Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2022 – 01:17 pm BST

PDB ID	:	7AOO
Title	:	Plasmoredoxin, a redox-active protein unique for malaria parasites
Authors	:	Fritz-Wolf, K.; Bathke, J.; Rahlfs, S.; Becker, K.
Deposited on	:	2020-10-14
Resolution	:	1.60 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 (i) symbol.

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

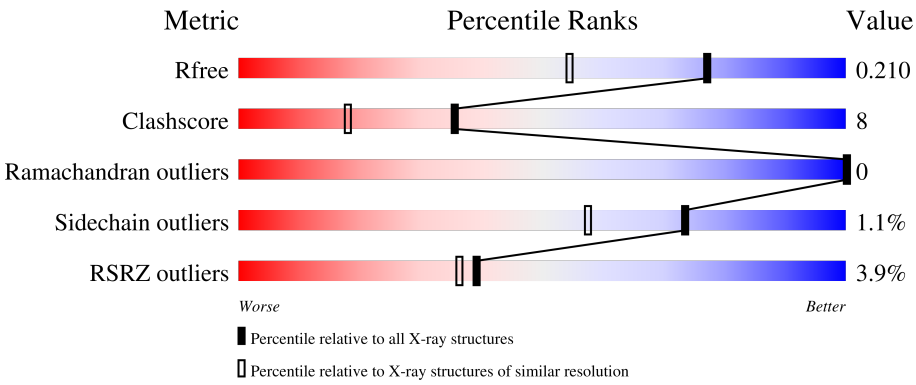
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	179	3% 77% 17% 6%
1	B	179	4% 75% 17% • 8%
1	C	179	4% 76% 11% 13%
1	D	179	2% 77% 11% • 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
3	PEG	B	203	-	-	X	-
3	PEG	B	206	-	-	X	-
3	PEG	B	207	-	-	X	-
3	PEG	D	204	-	-	X	-

2 Entry composition (i)

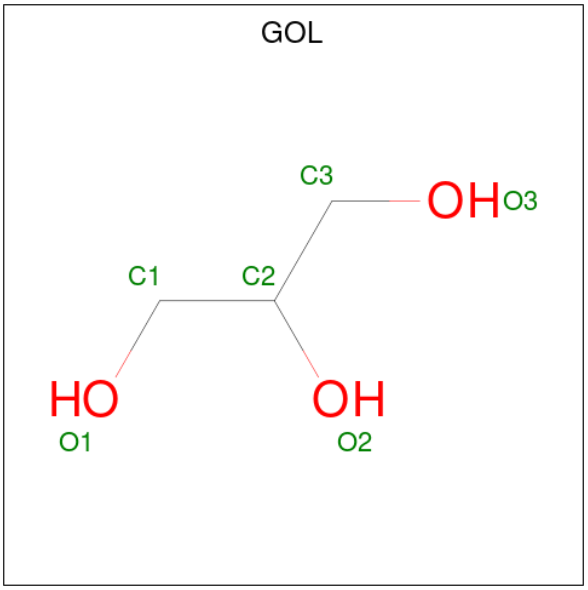
There are 6 unique types of molecules in this entry. The entry contains 6181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Plasmoredoxin.

