



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2021 – 08:08 PM JST

PDB ID : 7CZC
Title : Crystal structure of apo-FabG from *Vibrio harveyi*
Authors : Singh, B.K.; Kumar, A.; Paul, B.; Biswas, R.; Das, A.K.
Deposited on : 2020-09-08
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

i

X-RAY DIFFRACTION

A.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	<div> <div></div> <div>3%</div> <div>88%</div> <div>8%</div> <div></div> </div>
1	B	241	<div> <div></div> <div>6%</div> <div>93%</div> <div>7%</div> <div></div> </div>
1	C	241	<div> <div></div> <div>12%</div> <div>89%</div> <div>10%</div> <div></div> </div>
1	D	241	<div> <div></div> <div>5%</div> <div>94%</div> <div>5%</div> <div></div> </div>

2 Entry composition [i](#)

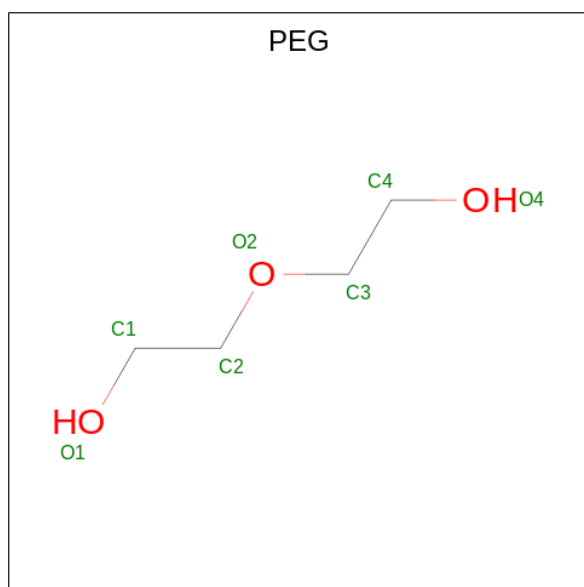
There are 3 unique types of molecules in this entry. The entry contains 14607 atoms, of which 7119 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-ACP reductase FabG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	H	N	O	S	0	0	0
			3476	1079	1746	311	329	11			
1	B	241	Total	C	H	N	O	S	0	0	0
			3592	1119	1797	324	341	11			
1	C	240	Total	C	H	N	O	S	0	0	0
			3516	1101	1748	320	337	10			
1	D	239	Total	C	H	N	O	S	0	0	0
			3605	1121	1808	324	340	12			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		

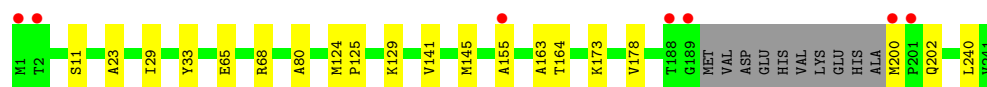
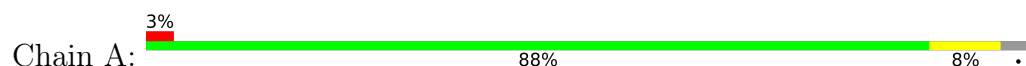
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total 104	O 104	0	0
3	B	90	Total 90	O 90	0	0
3	C	85	Total 85	O 85	0	0
3	D	105	Total 105	O 105	0	0

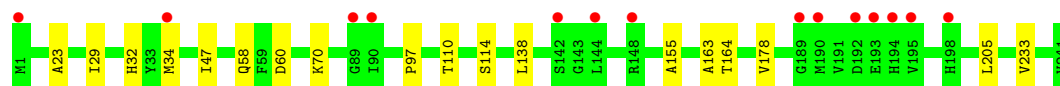
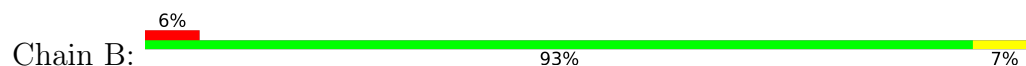
3 Residue-property plots [i](#)

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.

