



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:08 pm BST

PDB ID : 6A2S  
Title : Mycobacterium tuberculosis LexA C-domain S160A  
Authors : Chandran, A.V.; Srikalaivani, R.; Paul, A.; Vijayan, M.  
Deposited on : 2018-06-12  
Resolution : 2.50 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

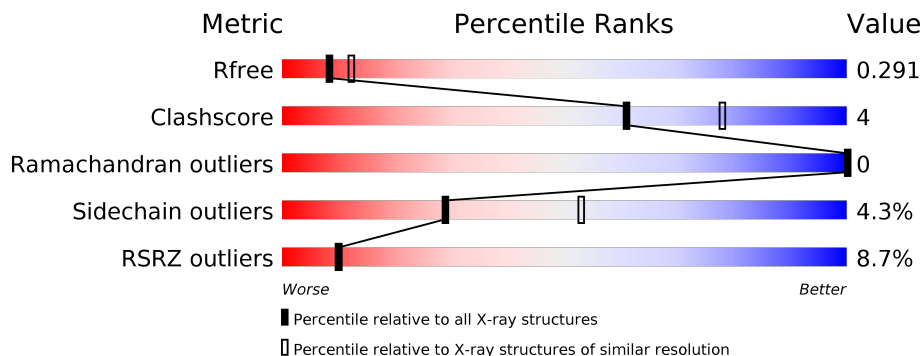
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	111	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">79% 11% 10%</p>
1	B	111	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">80% 10% 10%</p>
1	C	111	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">81% 9% 10%</p>
1	D	111	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">80% 10% 10%</p>
1	E	111	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">80% 10% 10%</p>
1	F	111	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 5px;">78% 11% 10%</p>

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Mol	Chain	Length	Quality of chain
1	G	111	23% 81% 8% • 10%
1	H	111	10% 80% 9% • 10%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6045 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 LexA repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	100	Total 739	C 476	N 125	O 133	S 5	0	0	0
1	B	100	Total 744	C 476	N 127	O 136	S 5	0	0	0
1	C	100	Total 746	C 479	N 125	O 137	S 5	0	0	0
1	D	100	Total 743	C 477	N 127	O 134	S 5	0	0	0
1	E	100	Total 731	C 467	N 127	O 133	S 4	0	0	0
1	F	100	Total 691	C 442	N 120	O 124	S 5	0	0	0
1	G	100	Total 677	C 426	N 121	O 126	S 4	0	0	0
1	H	100	Total 707	C 456	N 117	O 130	S 4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

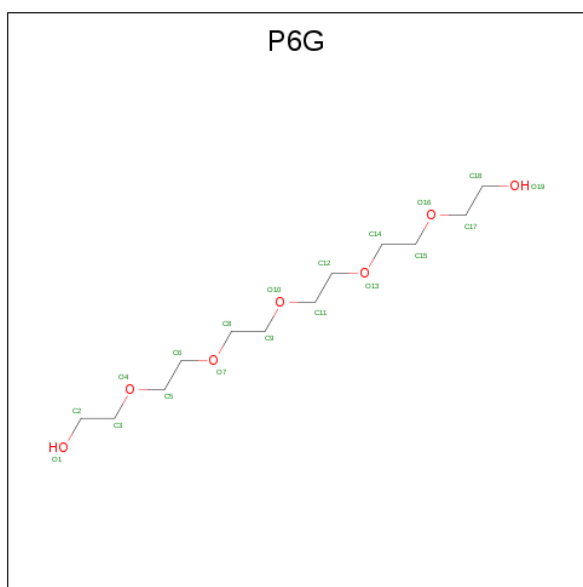
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ALA	SER	engineered mutation	UNP P9WHR7
B	160	ALA	SER	engineered mutation	UNP P9WHR7
C	160	ALA	SER	engineered mutation	UNP P9WHR7
D	160	ALA	SER	engineered mutation	UNP P9WHR7
E	160	ALA	SER	engineered mutation	UNP P9WHR7
F	160	ALA	SER	engineered mutation	UNP P9WHR7
G	160	ALA	SER	engineered mutation	UNP P9WHR7
H	160	ALA	SER	engineered mutation	UNP P9WHR7

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	A	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	E	1	Total C O 7 4 3	0	0
2	F	1	Total C O 7 4 3	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0

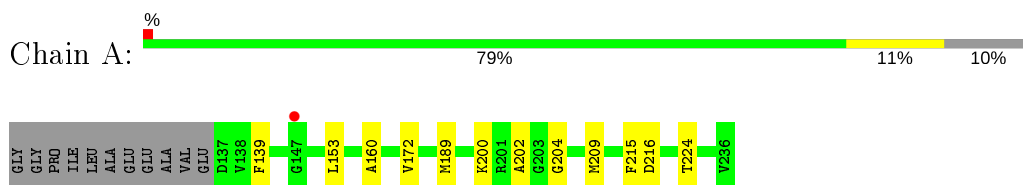
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	38	Total O 38 38	0	0
4	B	26	Total O 26 26	0	0
4	C	37	Total O 37 37	0	0
4	D	28	Total O 28 28	0	0
4	E	17	Total O 17 17	0	0
4	F	8	Total O 8 8	0	0
4	G	6	Total O 6 6	0	0
4	H	13	Total O 13 13	0	0