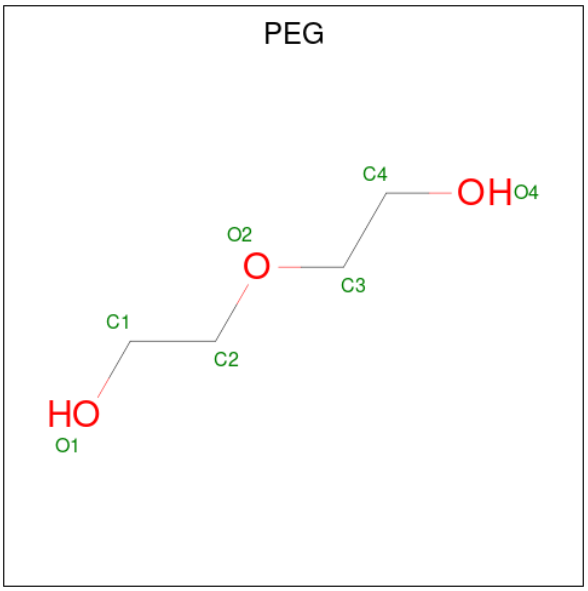
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	168	1467	973	227	262	5	0	2	0
1	B	165	1440	958	221	255	6	0	2	0
1	C	155	1344	896	207	236	5	0	0	0
1	D	160	1395	929	215	246	5	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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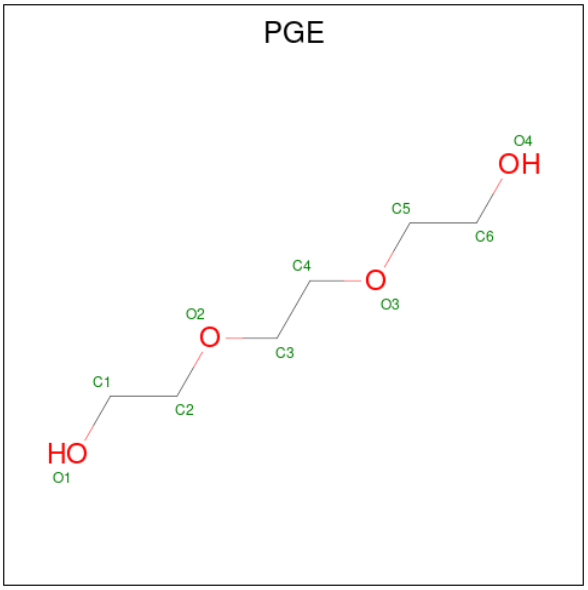
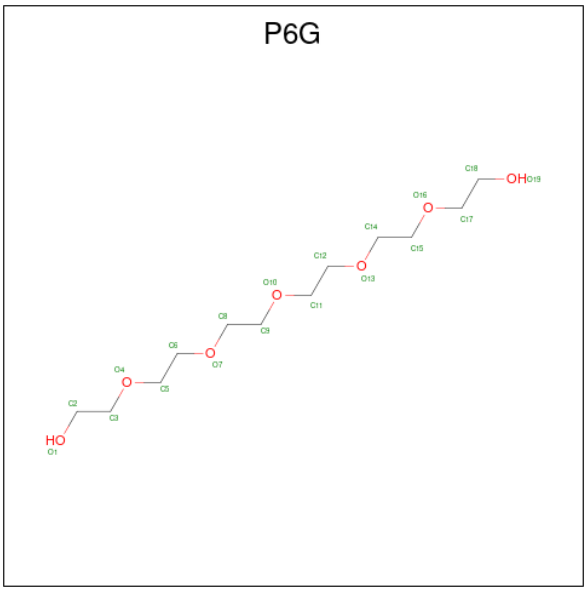
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	7	4	3	0	0
			Total	C	O		
3	D	1	7	4	3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
			Total	C	O		
4	B	1	10	6	4	0	0
			Total	C	O		
4	D	1	10	6	4	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	19	12	7	0	0
			Total	C	O		
5	C	1	19	12	7	0	0
			Total	C	O		
5	C	1	19	12	7	0	0
			Total	C	O		
5	D	1	19	12	7	0	0

- Molecule 6 is water.

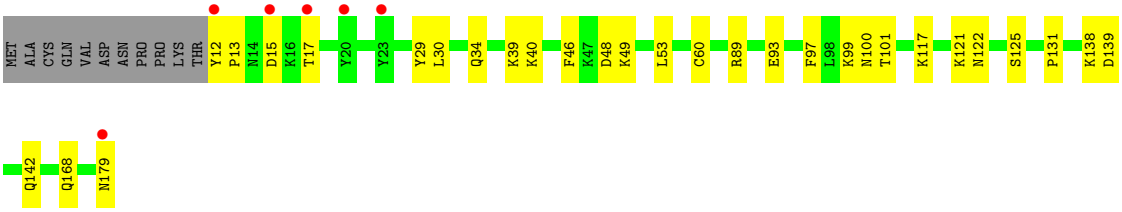
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	82	82	82	0	0
			Total	O		
6	B	80	80	80	0	0
			Total	O		
6	C	84	84	84	0	0
			Total	O		
6	D	65	65	65	0	0

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.

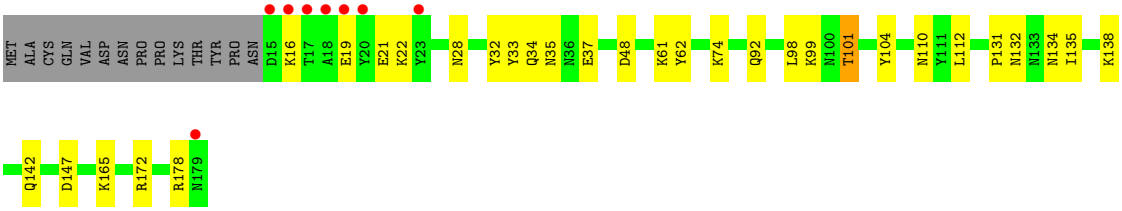
• Molecule 1: Plasmoredoxin

Chain A:



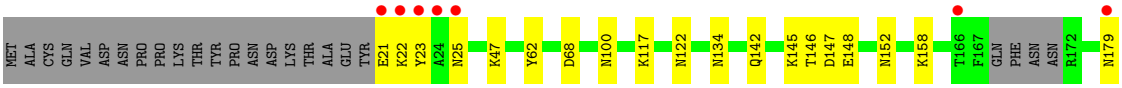
• Molecule 1: Plasmoredoxin

Chain B:



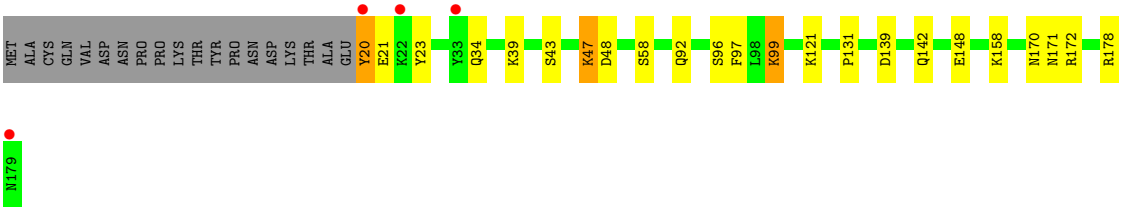
• Molecule 1: Plasmoredoxin

Chain C:



• Molecule 1: Plasmoredoxin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.75Å 122.73Å 72.86Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	46.26 – 1.60 46.26 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.26-1.60) 99.9 (46.26-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.178 , 0.210 0.178 , 0.210	Depositor DCC
R_{free} test set	5321 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6181	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, GOL, P6G, 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	0.81	0/1518	0.83	1/2053 (0.0%)
1	B	0.83	0/1489	0.87	3/2011 (0.1%)
1	C	0.81	0/1384	0.84	0/1868
1	D	0.80	0/1441	0.80	0/1947
All	All	0.81	0/5832	0.84	4/7879 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	53	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	B	172	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	101	THR	C-N-CA	-5.02	109.15	121.70