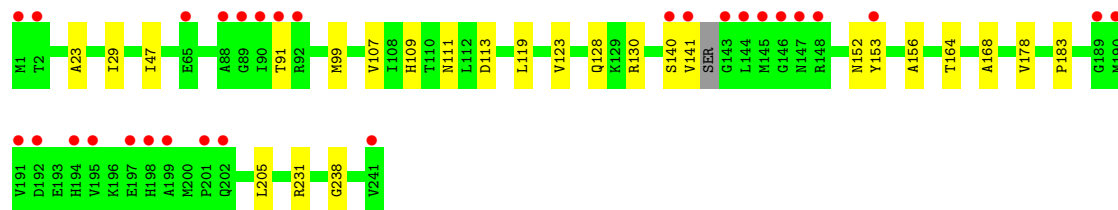
- Molecule 1: 3-oxoacyl-ACP reductase FabG



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.46Å 91.32Å 94.16Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	19.75 – 2.00 19.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.75-2.00) 98.5 (19.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.209 , 0.233 0.209 , 0.233	Depositor DCC
R_{free} test set	3161 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14607	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG

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	0.35	0/1754	0.53	0/2370
1	B	0.33	0/1821	0.53	0/2463
1	C	0.33	0/1792	0.52	0/2425
1	D	0.33	0/1823	0.52	0/2463
All	All	0.33	0/7190	0.52	0/9721

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

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	1730	1746	1745	13	0
1	B	1795	1797	1796	12	0
1	C	1768	1748	1747	17	0
1	D	1797	1808	1806	8	0
2	A	14	20	20	2	0
3	A	104	0	0	0	0
3	B	90	0	0	0	0
3	C	85	0	0	0	0
3	D	105	0	0	0	0
All	All	7488	7119	7114	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:VAL:HG13	1:C:183:PRO:O	2.01	0.60
1:C:140:SER:O	1:C:141:VAL:HG23	2.02	0.58
1:C:99:MET:HE1	1:C:152:ASN:HB3	1.87	0.57
1:D:148:ARG:HG2	1:D:148:ARG:O	2.05	0.56
1:D:164:THR:HG23	1:D:178:VAL:HG12	1.89	0.54
1:C:91:THR:HG22	1:C:153:TYR:CD1	2.43	0.54
1:C:141:VAL:HG12	1:C:141:VAL:O	2.07	0.54
1:B:23:ALA:HB1	1:B:47:ILE:HG23	1.89	0.53
1:A:23:ALA:HB2	1:A:29:ILE:HG13	1.92	0.52
1:A:141:VAL:HG22	1:A:145:MET:HE2	1.90	0.51
1:A:164:THR:HG23	1:A:178:VAL:HG12	1.93	0.51
1:C:109:HIS:O	1:C:113:ASP:HB2	2.11	0.50
1:C:128:GLN:O	1:C:130:ARG:NH1	2.45	0.50
1:C:205:LEU:HD12	1:C:238:GLY:HA2	1.94	0.50
1:A:202:GLN:HG3	1:A:240:LEU:HD21	1.94	0.49
1:B:58:GLN:O	1:B:70:LYS:HE3	2.12	0.49
1:B:205:LEU:HD23	1:D:172:ALA:HB1	1.93	0.48
1:B:34:MET:HG3	1:B:60:ASP:HA	1.95	0.47
1:A:11:SER:OG	2:A:301:PEG:H21	2.14	0.47
1:C:23:ALA:HB1	1:C:47:ILE:HG23	1.97	0.47
1:C:107:VAL:HG22	1:C:153:TYR:CE1	2.50	0.46
1:B:23:ALA:HB2	1:B:29:ILE:HG13	1.98	0.46
1:D:141:VAL:O	1:D:141:VAL:HG13	2.15	0.46
1:A:23:ALA:N	1:A:29:ILE:HD11	2.30	0.45
1:D:88:ALA:HB2	1:D:138:LEU:O	2.17	0.45
1:B:110:THR:O	1:B:114:SER:HB3	2.16	0.45
1:A:155:ALA:HB2	1:B:163:ALA:HB2	1.98	0.45
1:A:65:GLU:HG2	1:A:68:ARG:NH2	2.32	0.44
1:C:23:ALA:HB2	1:C:29:ILE:HG13	1.99	0.44
1:C:91:THR:HA	1:C:153:TYR:CE1	2.52	0.44
1:A:124:MET:HG3	1:B:97:PRO:HB3	1.98	0.43
1:D:23:ALA:HB1	1:D:47:ILE:HG23	2.01	0.43
1:C:119:LEU:O	1:C:123:VAL:HG23	2.19	0.42
1:A:125:PRO:O	1:A:129:LYS:HE2	2.18	0.42
1:C:111:ASN:HB2	1:C:156:ALA:HB1	2.02	0.42
1:A:80:ALA:HB2	1:A:129:LYS:HE2	2.00	0.42
1:D:83:GLY:HA2	1:D:134:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:HA	1:D:32:HIS:HB3	2.00	0.42
1:A:33:TYR:OH	2:A:302:PEG:H42	2.20	0.41
1:B:233:VAL:O	1:B:233:VAL:HG13	2.21	0.41
1:C:168:ALA:HB2	1:C:178:VAL:HB	2.01	0.41
1:B:23:ALA:N	1:B:29:ILE:HD11	2.36	0.41
1:C:164:THR:HG23	1:C:178:VAL:HG12	2.03	0.41
1:A:163:ALA:HB2	1:B:155:ALA:HB2	2.03	0.41
1:B:164:THR:HG23	1:B:178:VAL:HG12	2.03	0.40
1:C:231:ARG:HG2	1:C:231:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/241 (94%)	222 (98%)	5 (2%)	0	100	100
1	B	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
1	C	236/241 (98%)	234 (99%)	2 (1%)	0	100	100
1	D	235/241 (98%)	230 (98%)	5 (2%)	0	100	100
All	All	937/964 (97%)	917 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/192 (95%)	180 (99%)	2 (1%)	73	78
1	B	186/192 (97%)	184 (99%)	2 (1%)	73	78
1	C	179/192 (93%)	179 (100%)	0	100	100
1	D	189/192 (98%)	189 (100%)	0	100	100
All	All	736/768 (96%)	732 (100%)	4 (0%)	88	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
1	A	200	MET
1	B	32	HIS
1	B	138	LEU