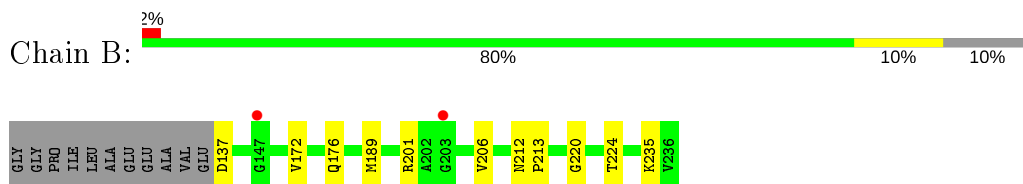
### 3 Residue-property plots [\(i\)](#)

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.

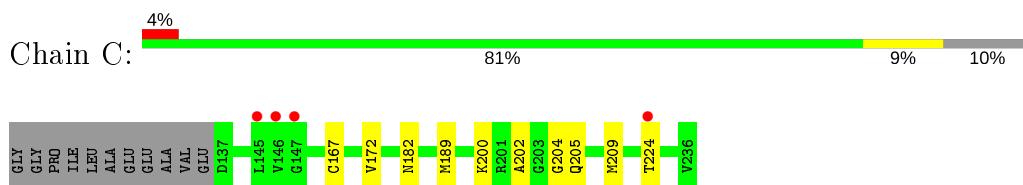
- Molecule 1: LexA repressor



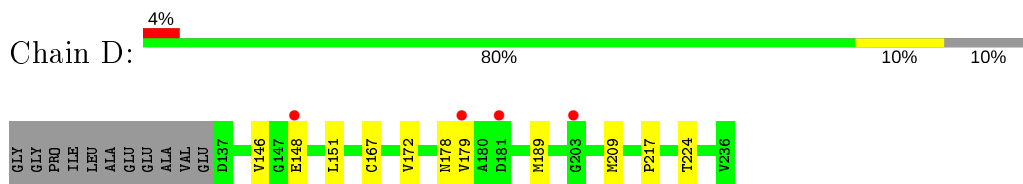
- Molecule 1: LexA repressor



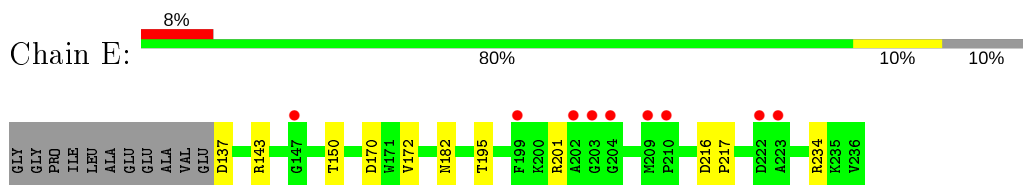
- Molecule 1: LexA repressor



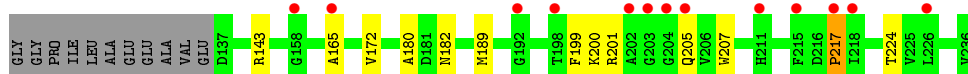
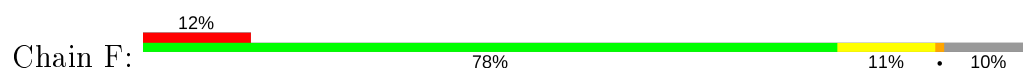
- Molecule 1: LexA repressor



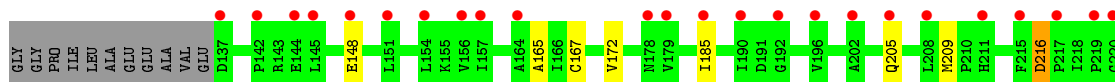
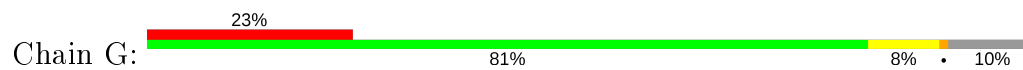
- Molecule 1: LexA repressor



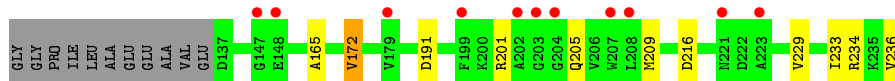
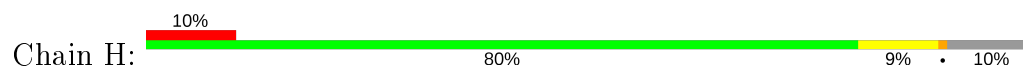
- Molecule 1: LexA repressor