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	1467	0	1430	24	0
1	B	1440	0	1416	31	1
1	C	1344	0	1322	15	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1395	0	1366	21	0
2	A	6	0	8	3	0
3	A	7	0	10	0	0
3	B	49	0	70	12	2
3	C	21	0	30	1	0
3	D	35	0	50	11	0
4	A	10	0	14	1	0
4	B	10	0	14	2	0
4	D	10	0	14	2	0
5	C	57	0	78	3	0
5	D	19	0	26	3	0
6	A	82	0	0	3	0
6	B	80	0	0	4	0
6	C	84	0	0	5	0
6	D	65	0	0	3	0
All	All	6181	0	5848	95	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 8.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLU:OE2	1:B:22:LYS:NZ	2.06	0.87
1:D:170:ASN:O	3:D:204:PEG:H41	1.84	0.78
1:B:74:LYS:NZ	3:B:207:PEG:H22	2.00	0.76
1:B:142:GLN:HE22	1:C:142:GLN:HE22	1.39	0.70
1:A:139:ASP:HB3	1:A:142:GLN:NE2	2.06	0.70
1:C:146:THR:OG1	1:C:148:GLU:HG3	1.92	0.69
1:A:122:ASN:OD1	6:A:301:HOH:O	2.12	0.66
4:D:207:PGE:O1	4:D:207:PGE:O4	2.13	0.66
1:D:47:LYS:HE2	3:D:204:PEG:O1	1.97	0.64
1:A:99:LYS:HD3	2:A:201:GOL:H31	1.79	0.63
1:A:139:ASP:HB3	1:A:142:GLN:HE21	1.62	0.63
1:A:34:GLN:HB3	1:A:39:LYS:HE3	1.81	0.62
1:B:138:LYS:H	3:B:203:PEG:H11	1.66	0.61
1:B:142:GLN:HE22	1:C:142:GLN:NE2	1.98	0.61
6:B:305:HOH:O	1:C:152:ASN:HB3	2.00	0.61
1:A:122:ASN:ND2	6:A:302:HOH:O	2.34	0.60
1:C:47:LYS:HE2	6:C:343:HOH:O	2.01	0.60
1:C:122:ASN:ND2	6:C:301:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ASP:HB3	1:D:142:GLN:NE2	2.18	0.59
1:C:117:LYS:NZ	1:C:179:ASN:HB2	2.18	0.58
1:B:101:THR:O	1:B:101:THR:OG1	2.18	0.57
1:D:172:ARG:H	3:D:204:PEG:H12	1.69	0.57
5:C:205:P6G:H142	6:C:325:HOH:O	2.04	0.57
5:C:206:P6G:H82	6:C:319:HOH:O	2.05	0.56
1:B:74:LYS:HZ3	3:B:207:PEG:H22	1.70	0.56
1:A:60:CYS:SG	6:C:375:HOH:O	2.57	0.56
1:B:110:ASN:HD21	5:D:206:P6G:H112	1.70	0.56
1:D:172:ARG:H	3:D:204:PEG:C1	2.20	0.55
1:D:20:TYR:HD2	1:D:21:GLU:H	1.55	0.55
1:B:74:LYS:HZ2	3:B:207:PEG:H22	1.70	0.55
1:D:172:ARG:N	3:D:204:PEG:H12	2.23	0.54
1:D:23:TYR:HE2	1:D:178:ARG:HH22	1.55	0.54
1:A:138:LYS:HZ1	3:D:201:PEG:H32	1.71	0.54
1:A:48:ASP:HA	1:A:131:PRO:HB3	1.90	0.54
1:D:58:SER:HB3	1:D:97:PHE:HB2	1.89	0.54
1:B:34:GLN:HG2	1:B:35:ASN:ND2	2.24	0.53
1:B:134:ASN:HB3	3:B:206:PEG:H31	1.91	0.52
1:C:134:ASN:OD1	3:C:203:PEG:H41	2.08	0.52
1:A:138:LYS:HZ2	3:D:201:PEG:H22	1.76	0.51
1:D:171:ASN:ND2	3:D:204:PEG:H32	2.26	0.51
1:D:92:GLN:H	1:D:92:GLN:CD	2.14	0.51
1:C:100:ASN:HB3	5:C:205:P6G:H91	1.92	0.51
1:A:122:ASN:OD1	1:A:125:SER:OG	2.26	0.50