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

Mol	Chain	Res	Type
1	B	42	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	A	302	-	6,6,6	0.99	0	5,5,5	0.26	0
2	PEG	A	301	-	6,6,6	0.91	0	5,5,5	0.39	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	A	302	-	-	1/4/4/4	-
2	PEG	A	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PEG	O2-C3-C4-O4
2	A	302	PEG	C4-C3-O2-C2
2	A	301	PEG	C1-C2-O2-C3
2	A	301	PEG	O1-C1-C2-O2

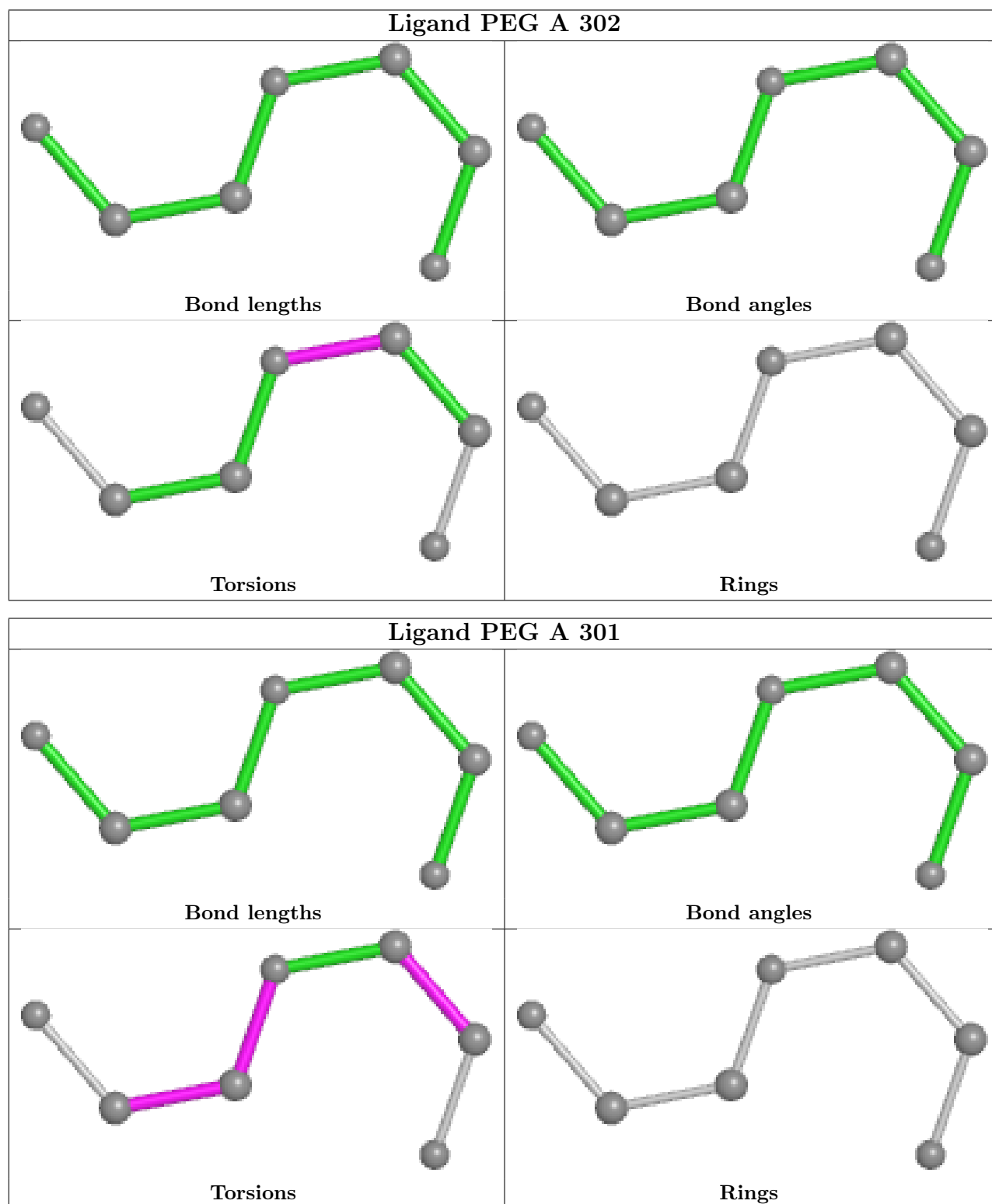
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	PEG	1	0
2	A	301	PEG	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	231/241 (95%)	0.00	7 (3%)	50	49	18, 23, 36, 71	0
1	B	241/241 (100%)	0.14	14 (5%)	23	22	18, 26, 54, 89	0
1	C	240/241 (99%)	0.34	29 (12%)	4	3	17, 27, 65, 78	0
1	D	239/241 (99%)	0.09	11 (4%)	32	31	17, 25, 55, 82	0
All	All	951/964 (98%)	0.15	61 (6%)	19	18	17, 25, 56, 89	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	ILE	6.2
1	D	146	GLY	6.0
1	A	1	MET	5.1
1	C	144	LEU	5.1