• Molecule 1: LexA repressor



• Molecule 1: LexA repressor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.61Å 104.20Å 88.10Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	66.16 – 2.50 66.08 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.16-2.50) 100.0 (66.08-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.241 , 0.290 0.243 , 0.291	Depositor DCC
$R_{free}$ test set	1709 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtrriage
Anisotropy	0.713	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: CME, PEG, P6G

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	0.50	0/742	0.68	0/1012
1	B	0.45	0/747	0.67	0/1017
1	C	0.51	0/749	0.72	0/1021
1	D	0.42	0/745	0.64	0/1014
1	E	0.40	0/733	0.61	0/997
1	F	0.38	0/692	0.65	0/945
1	G	0.41	0/675	0.65	0/914
1	H	0.41	0/710	0.60	0/971
All	All	0.44	0/5793	0.66	0/7891

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	739	0	747	6	0
1	B	744	0	745	4	0
1	C	746	0	753	7	0
1	D	743	0	750	9	0
1	E	731	0	723	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	691	0	656	9	0
1	G	677	0	617	10	0
1	H	707	0	673	11	0
2	A	14	0	20	0	0
2	B	14	0	20	1	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
2	E	7	0	10	0	0
2	F	7	0	10	0	0
3	A	19	0	26	3	0
3	C	19	0	26	0	0
4	A	38	0	0	1	0
4	B	26	0	0	0	0
4	C	37	0	0	1	0
4	D	28	0	0	0	0
4	E	17	0	0	1	0
4	F	8	0	0	0	0
4	G	6	0	0	0	0
4	H	13	0	0	0	0
All	All	6045	0	5796	52	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 (52) 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:G:185:ILE:HB	1:H:236:VAL:HG11	1.51	0.92
1:H:201:ARG:HA	1:H:205:GLN:O	1.88	0.72
1:G:165:ALA:O	1:H:234:ARG:NH1	2.22	0.72
1:F:217:PRO:HB2	1:G:209:MET:HE1	1.74	0.70
1:E:170:ASP:OD1	1:E:234:ARG:HD3	1.91	0.69
1:D:146:VAL:HG11	1:D:151:LEU:HG	1.74	0.69
1:C:189:MET:HB3	1:C:224:THR:OG1	1.97	0.64
1:A:189:MET:HB3	1:A:224:THR:OG1	1.98	0.64
1:A:204:GLY:HA3	4:A:404:HOH:O	2.03	0.58
1:E:217:PRO:HG3	1:H:209:MET:HE1	1.86	0.58
1:D:146:VAL:HG11	1:D:151:LEU:CD1	2.35	0.57
1:E:182:ASN:OD1	1:E:201:ARG:N	2.35	0.57
1:H:201:ARG:CA	1:H:205:GLN:O	2.52	0.56
1:D:146:VAL:HG11	1:D:151:LEU:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ASN:ND2	1:F:200:LYS:O	2.38	0.55
1:F:189:MET:HB3	1:F:224:THR:OG1	2.07	0.54
1:A:160:ALA:HB2	1:A:215:PHE:CE2	2.44	0.53
1:G:167:CME:CE	1:H:165:ALA:HB2	2.39	0.53
1:B:176:GLN:NE2	2:B:302:PEG:O1	2.43	0.52
1:C:182:ASN:OD1	1:C:200:LYS:HA	2.10	0.51
1:C:204:GLY:HA3	4:C:410:HOH:O	2.09	0.51
1:C:200:LYS:HG3	1:C:209:MET:HG3	1.93	0.51
1:G:232:VAL:O	1:H:233:ILE:HA	2.12	0.50
3:A:303:P6G:C18	1:C:167:CME:HE3	2.42	0.49
1:B:212:ASN:OD1	1:B:213:PRO:HD2	2.12	0.49
1:F:201:ARG:HA	1:F:205:GLN:O	2.13	0.49
1:B:189:MET:HB3	1:B:224:THR:OG1	2.13	0.48
1:D:146:VAL:CG1	1:D:151:LEU:CD1	2.91	0.48
1:F:180:ALA:HB3	1:F:199:PHE:CD1	2.49	0.48
1:D:178:ASN:N	1:D:178:ASN:OD1	2.46	0.48
1:G:232:VAL:HB	1:H:234:ARG:HB3	1.95	0.48
1:A:200:LYS:HG3	1:A:209:MET:HG3	1.95	0.47
1:D:189:MET:HB3	1:D:224:THR:OG1	2.15	0.46
1:F:180:ALA:HB3	1:F:199:PHE:CE1	2.51	0.46
1:B:206:VAL:O	1:B:220:GLY:N	2.44	0.46
1:F:217:PRO:HB2	1:G:209:MET:CE	2.43	0.46
1:D:146:VAL:HG12	1:D:148:GLU:H	1.81	0.46
1:E:234:ARG:HH22	1:F:165:ALA:C	2.20	0.45
1:G:185:ILE:HB	1:H:236:VAL:CG1	2.35	0.45
1:F:200:LYS:CB	1:F:207:TRP:H	2.30	0.44
1:G:216:ASP:OD1	1:G:216:ASP:N	2.51	0.44
1:E:143:ARG:HD3	1:E:150:THR:OG1	2.18	0.43
1:A:202:ALA:O	1:A:204:GLY:N	2.52	0.42
1:A:139:PHE:HB2	1:A:153:LEU:HB2	2.02	0.42
3:A:303:P6G:H182	1:C:167:CME:HE3	2.01	0.42
1:G:185:ILE:CB	1:H:236:VAL:HG11	2.37	0.42
1:C:202:ALA:O	1:C:204:GLY:N	2.52	0.42
1:D:209:MET:SD	1:D:217:PRO:HB3	2.60	0.41
1:H:172:VAL:HG21	1:H:229:VAL:HG22	2.02	0.41
1:E:195:THR:HG22	4:E:417:HOH:O	2.21	0.41
1:E:170:ASP:OD1	1:E:234:ARG:CD	2.63	0.40
3:A:303:P6G:H141	1:D:167:CME:HE3	2.03	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	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	B	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	C	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
1	D	97/111 (87%)	93 (96%)	4 (4%)	0	100	100
1	E	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
1	F	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
1	G	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
1	H	97/111 (87%)	92 (95%)	5 (5%)	0	100	100
All	All	776/888 (87%)	730 (94%)	46 (6%)	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	75/86 (87%)	73 (97%)	2 (3%)	44	71
1	B	75/86 (87%)	71 (95%)	4 (5%)	22	43
1	C	77/86 (90%)	75 (97%)	2 (3%)	46	72
1	D	75/86 (87%)	73 (97%)	2 (3%)	44	71
1	E	72/86 (84%)	69 (96%)	3 (4%)	30	54
1	F	62/86 (72%)	59 (95%)	3 (5%)	25	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	59/86 (69%)	54 (92%)	5 (8%)	10	21
1	H	65/86 (76%)	62 (95%)	3 (5%)	27	50
All	All	560/688 (81%)	536 (96%)	24 (4%)	29	53

