-	-	3/6/14/14	0/1/1/1
2	PE5	C	302	-	-	14/21/21/24	-
2	PE5	A	301	-	-	15/21/21/24	-
4	BNG	B	301	-	-	6/12/32/32	0/1/1/1
2	PE5	A	302	-	-	11/21/21/24	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	MES	C8-S	-7.33	1.67	1.77
4	B	301	BNG	O5-C1	2.93	1.49	1.41
2	A	301	PE5	C12-C11	2.07	1.59	1.49
2	C	301	PE5	C12-C11	2.07	1.59	1.49
2	B	302	PE5	C12-C11	2.01	1.59	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	MES	C5-N4-C3	3.99	117.81	108.83
4	B	301	BNG	O5-C1-C2	3.23	117.19	110.35
3	A	303	MES	O1S-S-C8	3.09	110.64	106.92
3	A	303	MES	C6-C5-N4	-3.09	105.42	110.10
3	A	303	MES	O3S-S-C8	2.97	110.58	105.77
4	B	301	BNG	C1-C2-C3	2.93	116.09	110.00
3	A	303	MES	C7-N4-C5	2.54	117.73	111.23
3	A	303	MES	C7-N4-C3	2.32	117.17	111.23
4	B	301	BNG	C4-C3-C2	2.27	114.78	110.82



There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	PE5	C14-C13-O7-C12
2	A	302	PE5	C14-C13-O7-C12
2	A	301	PE5	O7-C13-C14-O8
2	A	302	PE5	O1-C1-C2-O2
2	C	302	PE5	O4-C7-C8-O5
2	A	301	PE5	O3-C5-C6-O4
2	C	301	PE5	C12-C11-O6-C10
2	C	302	PE5	O7-C13-C14-O8
2	C	302	PE5	O3-C5-C6-O4
2	A	301	PE5	O6-C10-C9-O5
2	A	301	PE5	O6-C11-C12-O7
2	C	301	PE5	O6-C10-C9-O5
2	B	302	PE5	O2-C3-C4-O3
4	B	301	BNG	C2-C1-O1-C1'
2	B	302	PE5	O4-C7-C8-O5
2	C	302	PE5	O1-C1-C2-O2
2	C	302	PE5	C13-C14-O8-C15
2	B	302	PE5	O1-C1-C2-O2
3	A	303	MES	C7-C8-S-O3S
2	B	302	PE5	O3-C5-C6-O4
4	B	301	BNG	O1-C1'-C2'-C3'
4	B	301	BNG	C3'-C4'-C5'-C6'
2	C	301	PE5	O4-C7-C8-O5
2	C	301	PE5	O3-C5-C6-O4
2	A	301	PE5	O4-C7-C8-O5
2	C	301	PE5	C13-C14-O8-C15
4	B	301	BNG	C2'-C1'-O1-C1
2	B	302	PE5	O6-C11-C12-O7
2	A	302	PE5	O7-C13-C14-O8
4	B	301	BNG	C1'-C2'-C3'-C4'
2	A	302	PE5	O2-C3-C4-O3
2	C	302	PE5	O2-C3-C4-O3
2	A	301	PE5	O1-C1-C2-O2
4	B	301	BNG	C5'-C6'-C7'-C8'
2	C	302	PE5	C5-C6-O4-C7
2	A	302	PE5	O4-C7-C8-O5
2	A	301	PE5	C2-C1-O1-C50
2	A	301	PE5	C13-C14-O8-C15
2	B	302	PE5	C13-C14-O8-C15
2	C	301	PE5	O2-C3-C4-O3

