



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:17 PM UTC

PDB ID : 7P8Y / pdb_00007p8y
Title : Short wilavidin apo form
Authors : Avraham, O.; Livnah, O.
Deposited on : 2021-07-23
Resolution : 2.18 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

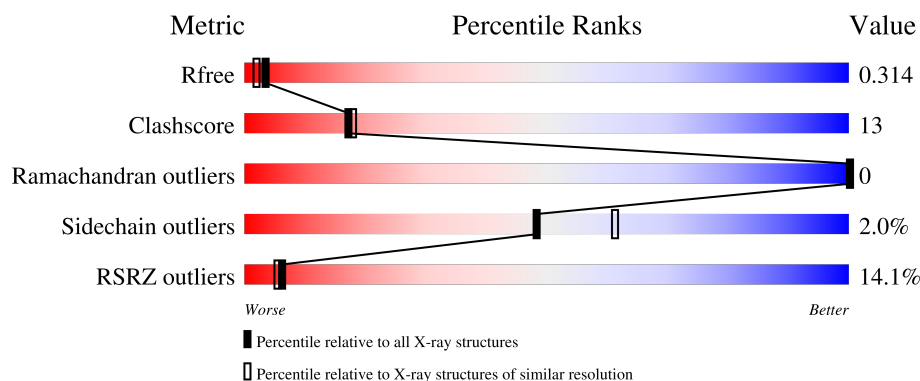
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	119	7% 71% 18% • 10%
1	B	119	12% 72% 18% 10%
1	C	119	20% 67% 19% • 11%
1	D	119	12% 71% 18% • 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
2	1PE	C	201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3634 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 Wilavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			823	526	129	166	2			
1	B	107	Total	C	N	O	S	0	0	0
			823	526	129	166	2			
1	C	106	Total	C	N	O	S	0	0	0
			815	520	128	165	2			
1	D	106	Total	C	N	O	S	0	0	0
			815	520	128	165	2			

There are 4 discrepancies between the modelled and reference sequences:

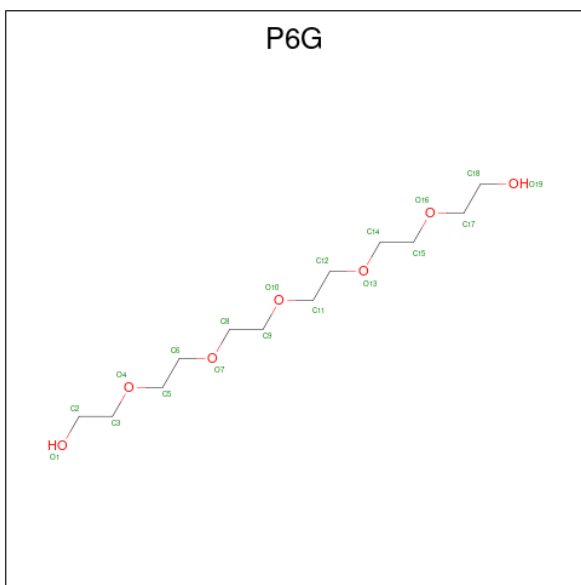
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A3A4VWA2
B	0	MET	-	initiating methionine	UNP A0A3A4VWA2
C	0	MET	-	initiating methionine	UNP A0A3A4VWA2
D	0	MET	-	initiating methionine	UNP A0A3A4VWA2

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



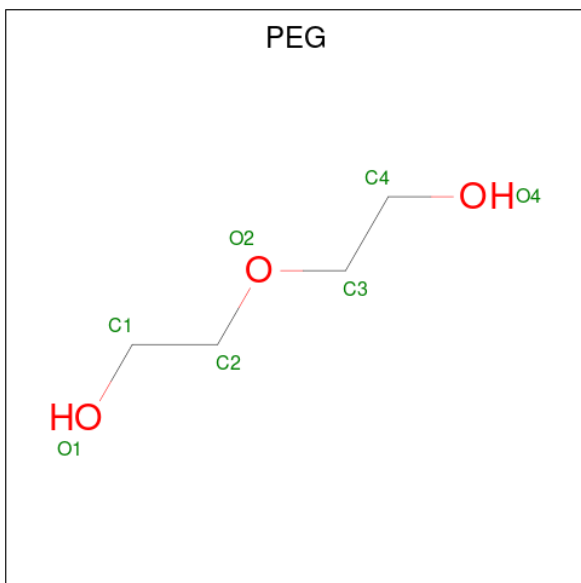
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		
2	B	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



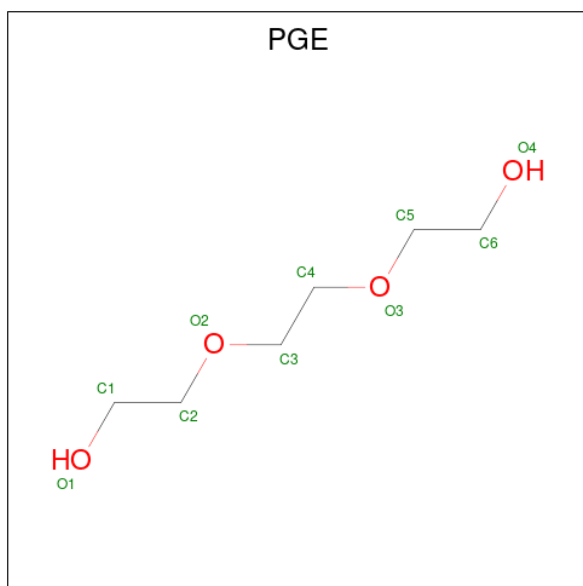
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