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	216	ASP
1	B	137	ASP
1	B	172	VAL
1	B	201	ARG
1	B	235	LYS
1	C	172	VAL
1	C	205	GLN
1	D	172	VAL
1	D	179	VAL
1	E	137	ASP
1	E	172	VAL
1	E	216	ASP
1	F	143	ARG
1	F	172	VAL
1	F	217	PRO
1	G	148	GLU
1	G	172	VAL
1	G	205	GLN
1	G	216	ASP
1	G	235	LYS
1	H	172	VAL
1	H	191	ASP
1	H	216	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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
1	CME	B	167	1	8,9,10	1.02	1 (12%)	5,9,11	1.53	1 (20%)
1	CME	D	167	1	8,9,10	0.92	0	5,9,11	1.55	1 (20%)
1	CME	G	167	1	8,9,10	0.79	0	5,9,11	1.33	1 (20%)
1	CME	E	167	1	8,9,10	0.88	0	5,9,11	1.08	0
1	CME	C	167	1	8,9,10	0.65	0	5,9,11	1.79	1 (20%)
1	CME	F	167	1	8,9,10	0.79	0	5,9,11	1.29	1 (20%)
1	CME	A	167	1	8,9,10	0.74	0	5,9,11	1.79	1 (20%)
1	CME	H	167	1	8,9,10	0.88	0	5,9,11	1.02	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
1	CME	B	167	1	-	3/5/8/10	-
1	CME	D	167	1	-	3/5/8/10	-
1	CME	G	167	1	-	3/5/8/10	-
1	CME	E	167	1	-	2/5/8/10	-
1	CME	C	167	1	-	3/5/8/10	-
1	CME	F	167	1	-	3/5/8/10	-
1	CME	A	167	1	-	3/5/8/10	-
1	CME	H	167	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	CME	CB-SG	-2.23	1.74	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	CME	CB-SG-SD	-3.63	94.41	103.82
1	A	167	CME	CB-SG-SD	-3.59	94.51	103.82
1	D	167	CME	CB-SG-SD	-2.96	96.14	103.82
1	B	167	CME	CB-SG-SD	-2.55	97.20	103.82
1	G	167	CME	CB-SG-SD	-2.55	97.22	103.82
1	F	167	CME	CB-SG-SD	-2.46	97.44	103.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	167	CME	N-CA-CB-SG
1	B	167	CME	SD-CE-CZ-OH
1	D	167	CME	N-CA-CB-SG
1	D	167	CME	SD-CE-CZ-OH
1	G	167	CME	N-CA-CB-SG
1	G	167	CME	SD-CE-CZ-OH
1	E	167	CME	N-CA-CB-SG
1	E	167	CME	SD-CE-CZ-OH
1	C	167	CME	N-CA-CB-SG
1	C	167	CME	SD-CE-CZ-OH
1	F	167	CME	N-CA-CB-SG
1	F	167	CME	SD-CE-CZ-OH
1	A	167	CME	N-CA-CB-SG
1	A	167	CME	SD-CE-CZ-OH
1	H	167	CME	N-CA-CB-SG
1	H	167	CME	SD-CE-CZ-OH
1	B	167	CME	CZ-CE-SD-SG
1	D	167	CME	CZ-CE-SD-SG
1	G	167	CME	CZ-CE-SD-SG
1	C	167	CME	CZ-CE-SD-SG
1	F	167	CME	CZ-CE-SD-SG
1	A	167	CME	CZ-CE-SD-SG
1	H	167	CME	CZ-CE-SD-SG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	167	CME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	167	CME	1	0
1	C	167	CME	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	PEG	B	301	-	6,6,6	0.50	0	5,5,5	0.30	0
2	PEG	D	301	-	6,6,6	0.59	0	5,5,5	0.34	0
2	PEG	B	302	-	6,6,6	0.43	0	5,5,5	0.31	0
2	PEG	A	302	-	6,6,6	0.80	0	5,5,5	0.69	0
2	PEG	E	301	-	6,6,6	0.53	0	5,5,5	0.24	0
3	P6G	A	303	-	18,18,18	0.56	0	17,17,17	0.47	0
2	PEG	A	301	-	6,6,6	0.50	0	5,5,5	0.20	0
2	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.39	0
3	P6G	C	302	-	18,18,18	0.58	0	17,17,17	0.39	0
2	PEG	F	301	-	6,6,6	0.49	0	5,5,5	0.21	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	PEG	B	301	-	-	3/4/4/4	-
2	PEG	D	301	-	-	3/4/4/4	-
2	PEG	B	302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	302	-	-	1/4/4/4	-
2	PEG	E	301	-	-	3/4/4/4	-
3	P6G	A	303	-	-	11/16/16/16	-
2	PEG	A	301	-	-	1/4/4/4	-
2	PEG	C	301	-	-	2/4/4/4	-
3	P6G	C	302	-	-	11/16/16/16	-
2	PEG	F	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	P6G	O13-C14-C15-O16
2	B	301	PEG	O1-C1-C2-O2
2	D	301	PEG	O2-C3-C4-O4
2	D	301	PEG	O1-C1-C2-O2
2	A	302	PEG	O2-C3-C4-O4
2	E	301	PEG	O1-C1-C2-O2
2	C	301	PEG	O1-C1-C2-O2
3	C	302	P6G	O1-C2-C3-O4
3	A	303	P6G	C8-C9-O10-C11
3	C	302	P6G	C14-C15-O16-C17
3	A	303	P6G	O1-C2-C3-O4
2	C	301	PEG	O2-C3-C4-O4
3	A	303	P6G	O7-C8-C9-O10
3	C	302	P6G	O4-C5-C6-O7
3	A	303	P6G	O4-C5-C6-O7
3	C	302	P6G	C18-C17-O16-C15
3	C	302	P6G	O10-C11-C12-O13
3	A	303	P6G	O16-C17-C18-O19
3	A	303	P6G	C12-C11-O10-C9
3	C	302	P6G	C15-C14-O13-C12
3	A	303	P6G	C2-C3-O4-C5
3	A	303	P6G	C15-C14-O13-C12
2	D	301	PEG	C1-C2-O2-C3
3	C	302	P6G	O16-C17-C18-O19
2	A	301	PEG	O1-C1-C2-O2
3	A	303	P6G	C18-C17-O16-C15