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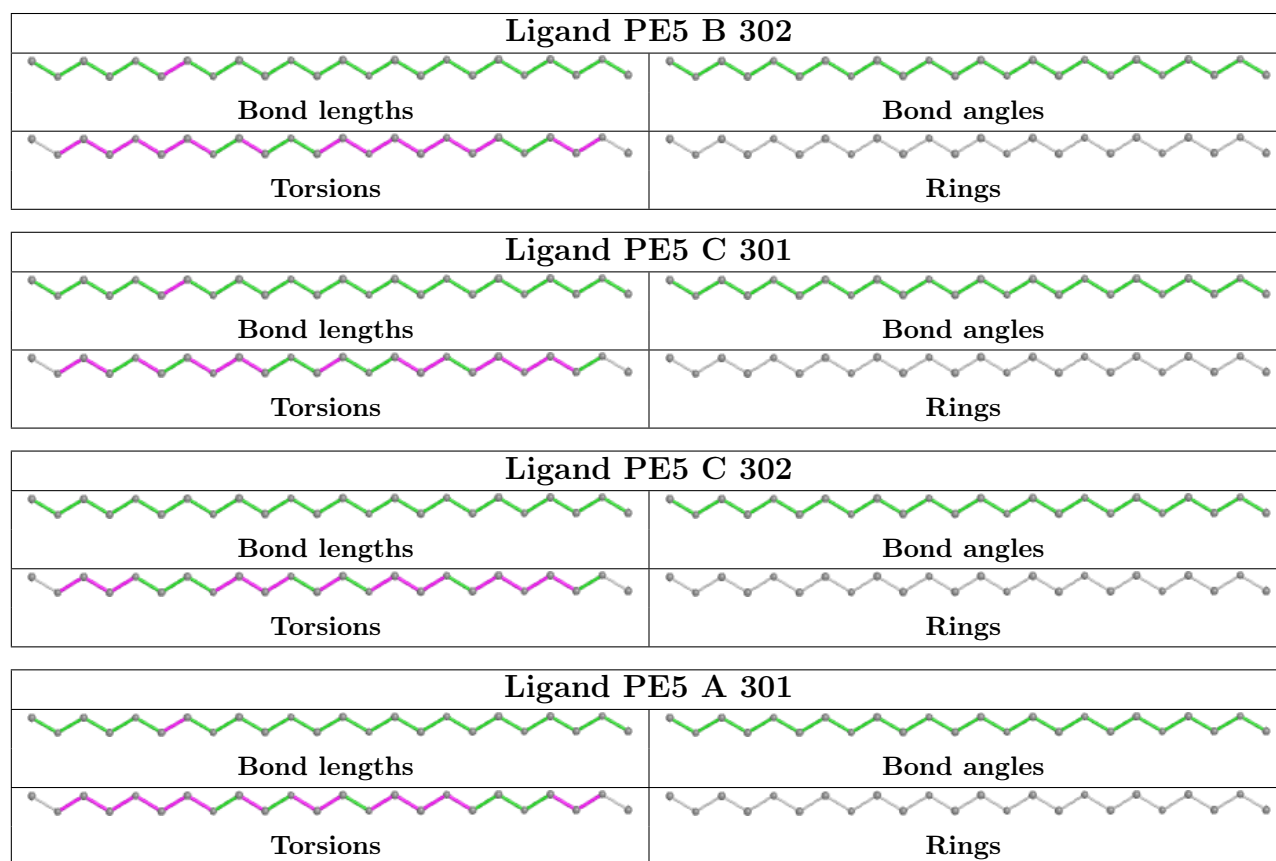
Mol	Chain	Res	Type	Atoms
2	C	302	PE5	O6-C10-C9-O5
2	A	302	PE5	C10-C9-O5-C8
2	C	302	PE5	C4-C3-O2-C2
2	A	301	PE5	C11-C12-O7-C13
2	A	301	PE5	C5-C6-O4-C7
2	B	302	PE5	C11-C12-O7-C13
2	B	302	PE5	C6-C5-O3-C4
2	C	301	PE5	C1-C2-O2-C3
2	A	301	PE5	C6-C5-O3-C4
2	C	301	PE5	C11-C12-O7-C13
3	A	303	MES	C7-C8-S-O1S
3	A	303	MES	C7-C8-S-O2S
2	C	301	PE5	C9-C10-O6-C11
2	A	302	PE5	C9-C10-O6-C11
2	B	302	PE5	C3-C4-O3-C5
2	B	302	PE5	C14-C13-O7-C12
2	C	302	PE5	C6-C5-O3-C4
2	B	302	PE5	C12-C11-O6-C10
2	A	302	PE5	C4-C3-O2-C2
2	B	302	PE5	C2-C1-O1-C50
2	A	301	PE5	C14-C13-O7-C12
2	A	302	PE5	O6-C11-C12-O7
2	C	301	PE5	O7-C13-C14-O8
2	C	302	PE5	C9-C10-O6-C11
2	B	302	PE5	C5-C6-O4-C7
2	C	301	PE5	C6-C5-O3-C4
2	A	301	PE5	C12-C11-O6-C10
2	C	302	PE5	C1-C2-O2-C3
2	C	301	PE5	C4-C3-O2-C2
2	C	301	PE5	O1-C1-C2-O2
2	C	302	PE5	C10-C9-O5-C8
2	B	302	PE5	O6-C10-C9-O5
2	A	302	PE5	O6-C10-C9-O5
2	A	302	PE5	C2-C1-O1-C50
2	A	301	PE5	C7-C8-O5-C9
2	A	301	PE5	C3-C4-O3-C5
2	B	302	PE5	C8-C7-O4-C6
2	B	302	PE5	O7-C13-C14-O8