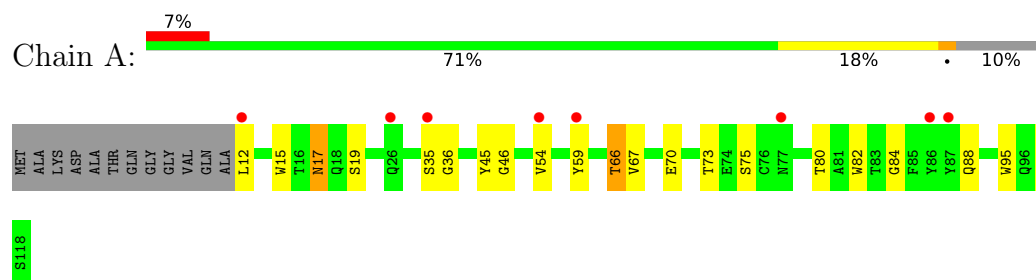
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	27	Total	O	0	0
			27	27		
6	C	40	Total	O	0	0
			40	40		
6	D	59	Total	O	0	0
			59	59		

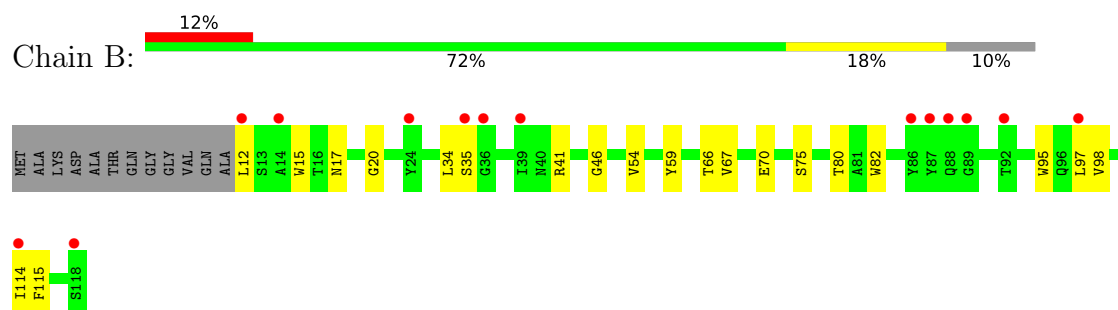
3 Residue-property plots [i](#)

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.

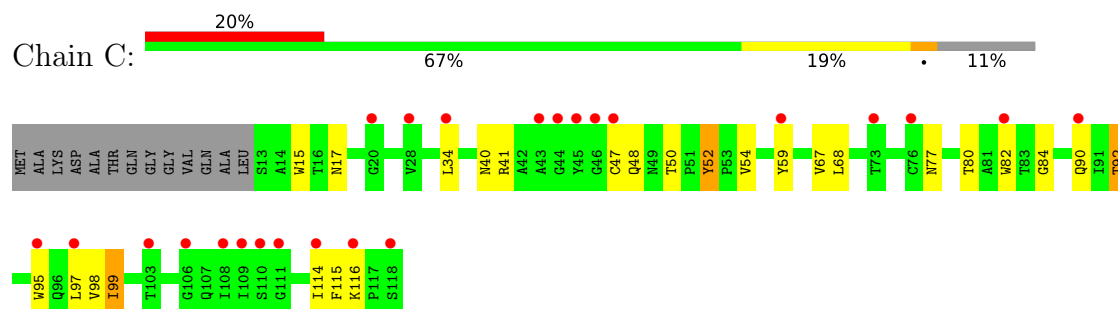
• Molecule 1: Wilavidin



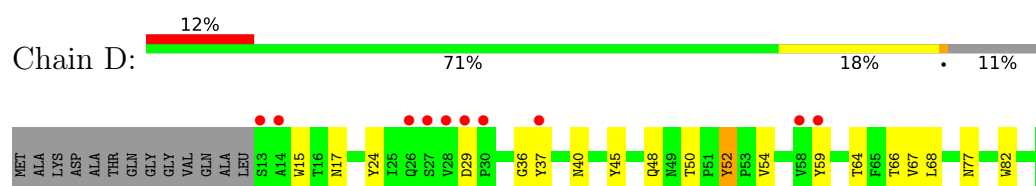
• Molecule 1: Wilavidin

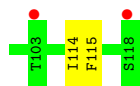


• Molecule 1: Wilavidin



• Molecule 1: Wilavidin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.67Å 67.69Å 77.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.71 – 2.18 58.71 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.71-2.18) 99.4 (58.71-2.18)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.52 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.249 , 0.306 0.256 , 0.314	Depositor DCC
R_{free} test set	1282 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3634	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5523e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: P6G, PEG, 1PE, PGE

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	1.12	3/847 (0.4%)	1.35	2/1162 (0.2%)
1	B	1.13	2/847 (0.2%)	1.39	0/1162
1	C	1.06	0/839	1.36	2/1151 (0.2%)
1	D	1.05	0/839	1.32	3/1151 (0.3%)
All	All	1.09	5/3372 (0.1%)	1.35	7/4626 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	GLY	C-O	7.46	1.31	1.23
1	A	84	GLY	C-O	5.80	1.29	1.23
1	B	35	SER	C-O	5.74	1.30	1.23
1	B	46	GLY	C-O	5.63	1.28	1.23
1	A	36	GLY	C-O	5.26	1.30	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	ASP	CA-CB-CG	7.66	120.25	112.60
1	C	92	THR	CB-CA-C	6.22	120.49	109.72
1	A	66	THR	CB-CA-C	6.11	120.35	109.65
1	D	52	TYR	CB-CA-C	5.91	117.74	108.63
1	C	52	TYR	CB-CA-C	5.35	116.86	108.63
1	A	73	THR	CA-CB-OG1	-5.18	101.82	109.60
1	D	66	THR	CB-CA-C	5.13	119.79	109.38