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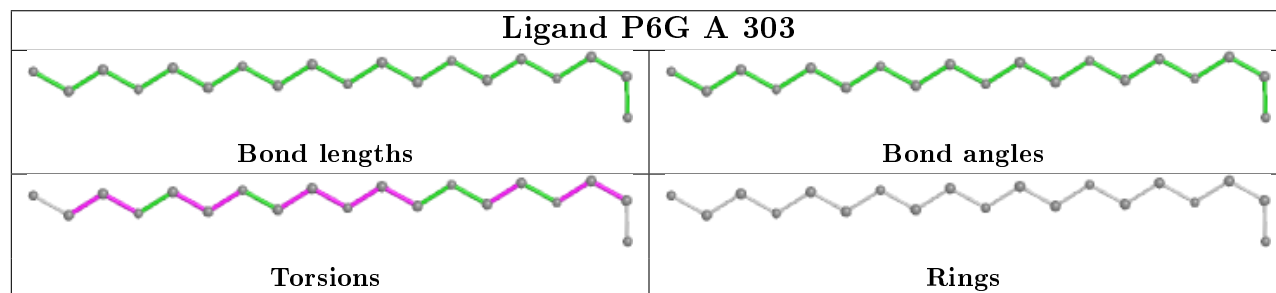
Mol	Chain	Res	Type	Atoms
2	E	301	PEG	C4-C3-O2-C2
3	A	303	P6G	O10-C11-C12-O13
3	C	302	P6G	C6-C5-O4-C3
2	F	301	PEG	C1-C2-O2-C3
2	B	301	PEG	C1-C2-O2-C3
2	E	301	PEG	C1-C2-O2-C3
3	C	302	P6G	O13-C14-C15-O16
2	F	301	PEG	O1-C1-C2-O2
3	C	302	P6G	C5-C6-O7-C8
3	C	302	P6G	C2-C3-O4-C5
2	B	301	PEG	C4-C3-O2-C2

