



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:25 PM UTC

PDB ID : 4KPT / pdb_00004kpt
Title : Crystal structure of substrate binding domain 1 (SBD1) OF ABC transporter GLNPQ from lactococcus lactis
Authors : Vujicic Zagar, A.; Guskov, A.; Schuurman-Wolters, G.K.; Slotboom, D.J.; Poolman, B.
Deposited on : 2013-05-14
Resolution : 1.40 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

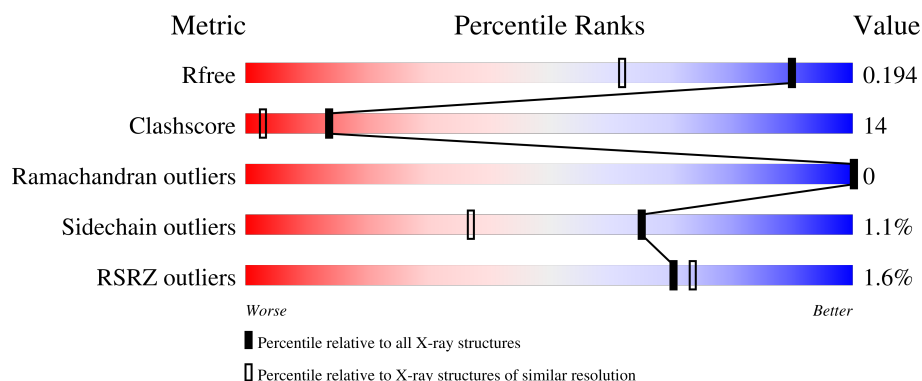
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	251	0% 77% 12% 11%
1	B	251	2% 76% 12% 11%

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
4	PG4	B	302	-	-	X	-
4	PG4	B	305	-	-	X	-
4	PG4	B	306	-	-	X	-
6	PEG	A	307	-	-	X	-
6	PEG	A	308	-	-	X	-
6	PEG	A	311	-	-	X	-
6	PEG	B	307	-	-	X	-

2 Entry composition [i](#)

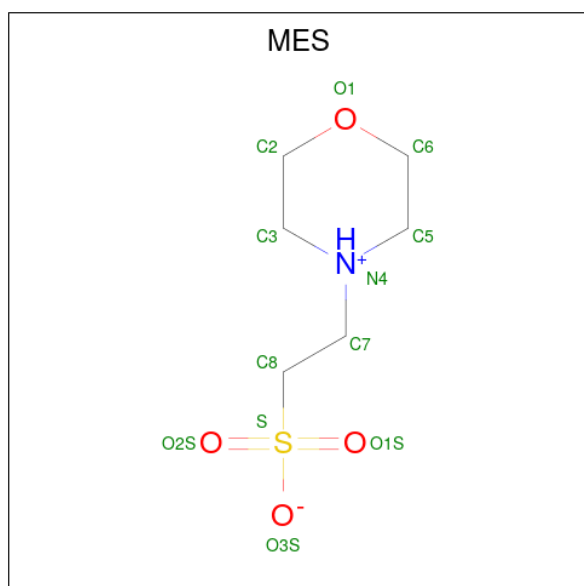
There are 7 unique types of molecules in this entry. The entry contains 4244 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine ABC transporter permease and substrate binding protein protein.

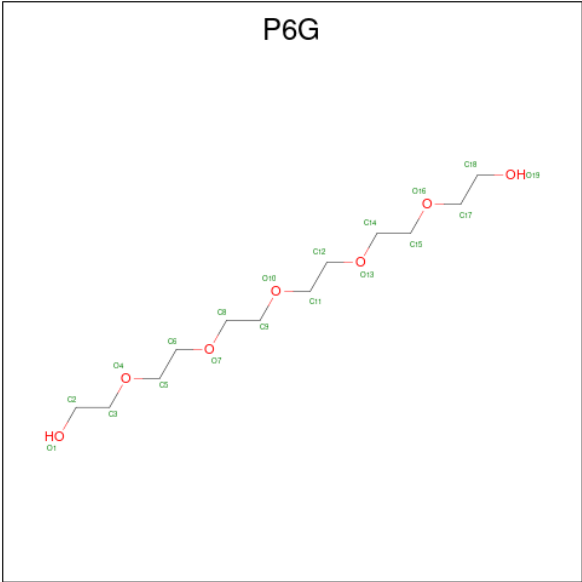
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	14	0
			1782	1136	281	355	10			
1	B	223	Total	C	N	O	S	0	7	0
			1738	1109	278	341	10			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