1:A:15:ASP:OD1	1:A:17:THR:HG23	2.12	0.50
1:C:117:LYS:HZ1	1:C:179:ASN:HB2	1.76	0.50
1:B:62:TYR:CE1	1:D:121:LYS:HD3	2.47	0.49
1:C:152:ASN:ND2	1:C:152:ASN:H	2.11	0.49
1:D:48:ASP:HA	1:D:131:PRO:HB3	1.94	0.48
1:A:117:LYS:NZ	1:A:179:ASN:OXT	2.30	0.48
1:D:34:GLN:HB3	1:D:39:LYS:HE3	1.96	0.48
1:B:138:LYS:CB	3:B:203:PEG:H11	2.44	0.47
1:B:32:TYR:CE2	4:B:208:PGE:H4	2.48	0.47
1:B:16:LYS:NZ	6:B:301:HOH:O	2.18	0.47
1:A:30:LEU:HD22	1:A:46:PHE:CE2	2.50	0.47
1:B:61:LYS:NZ	6:B:304:HOH:O	2.43	0.47
1:A:89:ARG:NH1	1:A:93:GLU:OE2	2.47	0.47
1:B:132:ASN:HB2	1:B:165:LYS:HG3	1.97	0.47
3:B:204:PEG:H22	3:B:204:PEG:H41	1.63	0.46
1:A:121:LYS:HD3	1:C:62:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:202:PEG:H11	6:D:324:HOH:O	2.15	0.46
1:A:12:TYR:HB3	1:A:13:PRO:HD3	1.97	0.46
1:D:23:TYR:HE2	1:D:178:ARG:NH2	2.13	0.46
1:B:16:LYS:HB3	1:B:19:GLU:HB2	1.97	0.46
1:A:99:LYS:HZ3	2:A:201:GOL:H32	1.81	0.46
3:B:205:PEG:H11	3:B:206:PEG:O4	2.15	0.45
1:D:43[B]:SER:OG	3:D:204:PEG:H22	2.16	0.45
1:B:112:LEU:HD11	5:D:206:P6G:H112	1.97	0.45
1:A:29:TYR:CD2	1:A:40:LYS:HE2	2.51	0.45
1:D:99:LYS:HB3	1:D:99:LYS:HE3	1.76	0.45
1:B:135:ILE:H	3:B:206:PEG:H41	1.82	0.44
1:B:138:LYS:H	3:B:203:PEG:C1	2.28	0.44
1:B:74:LYS:HB3	1:B:74:LYS:HE3	1.82	0.44
1:D:148:GLU:OE1	3:D:201:PEG:O4	2.21	0.44
4:D:207:PGE:HO4	4:D:207:PGE:HO1	1.61	0.44
1:D:47:LYS:N	6:D:308:HOH:O	2.51	0.43
1:D:158:LYS:HB3	1:D:158:LYS:HE3	1.69	0.43
1:B:110:ASN:HD21	5:D:206:P6G:C11	2.31	0.43
1:B:92:GLN:H	1:B:92:GLN:CD	2.20	0.43
1:B:33:TYR:CE1	1:B:99:LYS:HE2	2.53	0.43
1:A:168:GLN:NE2	6:A:306:HOH:O	2.51	0.43
1:B:48:ASP:HA	1:B:131:PRO:HB3	2.02	0.42
1:B:135:ILE:H	3:B:206:PEG:C4	2.32	0.42
1:B:21:GLU:OE2	6:B:302:HOH:O	2.22	0.42
1:C:146:THR:OG1	1:C:147:ASP:N	2.53	0.42
1:B:98[B]:LEU:HD23	1:B:98[B]:LEU:HA	1.80	0.42
1:D:96:SER:HB2	6:D:335:HOH:O	2.19	0.42
1:A:46:PHE:HA	1:A:49:LYS:HG3	2.00	0.42
1:C:22:LYS:O	1:C:25:ASN:HB2	2.21	0.41
1:B:104:TYR:OH	4:B:208:PGE:H5	2.20	0.41
1:A:100:ASN:ND2	4:A:203:PGE:O3	2.53	0.41
1:B:35:ASN:C	1:B:37:GLU:N	2.74	0.40
3:B:203:PEG:H11	3:B:203:PEG:H31	1.89	0.40
1:C:21:GLU:HG3	1:C:23:TYR:HE2	1.86	0.40
1:A:97:PHE:O	1:A:101:THR:HG23	2.21	0.40
1:A:99:LYS:CD	2:A:201:GOL:H31	2.51	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:C:68:ASP:OD1	3:B:207:PEG:C4[1_655]	1.38	0.82
1:B:35:ASN:ND2	1:C:145:LYS:O[1_455]	2.00	0.20
1:C:68:ASP:OD1	3:B:207:PEG:O4[1_655]	2.09	0.11