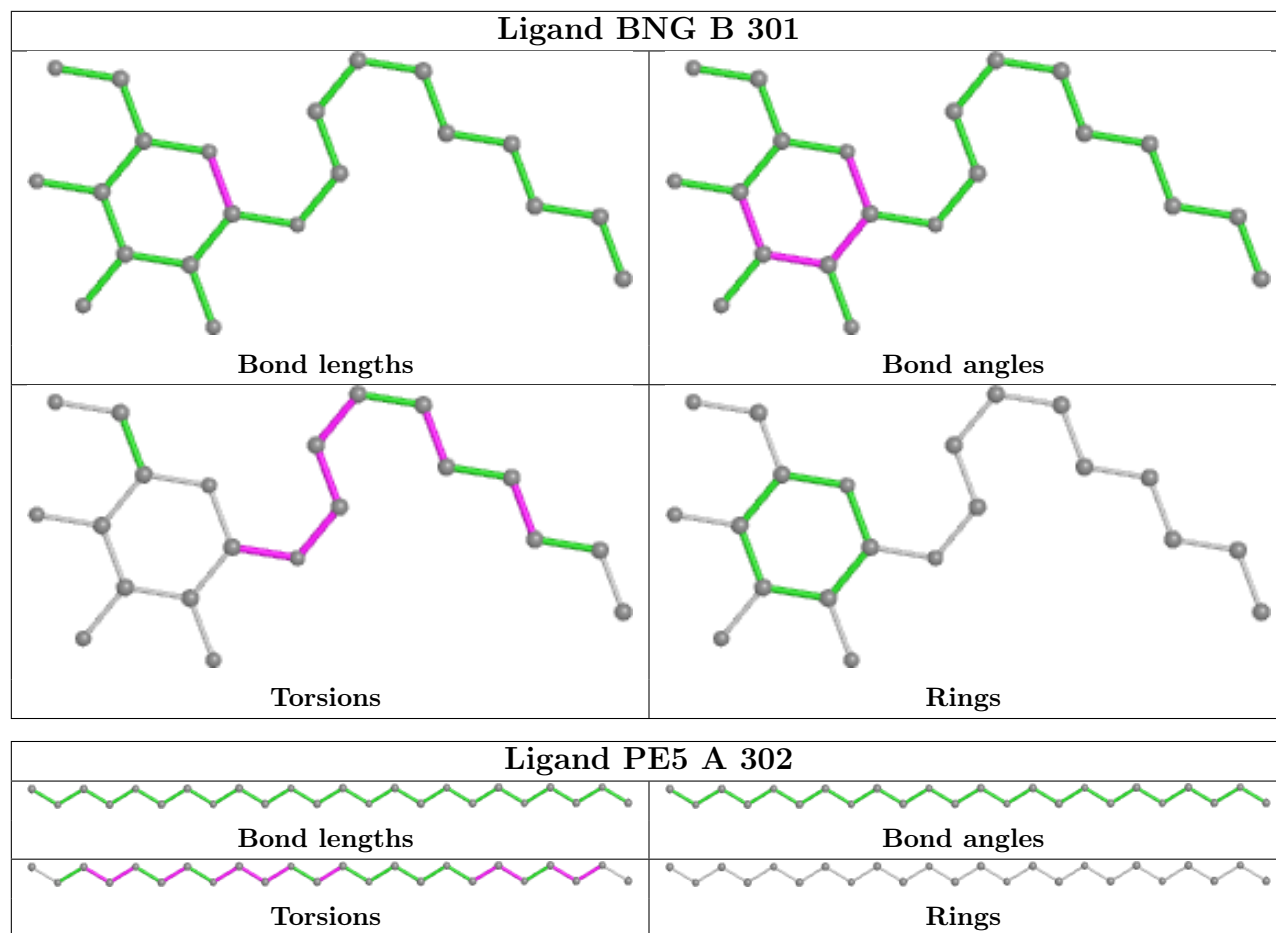
There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	PE5	1	0
3	A	303	MES	1	0
2	C	302	PE5	4	0
2	A	301	PE5	1	0
4	B	301	BNG	3	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 [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, 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	212/224 (94%)	0.04	3 (1%) 75 64	66, 135, 195, 295	0
1	B	215/224 (95%)	0.02	5 (2%) 60 48	64, 103, 158, 189	0
1	C	213/224 (95%)	0.31	8 (3%) 40 30	93, 161, 219, 247	0
All	All	640/672 (95%)	0.12	16 (2%) 57 45	64, 133, 207, 295	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	ARG	4.6
1	A	2	ASP	4.6
1	C	37	ALA	4.0
1	C	217	ASN	3.4
1	C	77	ASN	3.0
1	A	8	SER	2.6
1	C	180	SER	2.6
1	B	174	THR	2.4
1	B	16	GLY	2.4
1	C	214	TYR	2.4
1	B	166	MET	2.2
1	A	48	TYR	2.1
1	C	190	ASP	2.1
1	B	24	PHE	2.1
1	B	3	SER	2.1
1	C	178	SER	2.0