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	823	0	767	19	0
1	B	823	0	767	15	0
1	C	815	0	756	24	0
1	D	815	0	756	17	0
2	A	16	0	22	5	0
2	B	16	0	22	6	0
2	C	32	0	44	9	0
2	D	32	0	44	4	0
3	A	19	0	26	0	0
3	B	19	0	26	2	0
3	C	38	0	52	0	0
4	A	7	0	10	0	0
5	C	10	0	14	2	0
6	A	43	0	0	5	1
6	B	27	0	0	4	0
6	C	40	0	0	9	0
6	D	59	0	0	5	1
All	All	3634	0	3306	85	1

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 13.

All (85) 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:47:CYS:HB2	6:C:316:HOH:O	1.52	1.08
2:C:201:1PE:H222	2:C:201:1PE:OH4	1.47	1.08
2:C:201:1PE:OH4	2:C:201:1PE:C22	2.13	0.96
2:C:201:1PE:H232	6:C:322:HOH:O	1.67	0.94
1:D:77:ASN:CG	6:D:305:HOH:O	2.10	0.94
1:D:77:ASN:HB2	6:D:305:HOH:O	1.68	0.92
1:D:77:ASN:CB	6:D:305:HOH:O	2.19	0.90
2:A:201:1PE:H261	6:A:325:HOH:O	1.73	0.88
2:D:201:1PE:H232	6:D:323:HOH:O	1.87	0.73
1:A:75:SER:HB2	6:A:309:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ASN:HA	1:B:114:ILE:O	1.92	0.70
1:B:97:LEU:HD21	2:B:201:1PE:H232	1.75	0.69
2:C:201:1PE:H251	6:C:316:HOH:O	1.92	0.67
1:C:95:TRP:CB	6:C:305:HOH:O	2.42	0.67
1:C:99:ILE:HD13	1:C:99:ILE:N	2.11	0.66
1:A:70:GLU:HG3	6:A:309:HOH:O	1.95	0.66
1:C:95:TRP:CG	6:C:305:HOH:O	2.47	0.65
1:C:82:TRP:CE2	6:C:305:HOH:O	2.49	0.64
1:C:17:ASN:HA	1:C:114:ILE:O	2.00	0.61
1:A:17:ASN:C	1:A:17:ASN:HD22	2.09	0.61
1:A:17:ASN:HA	1:A:114:ILE:O	2.02	0.59
1:B:54:VAL:HG22	1:B:67:VAL:HG22	1.85	0.58
1:B:59:TYR:CZ	1:C:77:ASN:HA	2.40	0.57
1:B:70:GLU:HG3	1:B:75:SER:OG	2.07	0.55
1:C:95:TRP:HB2	6:C:305:HOH:O	2.03	0.55
1:C:80:THR:HG21	6:C:305:HOH:O	2.07	0.55
1:C:98:VAL:C	1:C:99:ILE:HD13	2.32	0.55
1:B:97:LEU:HD21	2:B:201:1PE:C23	2.36	0.55
1:B:82:TRP:CD1	1:B:95:TRP:HB3	2.42	0.54
2:D:201:1PE:H231	6:D:320:HOH:O	2.08	0.54
1:B:114:ILE:N	1:B:114:ILE:HD12	2.23	0.53
1:C:41:ARG:HD3	6:C:336:HOH:O	2.08	0.52
1:C:15:TRP:HB3	1:C:115:PHE:HB3	1.91	0.52
1:A:45:TYR:CD1	2:A:201:1PE:H252	2.46	0.51
2:B:201:1PE:H221	6:B:314:HOH:O	2.09	0.51
1:C:50:THR:HG23	1:C:52:TYR:CE2	2.46	0.51
1:B:20:GLY:O	1:B:41:ARG:HD2	2.12	0.50
1:A:75:SER:OG	1:D:59:TYR:OH	2.21	0.49
1:C:80:THR:OG1	1:C:97:LEU:HD13	2.11	0.49
2:B:201:1PE:C22	6:B:314:HOH:O	2.60	0.49
1:C:40:ASN:O	1:C:48:GLN:HA	2.12	0.49
1:D:45:TYR:CD1	2:D:201:1PE:H241	2.48	0.49
1:D:17:ASN:HA	1:D:114:ILE:O	2.13	0.49
1:A:59:TYR:CZ	1:D:77:ASN:HA	2.47	0.49
2:B:201:1PE:H242	6:B:314:HOH:O	2.13	0.47
1:A:15:TRP:HB3	1:A:115:PHE:HB3	1.95	0.47
1:B:15:TRP:HB3	1:B:115:PHE:HB3	1.96	0.47
1:B:34:LEU:HD23	1:B:34:LEU:C	2.39	0.47
2:B:201:1PE:H132	6:B:314:HOH:O	2.14	0.47
3:B:202:P6G:C18	3:B:202:P6G:H52	2.44	0.47
1:D:50:THR:HG23	1:D:52:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASN:ND2	1:A:19:SER:H	2.13	0.47
1:A:66:THR:HA	1:A:80:THR:O	2.14	0.46
1:C:54:VAL:HG22	1:C:67:VAL:HG22	1.98	0.46
1:A:97:LEU:HD21	2:A:201:1PE:C13	2.46	0.46
2:C:201:1PE:H222	2:C:201:1PE:C24	2.43	0.45
2:C:202:1PE:H161	5:C:203:PGE:O4	2.16	0.45
1:C:90:GLN:NE2	1:C:116:LYS:HE3	2.32	0.45
1:C:82:TRP:CZ2	2:C:201:1PE:H221	2.52	0.45
1:A:45:TYR:HB3	2:A:201:1PE:H251	1.99	0.45
1:A:88:GLN:NE2	6:A:304:HOH:O	2.42	0.44
2:C:202:1PE:OH7	5:C:203:PGE:H62	2.17	0.44
1:C:90:GLN:NE2	1:C:116:LYS:CE	2.81	0.44
1:B:66:THR:HA	1:B:80:THR:O	2.17	0.44
1:D:54:VAL:HG22	1:D:67:VAL:HG22	2.00	0.44
1:C:82:TRP:CD1	1:C:95:TRP:HB3	2.52	0.44
1:C:90:GLN:HE21	1:C:116:LYS:CE	2.31	0.43
1:A:17:ASN:HB3	1:A:115:PHE:CE1	2.53	0.43
1:A:70:GLU:CG	6:A:309:HOH:O	2.60	0.43
1:D:15:TRP:HB3	1:D:115:PHE:HB3	1.99	0.43
1:D:40:ASN:ND2	2:D:201:1PE:H242	2.34	0.43
1:A:54:VAL:HG22	1:A:67:VAL:HG22	2.00	0.43
1:A:97:LEU:HD21	2:A:201:1PE:H131	2.00	0.43
1:D:64:THR:HA	1:D:82:TRP:O	2.19	0.43
1:B:75:SER:HB3	1:C:59:TYR:OH	2.19	0.42
1:A:82:TRP:CD1	1:A:95:TRP:HB3	2.55	0.42
1:D:40:ASN:O	1:D:48:GLN:HA	2.19	0.42
1:A:59:TYR:CD2	1:D:68:LEU:HD11	2.56	0.41
3:B:202:P6G:H52	3:B:202:P6G:H181	2.03	0.41
2:C:201:1PE:C16	2:C:202:1PE:OH2	2.69	0.40
1:D:24:TYR:O	1:D:36:GLY:HA3	2.20	0.40
1:B:59:TYR:CD2	1:C:68:LEU:HD11	2.56	0.40
1:D:82:TRP:CD1	1:D:95:TRP:HB3	2.56	0.40
1:B:98:VAL:HG21	1:C:84:GLY:O	2.21	0.40
1:D:37:TYR:HA	1:D:52:TYR:O	2.21	0.40