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	168/179 (94%)	163 (97%)	5 (3%)	0	100	100
1	B	165/179 (92%)	159 (96%)	6 (4%)	0	100	100
1	C	151/179 (84%)	146 (97%)	5 (3%)	0	100	100
1	D	159/179 (89%)	156 (98%)	3 (2%)	0	100	100
All	All	643/716 (90%)	624 (97%)	19 (3%)	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	162/170 (95%)	162 (100%)	0	100	100
1	B	159/170 (94%)	156 (98%)	3 (2%)	57	34
1	C	148/170 (87%)	147 (99%)	1 (1%)	84	73
1	D	154/170 (91%)	151 (98%)	3 (2%)	57	34
All	All	623/680 (92%)	616 (99%)	7 (1%)	73	57

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

Mol	Chain	Res	Type
1	B	28	ASN
1	B	147	ASP
1	B	178	ARG
1	C	158	LYS
1	D	20	TYR
1	D	47	LYS
1	D	99	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	142	GLN
1	B	28	ASN
1	B	35	ASN
1	B	100	ASN
1	B	142	GLN
1	C	163	HIS
1	D	95	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	PEG	C	201	-	6,6,6	0.46	0	5,5,5	0.38	0
5	P6G	D	206	-	18,18,18	0.62	0	17,17,17	0.84	1 (5%)
4	PGE	B	208	-	9,9,9	0.32	0	8,8,8	0.37	0
5	P6G	C	205	-	18,18,18	0.54	0	17,17,17	0.57	0
3	PEG	D	204	-	6,6,6	0.51	0	5,5,5	1.06	0
3	PEG	B	205	-	6,6,6	0.45	0	5,5,5	0.32	0
3	PEG	C	202	-	6,6,6	0.47	0	5,5,5	0.54	0
3	PEG	D	205	-	6,6,6	0.50	0	5,5,5	0.43	0
5	P6G	C	206	-	18,18,18	0.51	0	17,17,17	0.59	0
3	PEG	B	206	-	6,6,6	0.55	0	5,5,5	0.54	0
4	PGE	A	203	-	9,9,9	0.33	0	8,8,8	0.43	0
5	P6G	C	204	-	18,18,18	0.56	0	17,17,17	0.36	0
3	PEG	D	201	-	6,6,6	0.51	0	5,5,5	0.76	0
3	PEG	D	202	-	6,6,6	0.51	0	5,5,5	0.34	0
3	PEG	B	204	-	6,6,6	0.53	0	5,5,5	0.39	0
2	GOL	A	201	-	5,5,5	1.01	0	5,5,5	0.89	0
3	PEG	D	203	-	6,6,6	0.53	0	5,5,5	0.48	0
3	PEG	B	202	-	6,6,6	0.50	0	5,5,5	0.64	0
3	PEG	B	201	-	6,6,6	0.43	0	5,5,5	0.30	0
4	PGE	D	207	-	9,9,9	0.42	0	8,8,8	0.79	0
3	PEG	B	207	-	6,6,6	0.57	0	5,5,5	0.67	0
3	PEG	A	202	-	6,6,6	0.51	0	5,5,5	0.44	0
3	PEG	B	203	-	6,6,6	0.73	0	5,5,5	0.31	0
3	PEG	C	203	-	6,6,6	0.49	0	5,5,5	0.54	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
3	PEG	C	201	-	-	2/4/4/4	-
5	P6G	D	206	-	-	8/16/16/16	-
4	PGE	B	208	-	-	5/7/7/7	-
5	P6G	C	205	-	-	6/16/16/16	-
3	PEG	D	204	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	205	-	-	3/4/4/4	-
3	PEG	C	202	-	-	2/4/4/4	-
3	PEG	D	205	-	-	2/4/4/4	-
5	P6G	C	206	-	-	11/16/16/16	-
3	PEG	B	206	-	-	1/4/4/4	-
4	PGE	A	203	-	-	3/7/7/7	-
5	P6G	C	204	-	-	4/16/16/16	-
3	PEG	D	201	-	-	2/4/4/4	-
3	PEG	D	202	-	-	4/4/4/4	-
3	PEG	B	204	-	-	2/4/4/4	-
2	GOL	A	201	-	-	2/4/4/4	-
3	PEG	D	203	-	-	1/4/4/4	-
3	PEG	B	202	-	-	2/4/4/4	-
3	PEG	B	201	-	-	2/4/4/4	-
4	PGE	D	207	-	-	4/7/7/7	-
3	PEG	B	207	-	-	2/4/4/4	-
3	PEG	A	202	-	-	3/4/4/4	-
3	PEG	B	203	-	-	3/4/4/4	-
3	PEG	C	203	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	206	P6G	O10-C11-C12	2.14	120.03	110.39

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	203	PEG	C1-C2-O2-C3
5	D	206	P6G	O7-C8-C9-O10
5	C	206	P6G	O4-C5-C6-O7
5	D	206	P6G	O10-C11-C12-O13
5	C	206	P6G	O10-C11-C12-O13
3	D	202	PEG	O1-C1-C2-O2
3	D	202	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	B	208	PGE	O3-C5-C6-O4
4	D	207	PGE	O1-C1-C2-O2
5	C	205	P6G	O1-C2-C3-O4
5	D	206	P6G	C5-C6-O7-C8
5	C	204	P6G	O4-C5-C6-O7
3	B	201	PEG	O1-C1-C2-O2
3	B	207	PEG	O1-C1-C2-O2
3	B	207	PEG	O2-C3-C4-O4
3	D	201	PEG	O2-C3-C4-O4
4	A	203	PGE	O1-C1-C2-O2
2	A	201	GOL	O1-C1-C2-C3
5	C	206	P6G	O16-C17-C18-O19
2	A	201	GOL	O1-C1-C2-O2
3	D	203	PEG	O2-C3-C4-O4
3	D	204	PEG	O2-C3-C4-O4
5	C	206	P6G	C8-C9-O10-C11
3	B	204	PEG	C4-C3-O2-C2
3	B	203	PEG	O1-C1-C2-O2
3	B	205	PEG	O1-C1-C2-O2
3	A	202	PEG	O1-C1-C2-O2
5	C	205	P6G	O4-C5-C6-O7
5	C	205	P6G	O13-C14-C15-O16
5	C	206	P6G	O13-C14-C15-O16
4	B	208	PGE	O1-C1-C2-O2
5	C	204	P6G	O7-C8-C9-O10
4	A	203	PGE	O2-C3-C4-O3
3	B	204	PEG	O2-C3-C4-O4
5	D	206	P6G	O16-C17-C18-O19
5	C	205	P6G	O16-C17-C18-O19
3	B	205	PEG	C4-C3-O2-C2
3	B	202	PEG	O2-C3-C4-O4
3	C	202	PEG	O2-C3-C4-O4
5	C	204	P6G	O1-C2-C3-O4
5	D	206	P6G	O1-C2-C3-O4
3	B	206	PEG	C4-C3-O2-C2
3	C	201	PEG	C4-C3-O2-C2
4	D	207	PGE	C1-C2-O2-C3
5	C	205	P6G	C11-C12-O13-C14
3	D	204	PEG	C1-C2-O2-C3
4	B	208	PGE	C3-C4-O3-C5
3	B	203	PEG	C4-C3-O2-C2
3	C	203	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	D	202	PEG	C1-C2-O2-C3
3	B	201	PEG	C1-C2-O2-C3
3	A	202	PEG	O2-C3-C4-O4
3	C	203	PEG	O1-C1-C2-O2
3	D	205	PEG	O1-C1-C2-O2
4	D	207	PGE	O3-C5-C6-O4
5	D	206	P6G	C11-C12-O13-C14
4	B	208	PGE	O2-C3-C4-O3
5	D	206	P6G	C18-C17-O16-C15
3	D	201	PEG	C1-C2-O2-C3
5	C	204	P6G	C8-C9-O10-C11
5	C	206	P6G	C14-C15-O16-C17
3	C	202	PEG	C1-C2-O2-C3
4	D	207	PGE	C3-C4-O3-C5
5	D	206	P6G	C9-C8-O7-C6
3	B	202	PEG	C1-C2-O2-C3
3	D	205	PEG	C1-C2-O2-C3
3	D	204	PEG	O1-C1-C2-O2
3	A	202	PEG	C4-C3-O2-C2
4	B	208	PGE	C1-C2-O2-C3
4	A	203	PGE	C3-C4-O3-C5
3	B	205	PEG	C1-C2-O2-C3
3	C	201	PEG	O1-C1-C2-O2
5	C	206	P6G	C11-C12-O13-C14
5	C	206	P6G	C18-C17-O16-C15
5	C	206	P6G	C15-C14-O13-C12
3	D	202	PEG	C4-C3-O2-C2
5	C	206	P6G	C5-C6-O7-C8
5	C	205	P6G	C2-C3-O4-C5
5	C	206	P6G	O7-C8-C9-O10