1	A	200	MET	5.0
1	A	201	PRO	4.9
1	A	189	GLY	4.7
1	B	198	HIS	4.5
1	B	190	MET	4.5
1	B	1	MET	4.1
1	C	1	MET	4.1
1	D	147	ASN	3.9
1	C	189	GLY	3.9
1	C	143	GLY	3.8
1	D	91	THR	3.8
1	C	91	THR	3.8
1	C	141	VAL	3.8
1	C	92	ARG	3.7
1	C	191	VAL	3.6
1	B	195	VAL	3.5
1	B	89	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	201	PRO	3.3
1	C	148	ARG	3.3
1	C	194	HIS	3.2
1	C	198	HIS	3.2
1	B	192	ASP	3.1
1	C	145	MET	3.1
1	C	192	ASP	3.0
1	C	89	GLY	3.0
1	D	92	ARG	3.0
1	D	145	MET	3.0
1	C	140	SER	3.0
1	C	195	VAL	2.9
1	C	190	MET	2.9
1	C	241	VAL	2.8
1	C	146	GLY	2.8
1	C	199	ALA	2.8
1	C	153	TYR	2.8
1	C	197	GLU	2.7
1	C	147	ASN	2.7
1	A	2	THR	2.7
1	D	90	ILE	2.6
1	D	190	MET	2.6
1	A	188	THR	2.6
1	B	189	GLY	2.5
1	C	2	THR	2.5
1	D	2	THR	2.5
1	D	148	ARG	2.4
1	B	193	GLU	2.4
1	B	148	ARG	2.4
1	C	202	GLN	2.3
1	C	88	ALA	2.3
1	D	198	HIS	2.2
1	A	155	ALA	2.1
1	C	65	GLU	2.1
1	D	109	HIS	2.1
1	B	142	SER	2.1
1	B	90	ILE	2.0
1	B	194	HIS	2.0
1	B	34	MET	2.0
1	B	144	LEU	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](#)