All (1) 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)
6:A:323:HOH:O	6:D:340:HOH:O[4_554]	2.18	0.02

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	105/119 (88%)	105 (100%)	0	0	100	100
1	B	105/119 (88%)	105 (100%)	0	0	100	100
1	C	104/119 (87%)	103 (99%)	1 (1%)	0	100	100
1	D	104/119 (87%)	102 (98%)	2 (2%)	0	100	100
All	All	418/476 (88%)	415 (99%)	3 (1%)	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	89/96 (93%)	86 (97%)	3 (3%)	32	41
1	B	89/96 (93%)	88 (99%)	1 (1%)	65	77
1	C	88/96 (92%)	85 (97%)	3 (3%)	32	41
1	D	88/96 (92%)	88 (100%)	0	100	100
All	All	354/384 (92%)	347 (98%)	7 (2%)	48	61

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	ASN

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Mol	Chain	Res	Type
1	A	35	SER
1	B	12	LEU
1	C	34	LEU
1	C	92	THR
1	C	99	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	B	88	GLN
1	B	90	GLN
1	C	48	GLN
1	C	90	GLN
1	C	96	GLN
1	D	90	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](#)

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](#)

12 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	1PE	A	201	-	15,15,15	0.88	0	14,14,14	0.84	0
3	P6G	A	202	-	18,18,18	0.83	1 (5%)	17,17,17	0.59	0
2	1PE	C	201	-	15,15,15	0.81	0	14,14,14	1.11	2 (14%)
4	PEG	A	203	-	6,6,6	0.24	0	5,5,5	0.10	0
5	PGE	C	203	-	9,9,9	0.24	0	8,8,8	0.19	0
3	P6G	C	205	-	18,18,18	0.74	0	17,17,17	0.73	0
2	1PE	C	202	-	15,15,15	0.64	0	14,14,14	0.61	0
3	P6G	C	204	-	18,18,18	0.98	0	17,17,17	0.99	0
2	1PE	B	201	-	15,15,15	0.76	0	14,14,14	0.90	1 (7%)
2	1PE	D	201	-	15,15,15	0.58	0	14,14,14	0.83	0
3	P6G	B	202	-	18,18,18	0.74	0	17,17,17	0.58	0
2	1PE	D	202	-	15,15,15	0.62	0	14,14,14	0.56	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	1PE	A	201	-	-	6/13/13/13	-
3	P6G	A	202	-	-	9/16/16/16	-
2	1PE	C	201	-	-	9/13/13/13	-
4	PEG	A	203	-	-	2/4/4/4	-
5	PGE	C	203	-	-	4/7/7/7	-
3	P6G	C	205	-	-	8/16/16/16	-
2	1PE	C	202	-	-	5/13/13/13	-
3	P6G	C	204	-	-	5/16/16/16	-
2	1PE	B	201	-	-	4/13/13/13	-
2	1PE	D	201	-	-	7/13/13/13	-
3	P6G	B	202	-	-	10/16/16/16	-
2	1PE	D	202	-	-	9/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	P6G	O4-C3	2.01	1.50	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	1PE	OH3-C22-C12	2.67	121.87	110.11
2	C	201	1PE	OH5-C25-C15	-2.27	99.99	110.35
2	B	201	1PE	OH3-C23-C13	2.08	119.81	110.35