There are no ring outliers.

16 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	206	P6G	3	0
4	B	208	PGE	2	0
5	C	205	P6G	2	0
3	D	204	PEG	7	0
3	B	205	PEG	1	0
5	C	206	P6G	1	0
3	B	206	PEG	4	0

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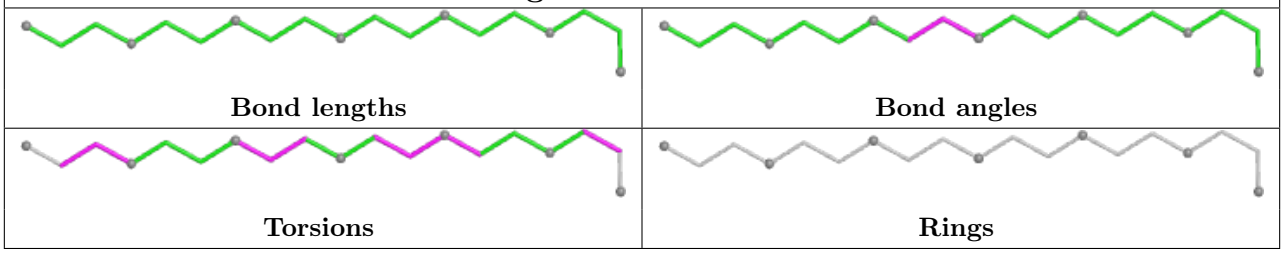
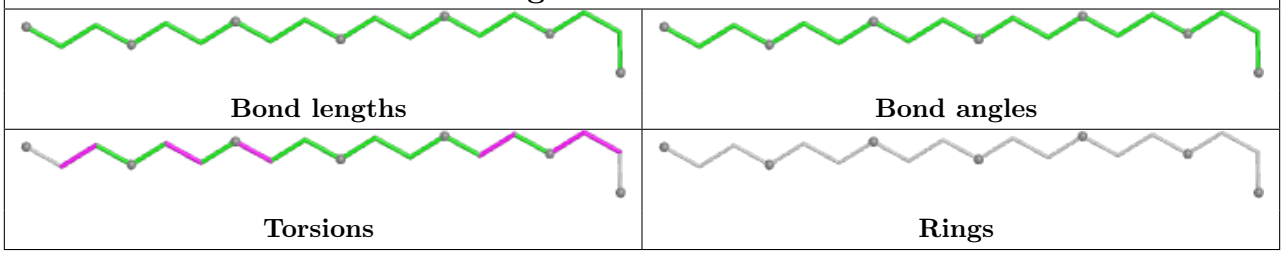
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	203	PGE	1	0
3	D	201	PEG	3	0
3	D	202	PEG	1	0
3	B	204	PEG	1	0
2	A	201	GOL	3	0
4	D	207	PGE	2	0
3	B	207	PEG	3	2
3	B	203	PEG	4	0
3	C	203	PEG	1	0