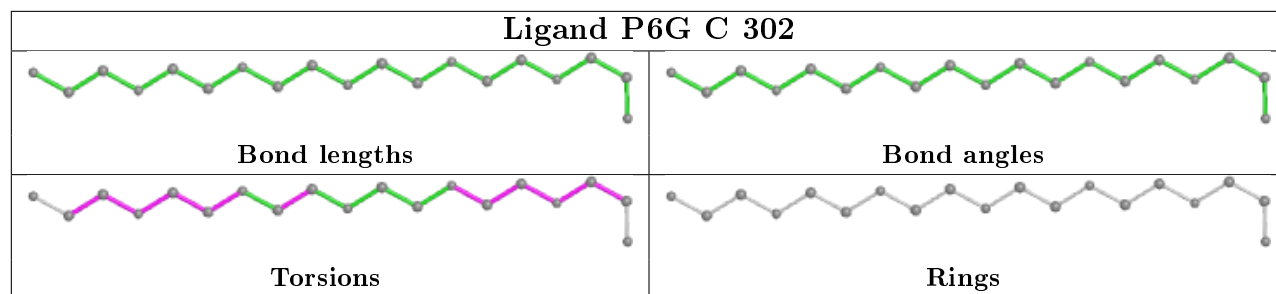
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	PEG	1	0
3	A	303	P6G	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

### 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	99/111 (89%)	0.40	1 (1%) 82 84	28, 40, 73, 114	0
1	B	99/111 (89%)	0.60	2 (2%) 65 68	27, 48, 92, 119	0
1	C	99/111 (89%)	0.32	4 (4%) 38 41	26, 39, 78, 110	0
1	D	99/111 (89%)	0.60	4 (4%) 38 41	28, 48, 91, 126	0
1	E	99/111 (89%)	0.74	9 (9%) 9 9	42, 65, 109, 116	0
1	F	99/111 (89%)	1.11	13 (13%) 3 3	42, 79, 113, 140	0
1	G	99/111 (89%)	1.44	25 (25%) 0 0	46, 79, 110, 132	0
1	H	99/111 (89%)	0.99	11 (11%) 5 5	44, 72, 119, 134	0
All	All	792/888 (89%)	0.78	69 (8%) 10 10	26, 60, 109, 140	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	204	GLY	6.9
1	F	202	ALA	5.9
1	E	147	GLY	5.7
1	H	147	GLY	5.6
1	B	203	GLY	5.1
1	H	223	ALA	5.0
1	G	202	ALA	4.8
1	F	203	GLY	4.8
1	H	207	TRP	4.7
1	H	202	ALA	4.1
1	G	215	PHE	4.1
1	G	217	PRO	4.0
1	G	223	ALA	4.0
1	G	145	LEU	3.9
1	G	190	ILE	3.8
1	G	208	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	178	ASN	3.6
1	H	204	GLY	3.6
1	H	179	VAL	3.6
1	E	223	ALA	3.3
1	H	148	GLU	3.3
1	G	196	VAL	3.3
1	H	203	GLY	3.3
1	E	204	GLY	3.2
1	E	210	PRO	3.2
1	E	222	ASP	3.2
1	G	157	ILE	3.1
1	G	156	VAL	3.1
1	G	219	PRO	3.0
1	E	202	ALA	3.0
1	F	192	GLY	3.0
1	H	199	PHE	3.0
1	E	199	PHE	2.9
1	G	164	ALA	2.9
1	F	158	GLY	2.9
1	H	208	LEU	2.8
1	F	218	ILE	2.8
1	H	221	ASN	2.7
1	G	220	GLY	2.7
1	F	198	THR	2.7
1	D	203	GLY	2.6
1	F	217	PRO	2.6
1	G	185	ILE	2.6
1	C	146	VAL	2.5
1	A	147	GLY	2.5
1	C	224	THR	2.5
1	D	181	ASP	2.5
1	G	144	GLU	2.5
1	G	192	GLY	2.4
1	G	137	ASP	2.4
1	B	147	GLY	2.4
1	G	205	GLN	2.3
1	G	148	GLU	2.2
1	C	147	GLY	2.2
1	E	209	MET	2.2
1	E	203	GLY	2.2
1	G	142	PRO	2.1
1	D	148	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	215	PHE	2.1
1	G	154	LEU	2.1
1	D	179	VAL	2.1
1	F	226	LEU	2.1
1	F	205	GLN	2.1
1	F	211	HIS	2.1
1	G	179	VAL	2.0
1	C	145	LEU	2.0
1	G	211	HIS	2.0
1	F	165	ALA	2.0
1	G	151	LEU	2.0