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	1PE	C13-C23-OH3-C22
5	C	203	PGE	O2-C3-C4-O3
2	D	201	1PE	OH5-C14-C24-OH4
3	C	205	P6G	O10-C11-C12-O13
3	C	204	P6G	O10-C11-C12-O13
3	B	202	P6G	O10-C11-C12-O13
4	A	203	PEG	C4-C3-O2-C2
3	B	202	P6G	O13-C14-C15-O16
2	D	201	1PE	OH7-C16-C26-OH6
3	A	202	P6G	O16-C17-C18-O19
3	B	202	P6G	O16-C17-C18-O19
4	A	203	PEG	O2-C3-C4-O4
5	C	203	PGE	O3-C5-C6-O4
2	B	201	1PE	OH4-C13-C23-OH3
2	A	201	1PE	OH2-C12-C22-OH3
2	A	201	1PE	OH7-C16-C26-OH6
2	C	201	1PE	OH6-C15-C25-OH5
2	A	201	1PE	OH5-C14-C24-OH4
2	C	201	1PE	OH7-C16-C26-OH6
3	C	205	P6G	O16-C17-C18-O19
2	C	202	1PE	OH5-C14-C24-OH4
2	D	202	1PE	OH4-C13-C23-OH3
3	B	202	P6G	O4-C5-C6-O7
3	B	202	P6G	O7-C8-C9-O10
2	C	201	1PE	OH5-C14-C24-OH4
2	C	201	1PE	OH4-C13-C23-OH3
2	B	201	1PE	OH2-C12-C22-OH3
2	C	201	1PE	OH2-C12-C22-OH3
3	A	202	P6G	O7-C8-C9-O10
2	C	201	1PE	C12-C22-OH3-C23
3	B	202	P6G	O1-C2-C3-O4
2	D	202	1PE	OH5-C14-C24-OH4
3	B	202	P6G	C15-C14-O13-C12
2	D	202	1PE	C13-C23-OH3-C22
3	A	202	P6G	O10-C11-C12-O13

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Mol	Chain	Res	Type	Atoms
2	A	201	1PE	C14-C24-OH4-C13
3	C	204	P6G	C18-C17-O16-C15
3	C	204	P6G	C11-C12-O13-C14
2	D	202	1PE	C12-C22-OH3-C23
2	C	201	1PE	C15-C25-OH5-C14
2	B	201	1PE	C23-C13-OH4-C24
3	C	205	P6G	C2-C3-O4-C5
3	C	205	P6G	C15-C14-O13-C12
2	C	202	1PE	C13-C23-OH3-C22
3	C	204	P6G	C9-C8-O7-C6
3	C	205	P6G	O4-C5-C6-O7
2	C	201	1PE	C24-C14-OH5-C25
2	D	201	1PE	C24-C14-OH5-C25
3	C	205	P6G	C5-C6-O7-C8
3	A	202	P6G	C11-C12-O13-C14
3	A	202	P6G	C6-C5-O4-C3
3	C	204	P6G	O16-C17-C18-O19
3	A	202	P6G	C2-C3-O4-C5
2	D	202	1PE	C16-C26-OH6-C15
2	B	201	1PE	OH6-C15-C25-OH5
2	D	201	1PE	OH4-C13-C23-OH3
2	D	201	1PE	C12-C22-OH3-C23
3	B	202	P6G	C8-C9-O10-C11
2	C	202	1PE	C23-C13-OH4-C24
3	A	202	P6G	C15-C14-O13-C12
2	C	202	1PE	C14-C24-OH4-C13
3	B	202	P6G	C6-C5-O4-C3
5	C	203	PGE	C1-C2-O2-C3
2	D	202	1PE	OH6-C15-C25-OH5
2	D	202	1PE	C24-C14-OH5-C25
5	C	203	PGE	C4-C3-O2-C2
2	D	201	1PE	C13-C23-OH3-C22
3	B	202	P6G	C11-C12-O13-C14
2	C	202	1PE	OH4-C13-C23-OH3
2	A	201	1PE	C25-C15-OH6-C26
2	D	202	1PE	C14-C24-OH4-C13
3	C	205	P6G	C12-C11-O10-C9
2	D	201	1PE	C14-C24-OH4-C13
3	A	202	P6G	C18-C17-O16-C15
2	D	202	1PE	OH2-C12-C22-OH3
2	A	201	1PE	OH6-C15-C25-OH5
3	C	205	P6G	O1-C2-C3-O4