### 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](#)

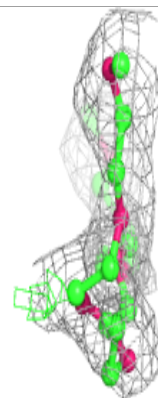
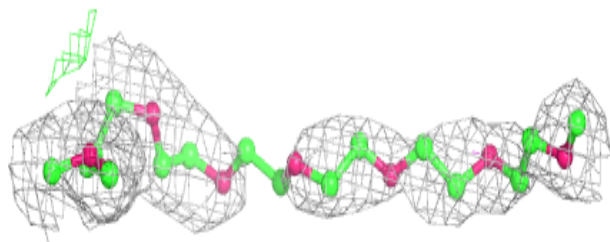
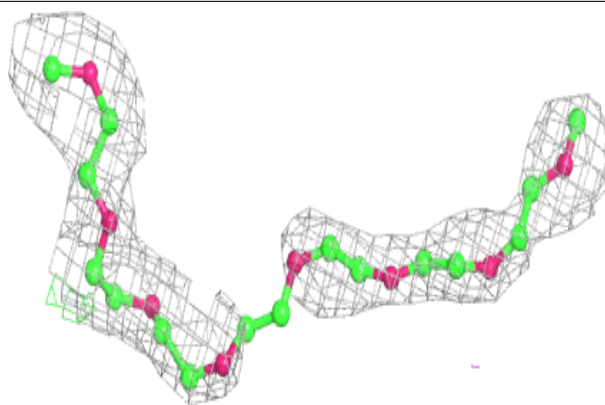
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	PE5	C	301	24/27	0.59	0.61	88,99,146,152	0
2	PE5	A	302	24/27	0.60	0.94	55,132,159,164	0
2	PE5	A	301	24/27	0.64	0.74	119,165,170,171	0
2	PE5	C	302	24/27	0.73	0.93	100,137,183,191	0
2	PE5	B	302	24/27	0.75	1.10	101,126,176,178	0
4	BNG	B	301	21/21	0.77	0.36	55,103,135,142	0
3	MES	A	303	12/12	0.80	0.29	176,180,192,192	0