## 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, 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
1	CME	G	167	10/11	0.83	0.24	66,73,89,105	0
1	CME	F	167	10/11	0.93	0.24	52,64,105,109	0
1	CME	H	167	10/11	0.93	0.18	61,66,108,109	0
1	CME	B	167	10/11	0.95	0.19	34,39,74,84	0
1	CME	C	167	10/11	0.95	0.21	35,46,77,83	0
1	CME	A	167	10/11	0.96	0.20	30,37,69,80	0
1	CME	E	167	10/11	0.96	0.16	52,57,84,92	0
1	CME	D	167	10/11	0.97	0.21	33,37,70,76	0

## 6.3 Carbohydrates [i](#)

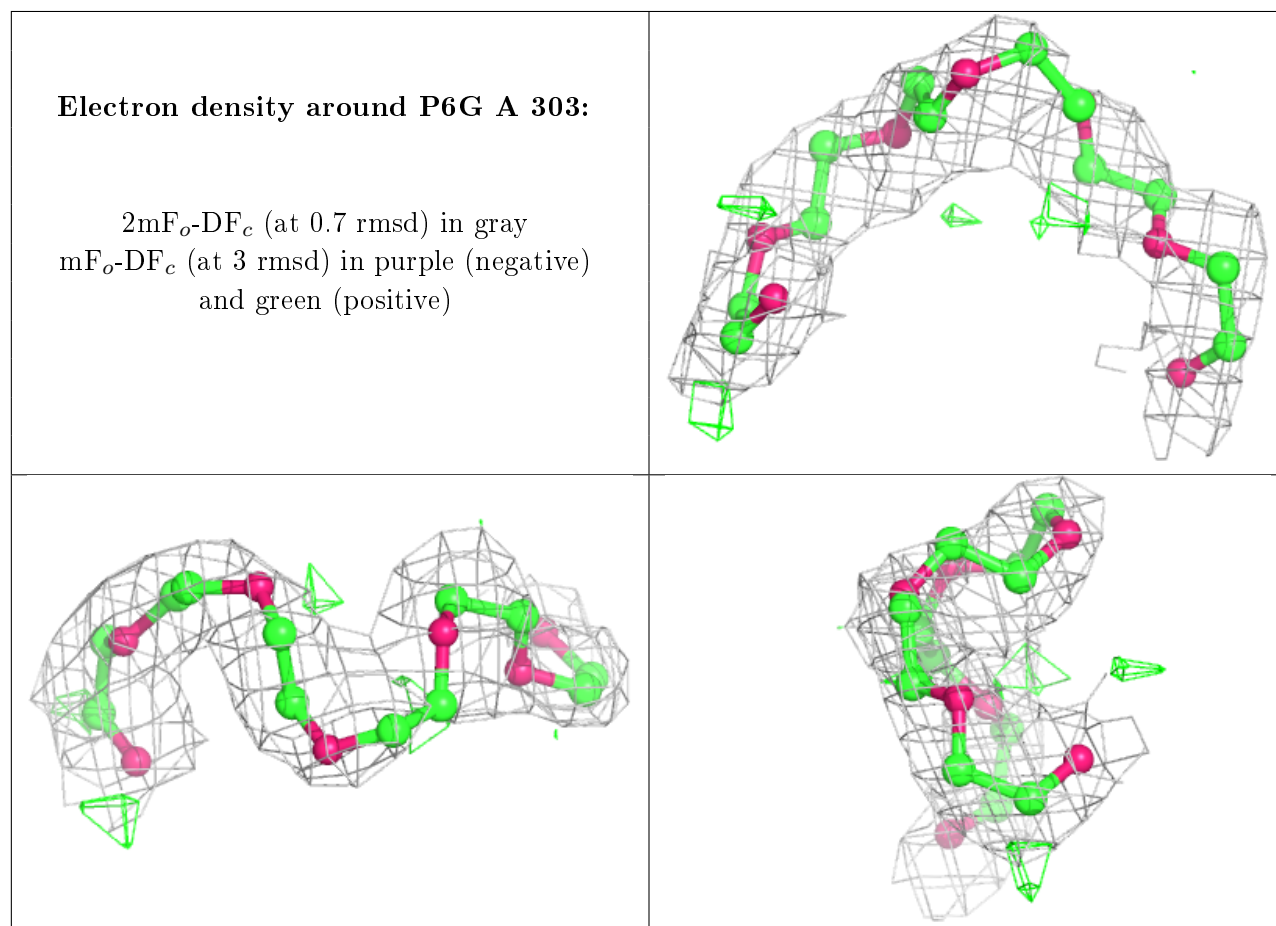
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