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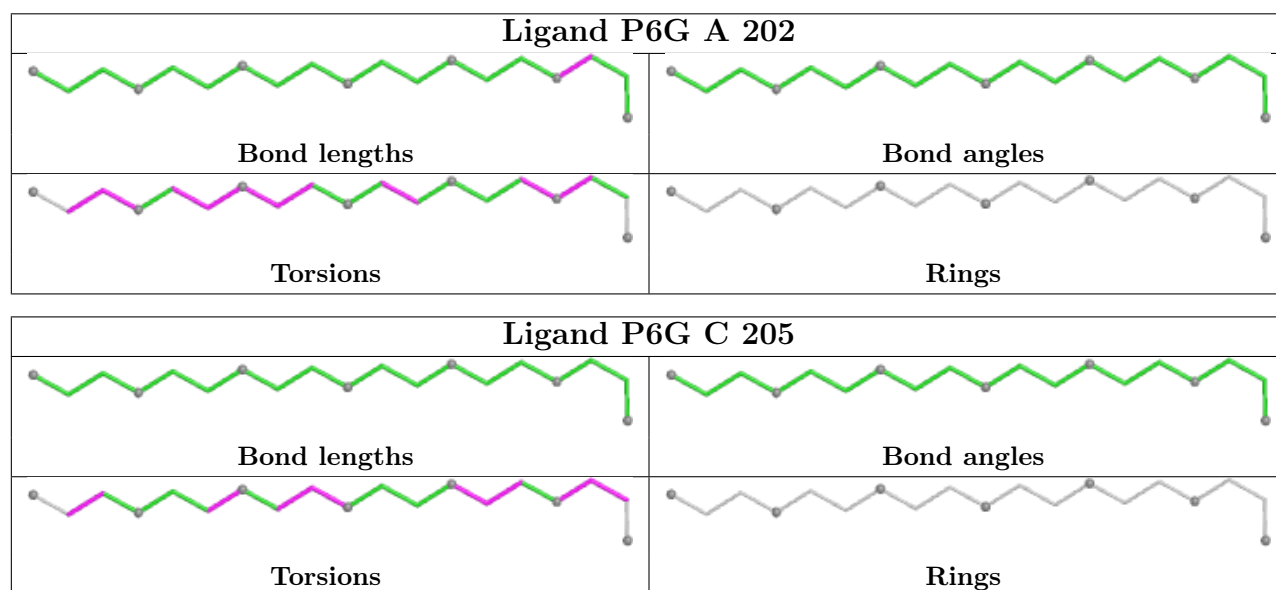
Mol	Chain	Res	Type	Atoms
3	A	202	P6G	O13-C14-C15-O16

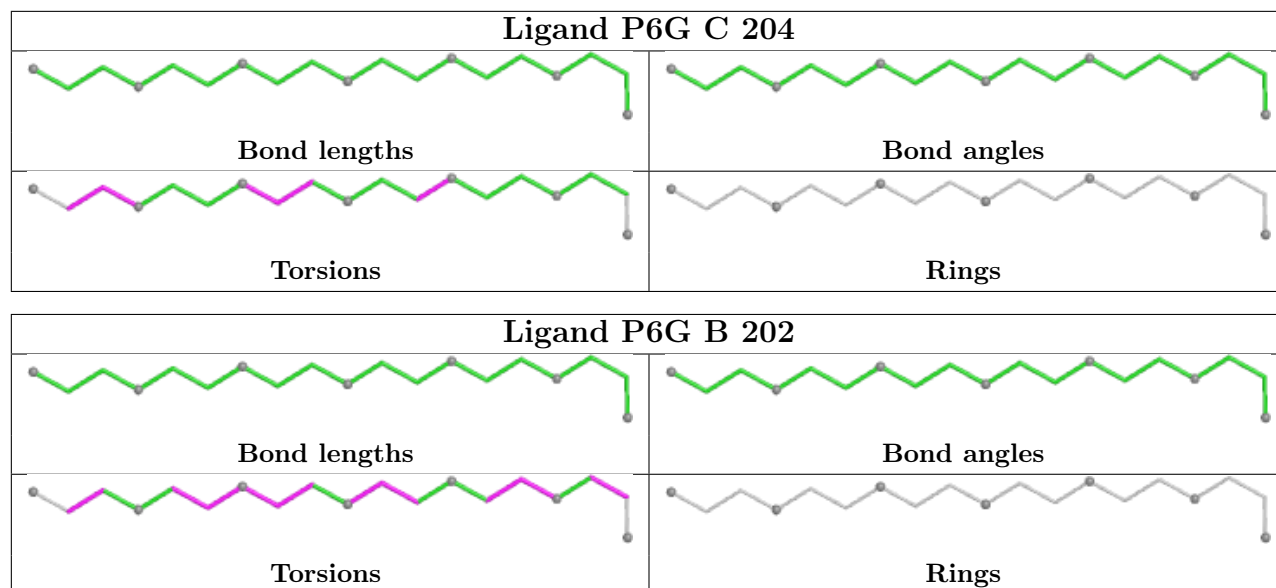
There are no ring outliers.

7 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	1PE	5	0
2	C	201	1PE	7	0
5	C	203	PGE	2	0
2	C	202	1PE	3	0
2	B	201	1PE	6	0
2	D	201	1PE	4	0
3	B	202	P6G	2	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	107/119 (89%)	0.86	8 (7%) 20 19	9, 17, 26, 44	0
1	B	107/119 (89%)	1.06	14 (13%) 7 6	9, 19, 29, 49	0
1	C	106/119 (89%)	1.22	24 (22%) 2 2	9, 20, 34, 49	0
1	D	106/119 (89%)	0.79	14 (13%) 7 6	9, 18, 32, 46	0
All	All	426/476 (89%)	0.98	60 (14%) 6 5	9, 19, 32, 49	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	5.5
1	D	29	ASP	5.2
1	B	12	LEU	5.2
1	D	59	TYR	4.4
1	B	87	TYR	3.7
1	B	24	TYR	3.6
1	A	59	TYR	3.3
1	C	45	TYR	3.2
1	D	28	VAL	3.2
1	C	108	ILE	3.2
1	C	20	GLY	3.0
1	C	111	GLY	3.0
1	B	89	GLY	3.0
1	C	34	LEU	2.9
1	B	14	ALA	2.9
1	B	39	ILE	2.8
1	D	13	SER	2.8
1	D	27	SER	2.8
1	C	106	GLY	2.8
1	D	30	PRO	2.8
1	C	47	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	43	ALA	2.7
1	C	59	TYR	2.6
1	C	90	GLN	2.6
1	C	46	GLY	2.6
1	C	109	ILE	2.6
1	C	114	ILE	2.5
1	D	86	TYR	2.5
1	D	118	SER	2.5
1	D	103	THR	2.5
1	C	73	THR	2.4
1	C	118	SER	2.4
1	B	97	LEU	2.4
1	C	76	CYS	2.4
1	A	86	TYR	2.4
1	D	14	ALA	2.4
1	D	37	TYR	2.3
1	B	35	SER	2.3
1	C	95	TRP	2.3
1	A	35	SER	2.3
1	B	114	ILE	2.2
1	A	77	ASN	2.2
1	C	97	LEU	2.2
1	C	82	TRP	2.2
1	B	92	THR	2.2
1	C	44	GLY	2.2
1	A	87	TYR	2.2
1	B	86	TYR	2.2
1	C	116	LYS	2.2
1	C	103	THR	2.2
1	B	36	GLY	2.1
1	B	88	GLN	2.1
1	C	110	SER	2.1
1	A	26	GLN	2.1
1	C	28	VAL	2.1
1	D	58	VAL	2.1
1	B	118	SER	2.1
1	D	26	GLN	2.0
1	D	90	GLN	2.0
1	A	54	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