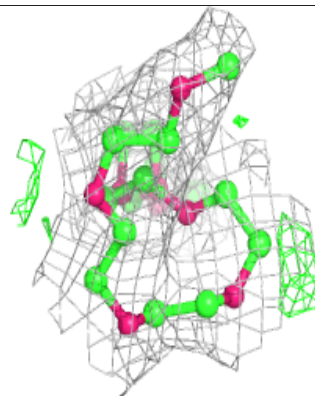
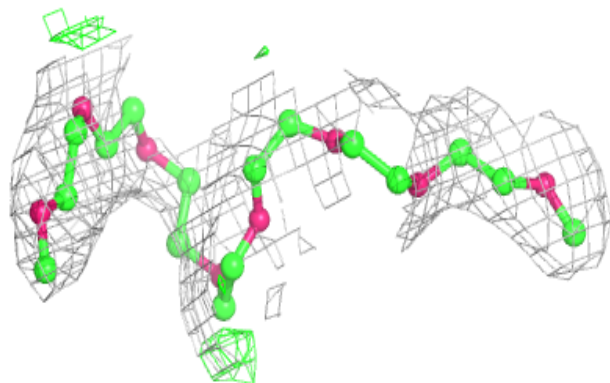
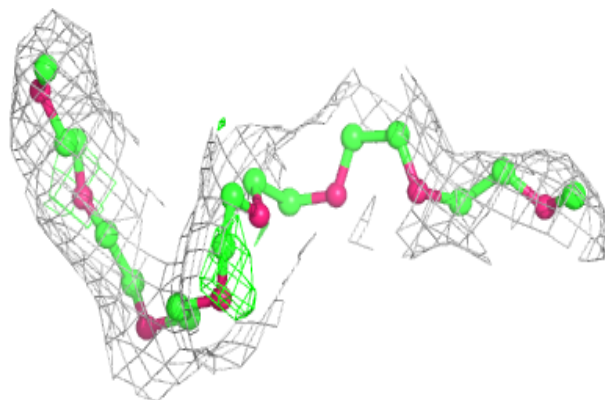
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PE5 C 301:**

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

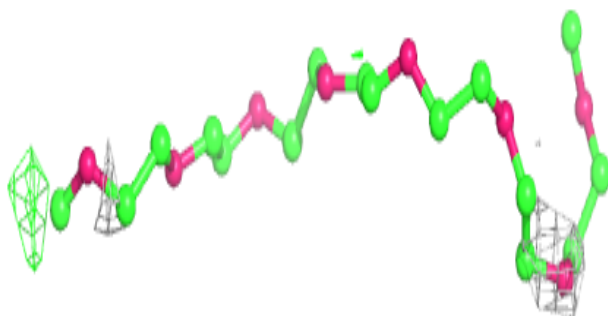
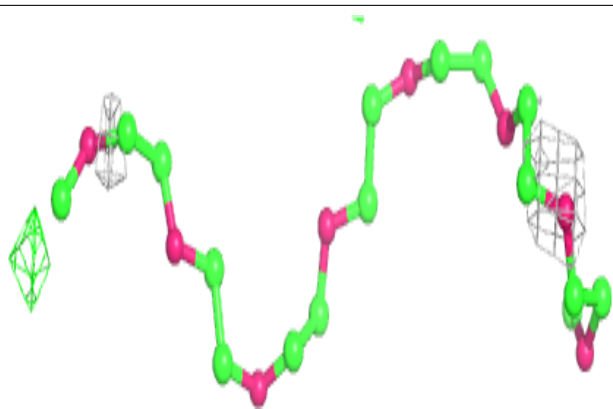
**Electron density around PE5 A 302:**

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

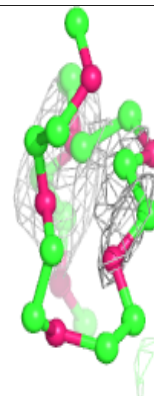
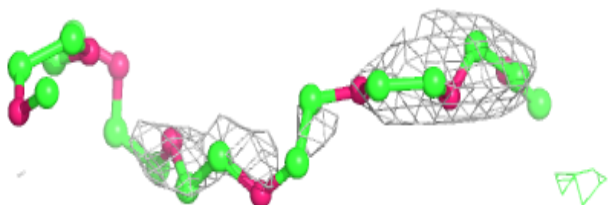
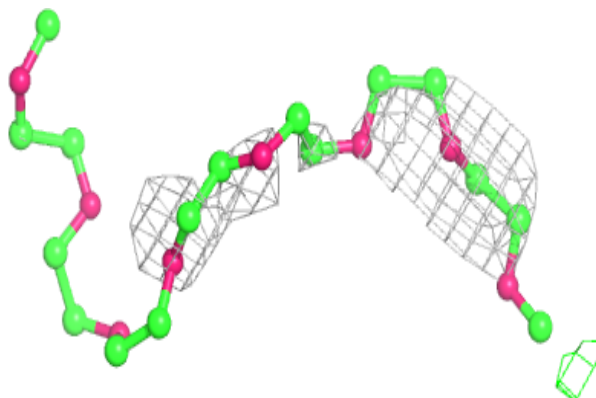