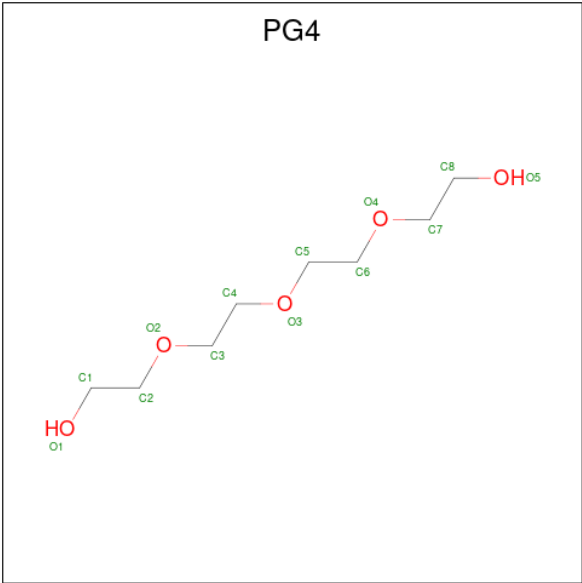
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



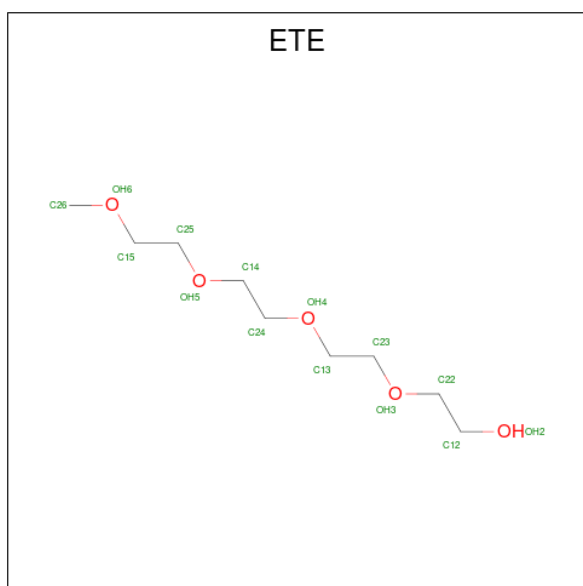
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is 2-{2-[2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

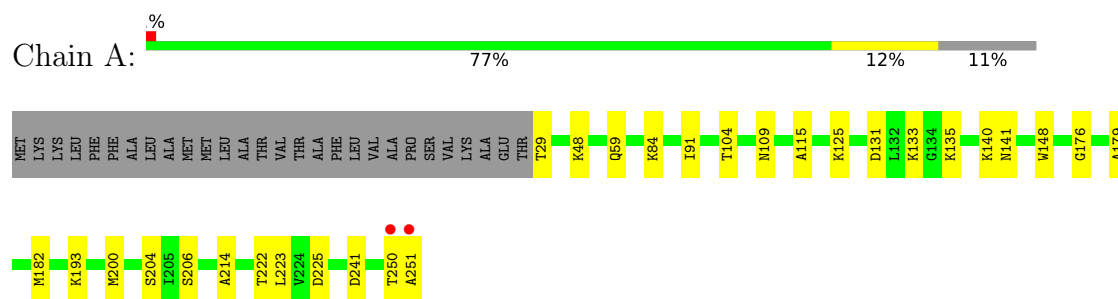
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	277	Total	O	0	7
			284	284		
7	B	240	Total	O	0	2
			242	242		

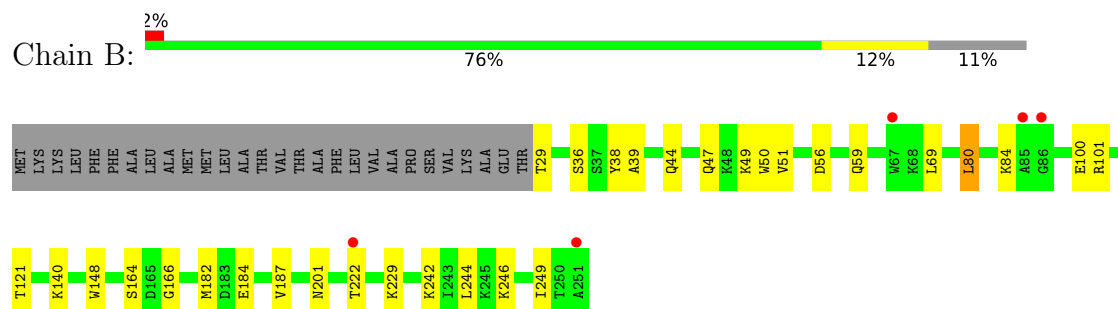
3 Residue-property plots

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: Glutamine ABC transporter permease and substrate binding protein protein