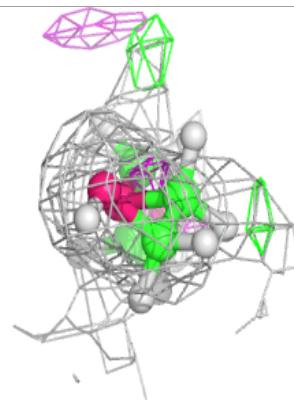
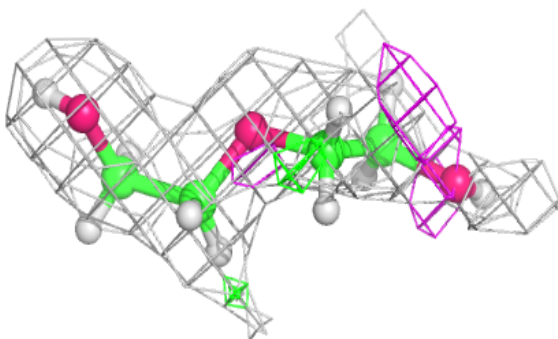
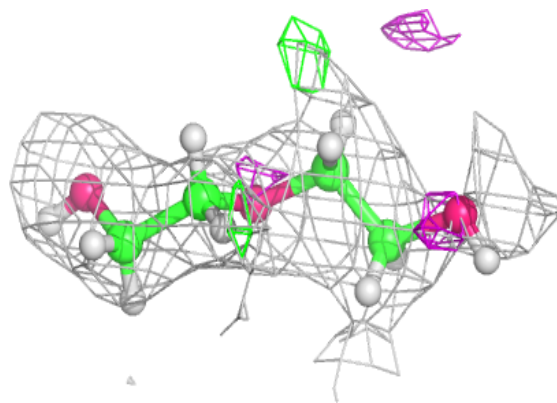
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	A	302	7/7	0.74	0.22	24,33,37,45	0
2	PEG	A	301	7/7	0.77	0.22	27,35,47,47	0

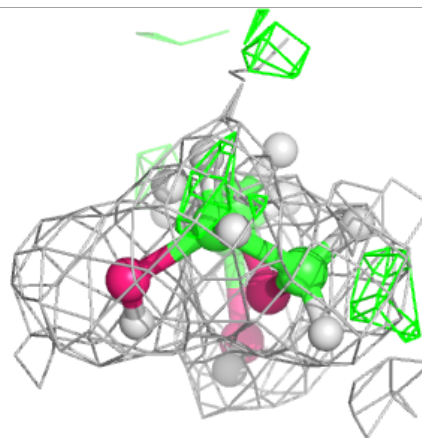
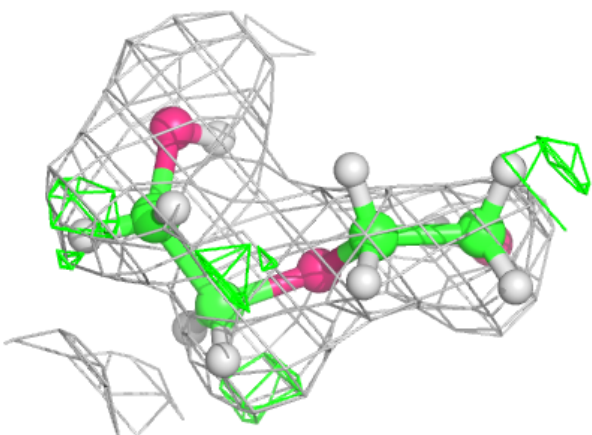
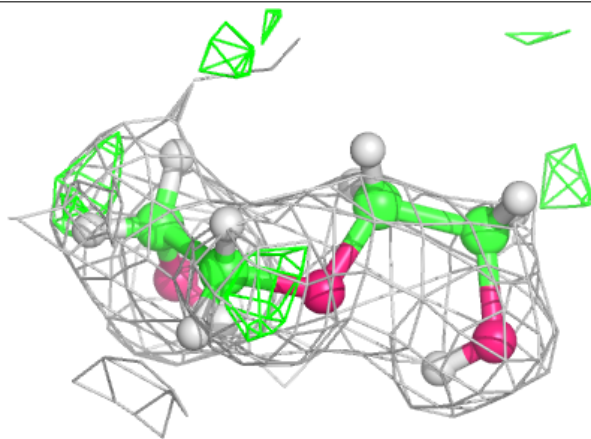
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEG 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 PEG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.