**Electron density around PE5 A 301:**

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

**Electron density around PE5 C 302:**

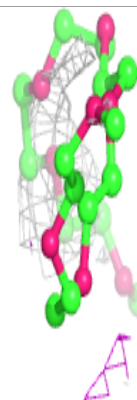
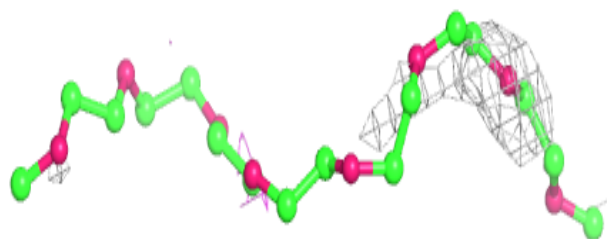
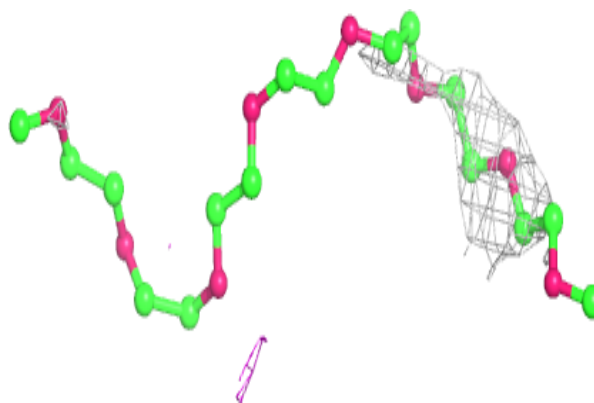
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



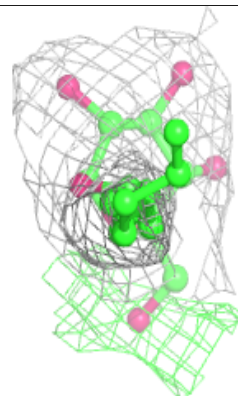
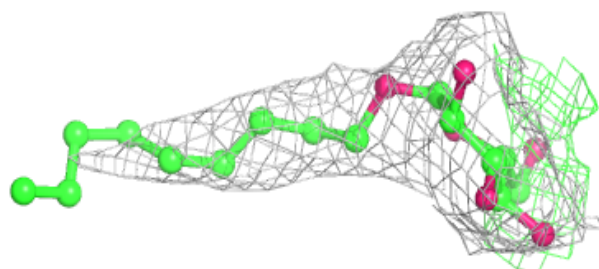
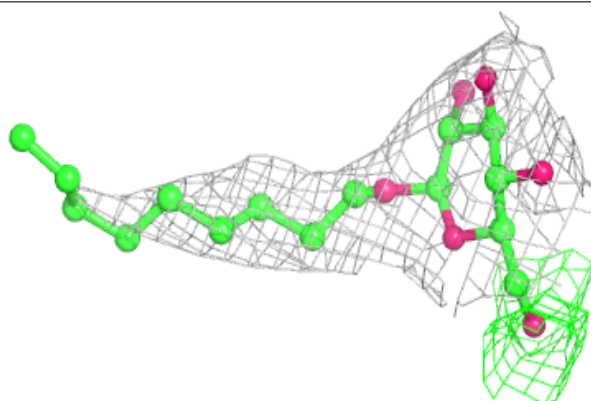


**Electron density around PE5 B 302:**

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

**Electron density around BNG B 301:**

$2mF_o-DF_c$  (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.