- Molecule 1: Glutamine ABC transporter permease and substrate binding protein protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.10Å 55.63Å 55.73Å 93.99° 89.71° 97.98°	Depositor
Resolution (Å)	17.94 – 1.40 17.94 – 1.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (17.94-1.40) 93.6 (17.94-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2)	Depositor
R, R_{free}	0.140 , 0.188 0.147 , 0.194	Depositor DCC
R_{free} test set	3857 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4244	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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, ETE, MES, PG4, 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	0.56	1/1848 (0.1%)	0.68	0/2489
1	B	0.52	0/1792	0.73	0/2410
All	All	0.54	1/3640 (0.0%)	0.71	0/4899

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	LYS	C-O	-5.57	1.17	1.23

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	1782	0	1781	43	2
1	B	1738	0	1742	48	1
2	A	12	0	13	0	0
2	B	12	0	12	0	0
3	A	38	0	52	12	0
4	A	26	0	36	7	0
4	B	33	0	44	45	0
5	A	14	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	42	0	60	19	1
6	B	21	0	30	13	0
7	A	284	0	0	12	0
7	B	242	0	0	5	1
All	All	4244	0	3790	109	3

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 14.

All (109) 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)
4:B:306:PG4:C5	6:B:307:PEG:H12	1.67	1.22
4:B:306:PG4:H52	6:B:307:PEG:C1	1.75	1.17
1:A:140:LYS:HB3	6:A:306:PEG:O4	1.63	0.99
4:B:305:PG4:H42	4:B:305:PG4:H82	1.45	0.98
4:B:302:PG4:H12	4:B:302:PG4:H41	1.53	0.91
1:B:56:ASP:OD1	4:B:302:PG4:H41	1.70	0.90
1:A:115:ALA:HB2	6:A:307:PEG:H12	1.51	0.89
4:B:306:PG4:H52	6:B:307:PEG:H12	0.89	0.88
1:A:48:LYS:HZ1	3:A:305:P6G:H51	1.44	0.82
6:A:307:PEG:O4	6:A:311:PEG:O4	2.00	0.80
1:A:206:SER:CB	6:A:307:PEG:H11	2.14	0.77
1:B:246:LYS:NZ	4:B:302:PG4:H52	2.00	0.76
1:A:59:GLN:NE2	7:A:639:HOH:O	2.18	0.76
1:A:223:LEU:HD21	6:A:310:PEG:H42	1.68	0.76
1:B:140[B]:LYS:NZ	4:B:305:PG4:O5	2.18	0.75
3:A:302:P6G:H61	3:A:302:P6G:H22	1.68	0.75
4:B:306:PG4:C6	6:B:307:PEG:H12	2.18	0.74
1:A:206:SER:HB2	6:A:307:PEG:H11	1.70	0.73
1:B:187:VAL:HG22	4:B:305:PG4:H41	1.71	0.73
1:B:121:THR:OG1	6:B:304:PEG:H42	1.90	0.71
1:A:135[B]:LYS:NZ	7:A:634:HOH:O	2.24	0.68
1:B:80:LEU:HB3	6:B:307:PEG:H31	1.74	0.68
1:B:187:VAL:HG21	4:B:305:PG4:C1	2.24	0.67
1:A:241[B]:ASP:OD1	7:A:618:HOH:O	2.11	0.66
1:B:56:ASP:OD1	4:B:302:PG4:H12	1.95	0.66
1:B:36:SER:O	6:B:303:PEG:H12	1.96	0.65
4:B:302:PG4:H41	4:B:302:PG4:C1	2.27	0.64
1:B:187:VAL:HG11	4:B:305:PG4:C8	2.27	0.64
1:A:222[B]:THR:HG21	6:A:310:PEG:H11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204[A]:SER:OG	6:A:307:PEG:H41	1.98	0.63
1:A:141:ASN:HD22	3:A:302:P6G:C14	2.12	0.62
1:A:48:LYS:HE2	3:A:305:P6G:H122	1.79	0.62
1:B:242:LYS:NZ	7:B:606:HOH:O	2.32	0.61
1:B:187:VAL:HG11	4:B:305:PG4:H82	1.84	0.58
1:B:84:LYS:NZ	6:B:307:PEG:O1	2.37	0.58
1:B:51:VAL:HA	4:B:302:PG4:H42	1.86	0.57
4:B:306:PG4:H62	6:B:307:PEG:H22	1.87	0.57
1:A:141:ASN:HD22	3:A:302:P6G:H142	1.69	0.57
1:A:179:ALA:CA	6:A:308:PEG:H11	2.35	0.57
1:B:38:TYR:CE1	4:B:305:PG4:H32	2.39	0.57
1:B:29:THR:N	7:B:586:HOH:O	2.37	0.56