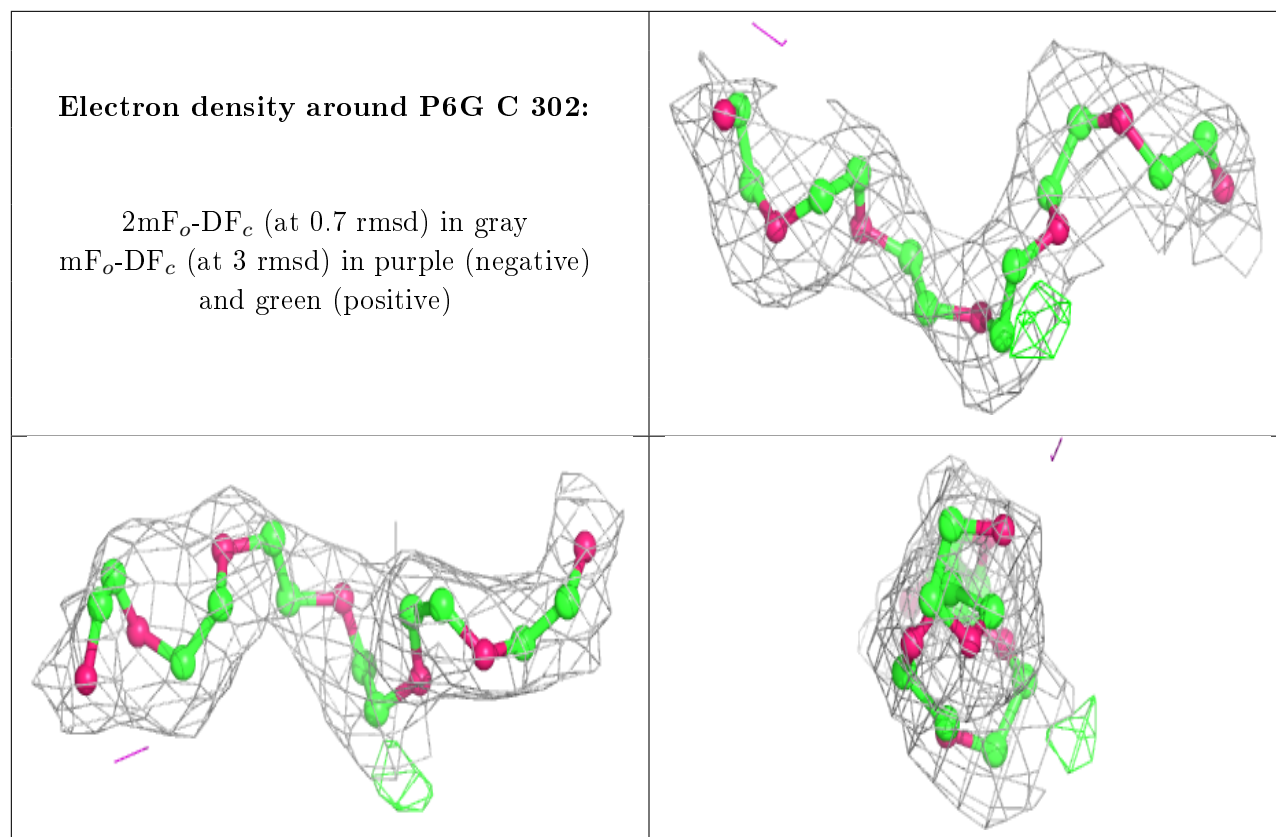
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	D	301	7/7	0.69	0.33	74,84,90,91	0
2	PEG	F	301	7/7	0.75	0.26	95,97,102,105	0
2	PEG	C	301	7/7	0.79	0.23	65,69,74,74	0
2	PEG	B	301	7/7	0.80	0.21	81,86,91,91	0
3	P6G	A	303	19/19	0.81	0.25	68,91,101,106	0
2	PEG	E	301	7/7	0.82	0.23	72,78,85,86	0
3	P6G	C	302	19/19	0.82	0.16	79,88,95,98	0
2	PEG	A	302	7/7	0.82	0.25	36,47,59,59	0
2	PEG	B	302	7/7	0.87	0.20	76,84,90,92	0
2	PEG	A	301	7/7	0.91	0.22	59,63,72,73	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.