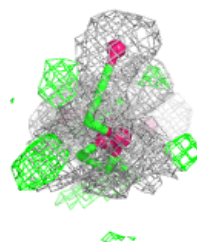
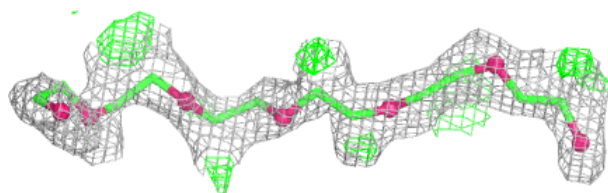
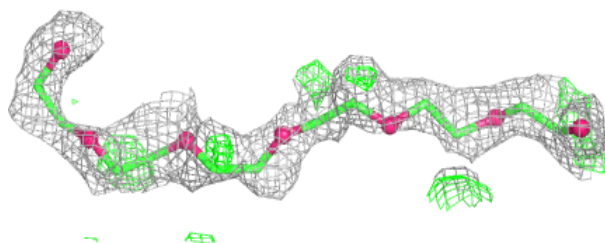
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	P6G	C	204	19/19	0.46	0.27	32,45,51,51	0
5	PGE	C	203	10/10	0.57	0.27	35,54,64,69	0
3	P6G	C	205	19/19	0.59	0.26	44,48,52,52	0
2	1PE	C	202	16/16	0.64	0.27	35,47,50,53	0
2	1PE	D	202	16/16	0.66	0.24	29,49,56,56	0
4	PEG	A	203	7/7	0.74	0.19	29,30,31,31	7
2	1PE	C	201	16/16	0.76	0.17	16,22,27,33	0
3	P6G	A	202	19/19	0.77	0.17	25,30,33,34	0
3	P6G	B	202	19/19	0.80	0.17	32,38,41,41	0
2	1PE	A	201	16/16	0.84	0.16	19,24,37,40	0
2	1PE	B	201	16/16	0.85	0.14	20,24,39,39	0
2	1PE	D	201	16/16	0.86	0.12	20,23,30,36	0

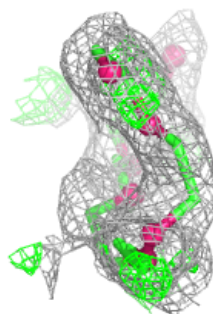
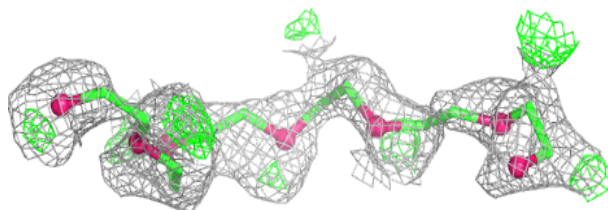
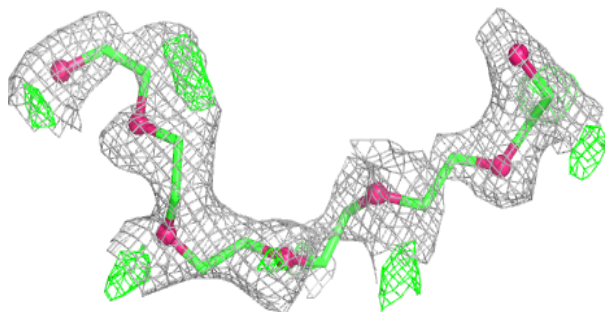
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G C 204:

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

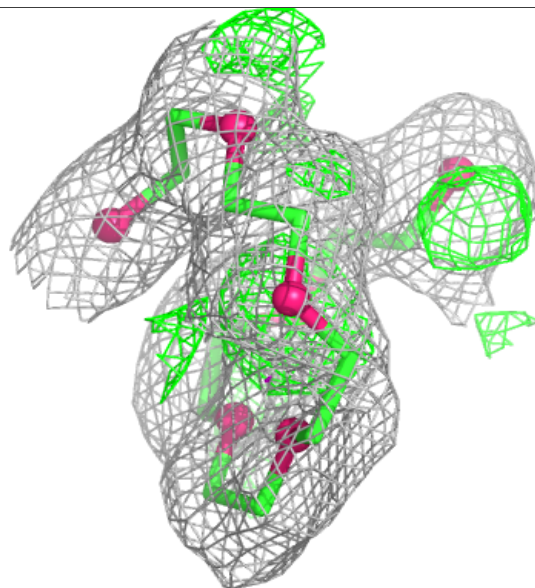
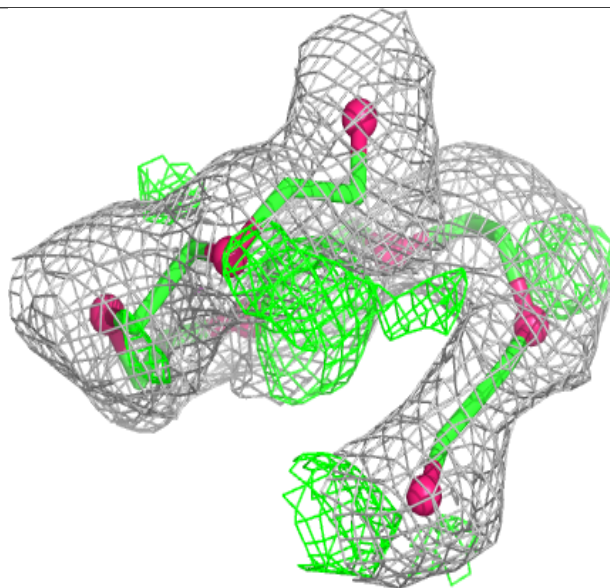
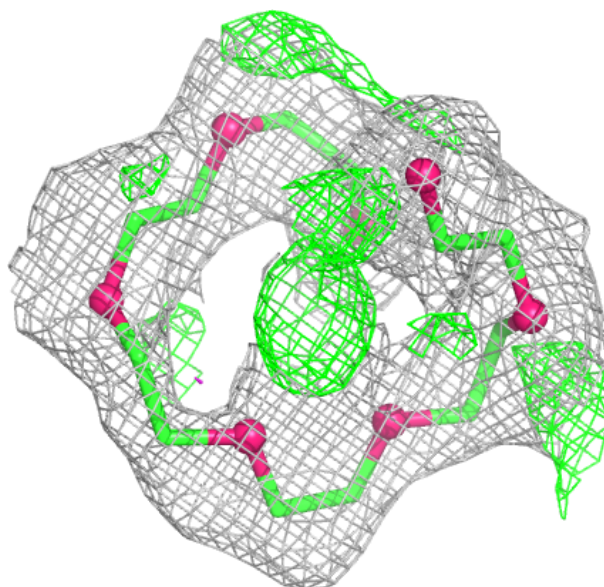
**Electron density around P6G C 205:**

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



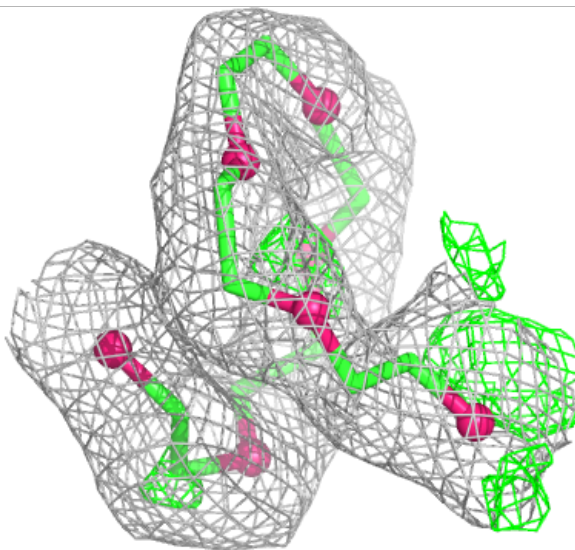
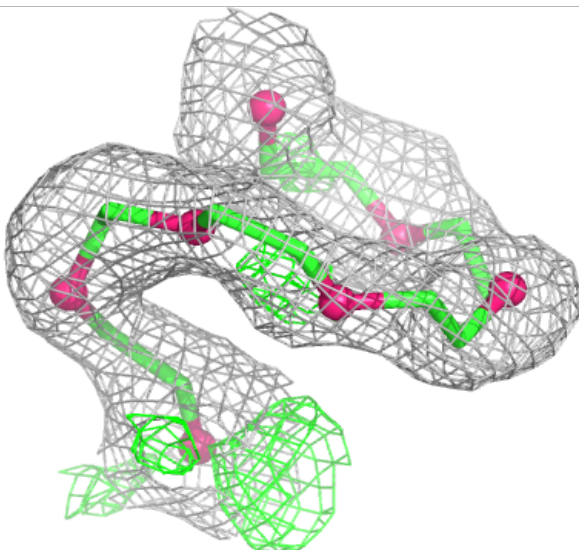
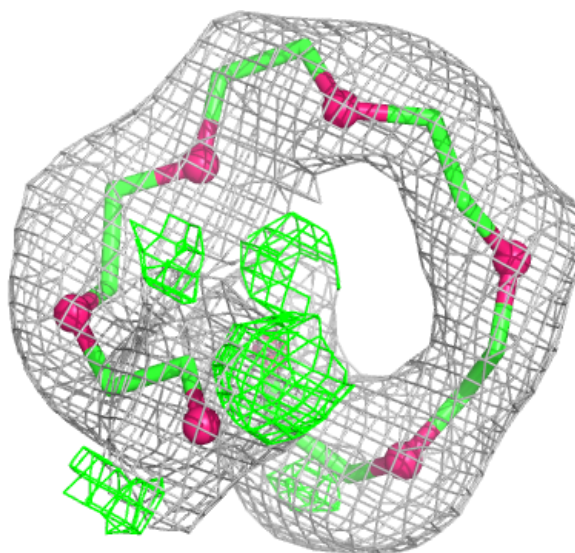
Electron density around P6G A 202:

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



Electron density around P6G B 202:

$2mF_o-DF_c$ (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.