1:B:187:VAL:HG13	4:B:305:PG4:H62	1.86	0.56
1:A:48:LYS:CE	3:A:305:P6G:H122	2.34	0.56
1:B:100:GLU:OE2	4:B:306:PG4:H31	2.05	0.56
1:A:251:ALA:O	7:A:659:HOH:O	2.18	0.55
1:B:246:LYS:HZ3	4:B:302:PG4:H52	1.69	0.55
1:B:56:ASP:OD1	4:B:302:PG4:C4	2.50	0.55
1:A:104:THR:HG21	4:A:303:PG4:H32	1.89	0.55
1:B:140[B]:LYS:CE	4:B:305:PG4:O5	2.55	0.54
1:A:200:MET:HB3	6:A:311:PEG:H22	1.89	0.54
1:B:187:VAL:HG11	4:B:305:PG4:H81	1.89	0.54
1:B:101:ARG:HH21	4:B:306:PG4:C8	2.21	0.54
1:A:59:GLN:HG3	7:A:467:HOH:O	2.07	0.53
1:B:80:LEU:HG	6:B:307:PEG:H21	1.91	0.53
1:A:131:ASP:OD2	7:A:635:HOH:O	2.19	0.53
1:B:39:ALA:O	4:B:305:PG4:H52	2.09	0.53
1:B:187:VAL:HG21	4:B:305:PG4:C2	2.40	0.52
1:B:246:LYS:HZ1	4:B:302:PG4:H52	1.74	0.52
1:B:187:VAL:HG21	4:B:305:PG4:H21	1.91	0.51
1:B:187:VAL:HG11	4:B:305:PG4:H21	1.92	0.51
4:B:305:PG4:H31	7:B:496:HOH:O	2.10	0.51
1:A:179:ALA:HA	6:A:308:PEG:H11	1.92	0.51
1:A:48:LYS:HZ1	3:A:305:P6G:H82	1.76	0.50
4:B:306:PG4:H71	6:B:307:PEG:H22	1.94	0.50
1:A:115:ALA:HB3	6:A:307:PEG:H42	1.94	0.49
1:A:204[A]:SER:HB3	6:A:311:PEG:HO1	1.77	0.49
1:B:187:VAL:CG2	4:B:305:PG4:H41	2.40	0.49
1:A:141:ASN:HD22	3:A:302:P6G:H141	1.78	0.49
1:A:193:LYS:NZ	7:A:675:HOH:O	2.45	0.49
1:B:38:TYR:HE1	4:B:305:PG4:H32	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ALA:O	4:B:305:PG4:H41	2.13	0.49
1:A:91[A]:ILE:CG2	1:A:214:ALA:HB3	2.43	0.48
4:B:305:PG4:H82	4:B:305:PG4:H21	1.95	0.48
1:A:48:LYS:NZ	3:A:305:P6G:H82	2.28	0.48
1:A:109:ASN:ND2	7:A:463[B]:HOH:O	2.30	0.47
1:A:84:LYS:NZ	4:A:303:PG4:H11	2.29	0.47
1:A:141:ASN:O	6:A:306:PEG:H41	2.13	0.47
1:A:176:GLY:O	6:A:308:PEG:H22	2.15	0.47
1:B:201:ASN:ND2	7:B:445:HOH:O	2.29	0.47
1:A:84:LYS:HZ1	4:A:303:PG4:H11	1.78	0.47
1:B:38:TYR:HD1	4:B:305:PG4:H31	1.81	0.46
1:B:166:GLY:HA3	4:B:305:PG4:H71	1.98	0.46
1:A:250[B]:THR:OG1	1:A:251:ALA:N	2.49	0.45
4:B:305:PG4:H32	4:B:305:PG4:H11	1.76	0.45
1:B:39:ALA:HB3	4:B:305:PG4:C5	2.47	0.45
1:B:140[A]:LYS:HD2	4:B:305:PG4:O5	2.16	0.45
1:A:141:ASN:HB3	3:A:302:P6G:H142	1.98	0.45
1:A:148:TRP:CE3	1:A:182[A]:MET:HE2	2.52	0.45
1:B:50:TRP:O	4:B:302:PG4:H31	2.17	0.44
3:A:305:P6G:H141	3:A:305:P6G:H171	1.77	0.44
1:A:84:LYS:HE3	4:A:303:PG4:H11	2.00	0.43
1:B:59:GLN:HG3	1:B:69:LEU:HD23	2.00	0.43
1:B:29:THR:CA	7:B:586:HOH:O	2.67	0.43
3:A:302:P6G:H171	1:B:164:SER:HA	2.01	0.43
6:A:306:PEG:H31	7:A:656:HOH:O	2.18	0.42
4:A:312:PG4:H12	7:A:640:HOH:O	2.18	0.42
1:B:39:ALA:HB3	4:B:305:PG4:H51	2.01	0.42
1:B:148:TRP:CE3	1:B:182[B]:MET:HE2	2.55	0.42
1:A:29:THR:N	7:A:640:HOH:O	2.52	0.42
1:A:251:ALA:HB3	6:A:311:PEG:H41	2.02	0.41
1:A:84:LYS:HZ2	4:A:303:PG4:H31	1.85	0.41
1:B:44:GLN:H	6:B:303:PEG:H11	1.85	0.41
1:A:204[B]:SER:OG	6:A:311:PEG:O1	2.27	0.41
1:B:244:LEU:HB3	1:B:249:ILE:HB	2.03	0.41
1:A:84:LYS:CE	4:A:303:PG4:H11	2.50	0.41
6:A:308:PEG:H41	7:A:445:HOH:O	2.20	0.41
1:B:184:GLU:OE1	4:B:305:PG4:C1	2.69	0.41
1:B:101:ARG:HH21	4:B:306:PG4:H81	1.87	0.40
1:B:44:GLN:HG3	6:B:303:PEG:H11	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225[A]:ASP:OD2	1:B:222:THR:OG1[1_544]	1.99	0.21
1:A:125:LYS:NZ	6:A:310:PEG:O4[1_556]	2.10	0.10
7:B:559:HOH:O	7:B:579:HOH:O[1_554]	2.17	0.03

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	236/251 (94%)	231 (98%)	5 (2%)	0	100	100
1	B	228/251 (91%)	223 (98%)	5 (2%)	0	100	100
All	All	464/502 (92%)	454 (98%)	10 (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	194/201 (96%)	194 (100%)	0	100	100
1	B	186/201 (92%)	182 (98%)	4 (2%)	45	14
All	All	380/402 (94%)	376 (99%)	4 (1%)	65	37

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

Mol	Chain	Res	Type
1	B	47	GLN

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Mol	Chain	Res	Type
1	B	49	LYS
1	B	80	LEU
1	B	229	LYS

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

Mol	Chain	Res	Type
1	A	177	ASN
1	A	220	ASN
1	B	82	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
4	PG4	B	305	-	12,12,12	0.45	0	11,11,11	0.28	0
2	MES	A	301	-	12,12,12	2.21	1 (8%)	15,16,16	1.69	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	311	-	6,6,6	0.44	0	5,5,5	0.31	0
6	PEG	B	304	-	6,6,6	0.43	0	5,5,5	0.30	0
4	PG4	B	302	-	9,9,12	0.44	0	8,8,11	0.29	0
4	PG4	A	303	-	12,12,12	0.45	0	11,11,11	0.28	0
3	P6G	A	305	-	18,18,18	0.46	0	17,17,17	0.27	0
6	PEG	A	308	-	6,6,6	0.44	0	5,5,5	0.31	0
6	PEG	B	307	-	6,6,6	0.43	0	5,5,5	0.31	0
4	PG4	B	306	-	9,9,12	0.44	0	8,8,11	0.28	0
2	MES	B	301	-	12,12,12	2.18	1 (8%)	15,16,16	1.87	3 (20%)
6	PEG	B	303	-	6,6,6	0.44	0	5,5,5	0.31	0
6	PEG	A	306	-	6,6,6	0.44	0	5,5,5	0.31	0
6	PEG	A	310	-	6,6,6	0.43	0	5,5,5	0.30	0
6	PEG	A	307	-	6,6,6	0.44	0	5,5,5	0.31	0
4	PG4	A	312	-	12,12,12	0.46	0	11,11,11	0.28	0
3	P6G	A	302	-	18,18,18	0.46	0	17,17,17	0.27	0
6	PEG	A	309	-	6,6,6	0.43	0	5,5,5	0.31	0
5	ETE	A	304	-	13,13,13	0.46	0	12,12,12	0.25	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
4	PG4	B	305	-	-	5/10/10/10	-
2	MES	A	301	-	-	2/6/14/14	0/1/1/1
6	PEG	A	311	-	-	2/4/4/4	-
6	PEG	B	304	-	-	1/4/4/4	-
4	PG4	B	302	-	-	5/7/7/10	-
4	PG4	A	303	-	-	2/10/10/10	-
3	P6G	A	305	-	-	10/16/16/16	-
6	PEG	A	308	-	-	2/4/4/4	-
6	PEG	B	307	-	-	1/4/4/4	-
4	PG4	B	306	-	-	3/7/7/10	-
2	MES	B	301	-	-	4/6/14/14	0/1/1/1
6	PEG	B	303	-	-	2/4/4/4	-
6	PEG	A	306	-	-	1/4/4/4	-
6	PEG	A	310	-	-	1/4/4/4	-
6	PEG	A	307	-	-	4/4/4/4	-
4	PG4	A	312	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P6G	A	302	-	-	8/16/16/16	-
6	PEG	A	309	-	-	2/4/4/4	-
5	ETE	A	304	-	-	3/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MES	C8-S	-7.48	1.67	1.77
2	B	301	MES	C8-S	-7.17	1.67	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	MES	O1S-S-C8	4.20	113.08	106.73
2	A	301	MES	C5-N4-C3	3.94	117.32	108.84
2	B	301	MES	C5-N4-C3	3.86	117.16	108.84
2	A	301	MES	O1S-S-C8	3.36	111.80	106.73
2	B	301	MES	C7-N4-C5	2.29	117.35	111.24
2	A	301	MES	O3S-S-O1S	-2.12	106.10	111.40
2	A	301	MES	O2S-S-C8	2.07	109.86	106.73

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MES	C8-C7-N4-C3
2	B	301	MES	C7-C8-S-O2S
4	A	303	PG4	O2-C3-C4-O3
4	A	312	PG4	O3-C5-C6-O4
4	B	302	PG4	O2-C3-C4-O3
4	B	302	PG4	O1-C1-C2-O2
4	B	305	PG4	O4-C7-C8-O5
6	A	308	PEG	O2-C3-C4-O4
6	B	303	PEG	O1-C1-C2-O2
6	B	307	PEG	O1-C1-C2-O2
5	A	304	ETE	OH6-C15-C25-OH5
4	B	305	PG4	O2-C3-C4-O3
4	B	306	PG4	O2-C3-C4-O3
6	A	310	PEG	O1-C1-C2-O2
6	A	311	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	302	P6G	O7-C8-C9-O10
3	A	305	P6G	O10-C11-C12-O13
2	B	301	MES	C7-C8-S-O3S
5	A	304	ETE	OH2-C12-C22-OH3
3	A	302	P6G	O10-C11-C12-O13
3	A	305	P6G	O16-C17-C18-O19
4	A	303	PG4	O4-C7-C8-O5
4	B	302	PG4	O3-C5-C6-O4
3	A	305	P6G	O13-C14-C15-O16
2	A	301	MES	C8-C7-N4-C5
2	B	301	MES	C8-C7-N4-C3
4	B	306	PG4	O3-C5-C6-O4
6	A	307	PEG	O2-C3-C4-O4
2	B	301	MES	C7-C8-S-O1S
6	A	311	PEG	C1-C2-O2-C3
3	A	305	P6G	C12-C11-O10-C9
6	A	308	PEG	O1-C1-C2-O2
4	A	312	PG4	C5-C6-O4-C7
4	A	312	PG4	C8-C7-O4-C6
4	B	302	PG4	C6-C5-O3-C4
3	A	302	P6G	O1-C2-C3-O4
6	A	306	PEG	C1-C2-O2-C3
4	B	305	PG4	O3-C5-C6-O4
6	A	307	PEG	O1-C1-C2-O2
3	A	302	P6G	O16-C17-C18-O19
5	A	304	ETE	C24-C14-OH5-C25
6	A	309	PEG	C1-C2-O2-C3
3	A	305	P6G	C11-C12-O13-C14
3	A	305	P6G	C14-C15-O16-C17
4	B	306	PG4	C8-C7-O4-C6
3	A	302	P6G	C14-C15-O16-C17
3	A	302	P6G	C11-C12-O13-C14
3	A	305	P6G	O7-C8-C9-O10
4	B	305	PG4	C1-C2-O2-C3
4	B	302	PG4	C3-C4-O3-C5
6	A	307	PEG	C1-C2-O2-C3
3	A	305	P6G	O1-C2-C3-O4
4	B	305	PG4	C6-C5-O3-C4
6	B	303	PEG	O2-C3-C4-O4
3	A	305	P6G	C15-C14-O13-C12
6	A	307	PEG	C4-C3-O2-C2
6	A	309	PEG	C4-C3-O2-C2

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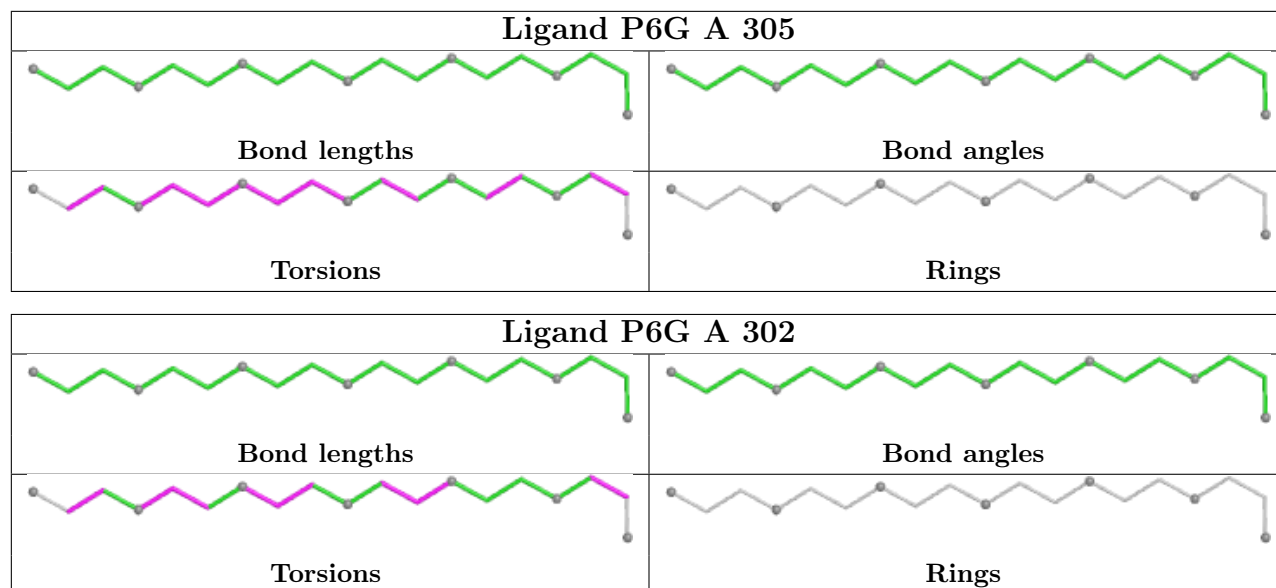
Mol	Chain	Res	Type	Atoms
3	A	302	P6G	O13-C14-C15-O16
3	A	302	P6G	C9-C8-O7-C6
3	A	305	P6G	O4-C5-C6-O7
6	B	304	PEG	C1-C2-O2-C3

There are no ring outliers.

15 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	305	PG4	26	0
6	A	311	PEG	5	0
6	B	304	PEG	1	0
4	B	302	PG4	10	0
4	A	303	PG4	6	0
3	A	305	P6G	6	0
6	A	308	PEG	4	0
6	B	307	PEG	9	0
4	B	306	PG4	9	0
6	B	303	PEG	3	0
6	A	306	PEG	3	0
6	A	310	PEG	2	1
6	A	307	PEG	6	0
4	A	312	PG4	1	0
3	A	302	P6G	6	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, 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	223/251 (88%)	-0.18	2 (0%) 81 84	9, 20, 31, 47	14 (6%)
1	B	223/251 (88%)	0.17	5 (2%) 62 65	10, 25, 43, 51	7 (3%)
All	All	446/502 (88%)	-0.00	7 (1%) 70 73	9, 22, 41, 51	21 (4%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	ALA	3.5
1	B	251	ALA	3.1
1	B	67	TRP	2.7
1	B	85	ALA	2.4
1	B	86	GLY	2.4
1	A	250[A]	THR	2.4
1	B	222	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

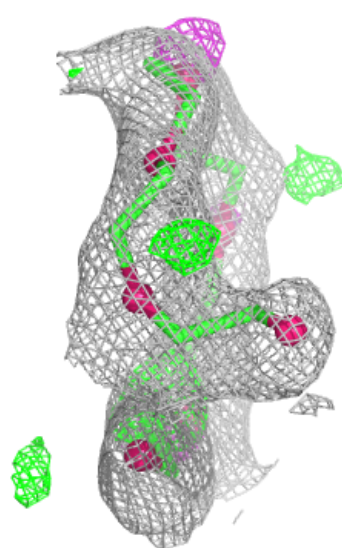
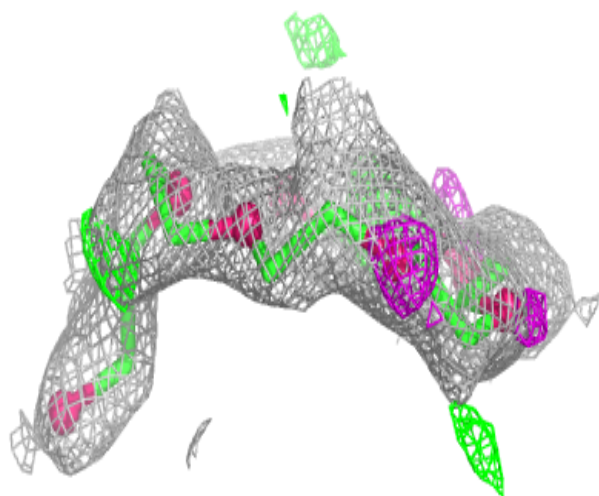
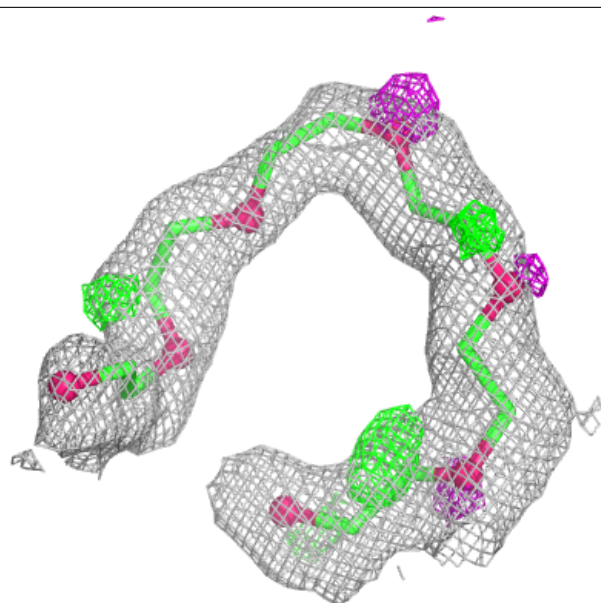
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	A	312	13/13	0.75	0.13	48,49,49,49	0
4	PG4	B	305	13/13	0.79	0.15	28,32,33,34	13
6	PEG	A	307	7/7	0.79	0.13	43,45,46,47	0
6	PEG	A	310	7/7	0.79	0.11	58,58,59,59	0
6	PEG	B	303	7/7	0.81	0.12	48,50,53,53	0
6	PEG	A	311	7/7	0.84	0.13	43,44,47,48	0
4	PG4	B	302	10/13	0.85	0.12	51,53,55,55	0
6	PEG	B	307	7/7	0.85	0.10	54,56,58,58	0
6	PEG	B	304	7/7	0.86	0.10	62,63,64,65	0
3	P6G	A	302	19/19	0.87	0.11	34,40,46,46	0
4	PG4	B	306	10/13	0.87	0.10	49,50,52,53	0
6	PEG	A	306	7/7	0.87	0.12	59,59,60,62	0
6	PEG	A	309	7/7	0.88	0.10	40,41,43,43	0
4	PG4	A	303	13/13	0.88	0.12	45,47,49,49	0
3	P6G	A	305	19/19	0.89	0.11	54,55,56,56	0
5	ETE	A	304	14/14	0.89	0.09	37,40,43,43	0
6	PEG	A	308	7/7	0.89	0.09	54,56,57,57	0
2	MES	B	301	12/12	0.96	0.08	28,30,33,35	0
2	MES	A	301	12/12	0.96	0.08	28,30,32,35	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.

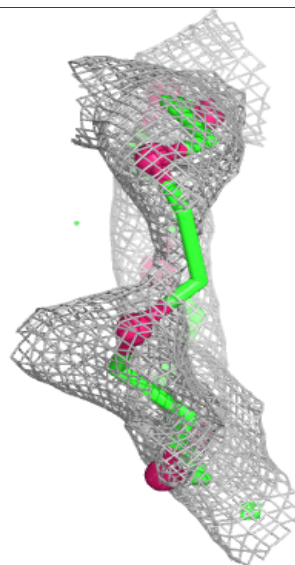
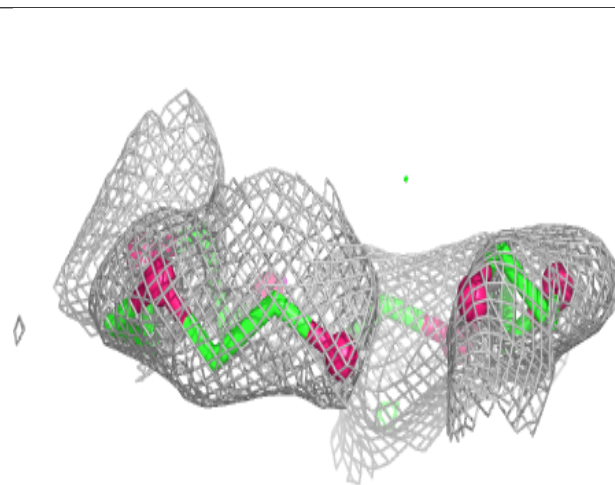
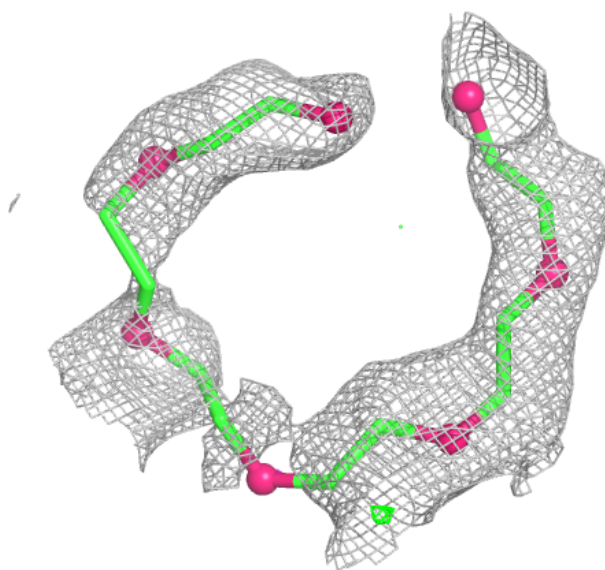
Electron density around P6G A 302:

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



Electron density around P6G A 305:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.