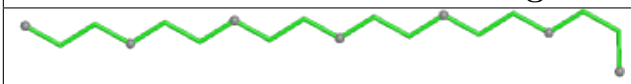
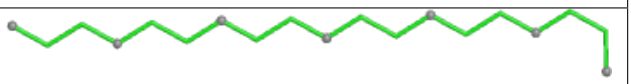
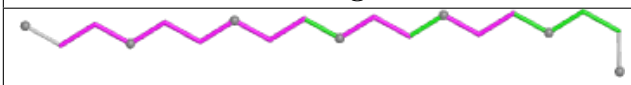
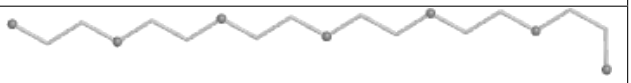
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

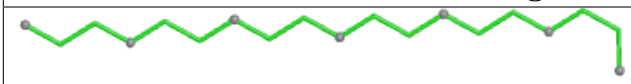
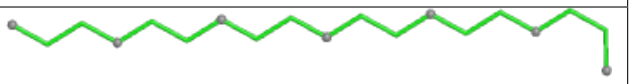
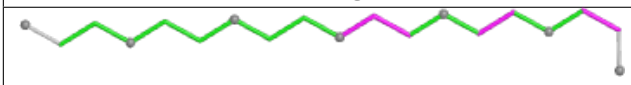
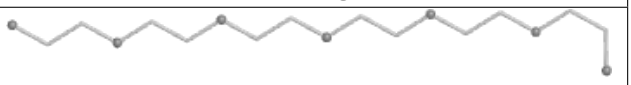
Ligand P6G D 206



Ligand P6G C 205



Ligand P6G C 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand P6G C 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	168/179 (93%)	-0.00	6 (3%)	42	40	19, 30, 57, 76	0
1	B	165/179 (92%)	0.29	8 (4%)	30	28	20, 29, 56, 81	0
1	C	155/179 (86%)	0.12	7 (4%)	33	30	19, 29, 53, 82	0
1	D	160/179 (89%)	-0.07	4 (2%)	57	55	20, 32, 55, 78	0
All	All	648/716 (90%)	0.09	25 (3%)	39	36	19, 30, 56, 82	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	7.4
1	B	179	ASN	7.3
1	C	23	TYR	7.1
1	C	24	ALA	5.7
1	C	179	ASN	5.7
1	B	15	ASP	5.4
1	B	16	LYS	5.4
1	A	179	ASN	5.1
1	D	179	ASN	5.1
1	B	17	THR	5.1
1	B	19	GLU	4.9
1	D	20	TYR	4.6
1	C	22	LYS	4.3
1	C	21	GLU	3.9
1	C	25	ASN	3.5
1	B	23	TYR	3.4
1	C	166	THR	3.4
1	A	15	ASP	3.4
1	A	23	TYR	3.4
1	B	18	ALA	3.3
1	A	17	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	20	TYR	2.9
1	D	22	LYS	2.4
1	A	20	TYR	2.3
1	D	33	TYR	2.1

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(Å^2)	Q<0.9
3	PEG	B	207	7/7	0.57	0.25	37,50,53,54	0
3	PEG	B	204	7/7	0.64	0.22	53,56,59,64	0
3	PEG	D	204	7/7	0.75	0.30	37,40,52,59	0
2	GOL	A	201	6/6	0.76	0.38	49,60,67,71	0
3	PEG	B	201	7/7	0.78	0.11	43,52,59,65	0
4	PGE	A	203	10/10	0.81	0.20	51,62,72,74	0
3	PEG	B	205	7/7	0.82	0.19	56,59,64,67	0
5	P6G	C	206	19/19	0.83	0.22	30,53,67,77	0
4	PGE	D	207	10/10	0.84	0.10	44,48,61,62	0
3	PEG	C	201	7/7	0.84	0.12	40,49,59,61	0
3	PEG	A	202	7/7	0.85	0.35	37,53,61,61	0
3	PEG	B	203	7/7	0.85	0.19	28,39,51,63	0
4	PGE	B	208	10/10	0.86	0.10	44,54,65,66	0
3	PEG	C	203	7/7	0.87	0.17	43,63,72,73	0
5	P6G	C	205	19/19	0.89	0.12	41,57,64,68	0
3	PEG	D	203	7/7	0.89	0.25	48,51,63,66	0
3	PEG	D	205	7/7	0.90	0.31	44,51,59,71	0
3	PEG	D	201	7/7	0.90	0.16	46,49,59,66	0
3	PEG	B	202	7/7	0.91	0.19	32,50,60,61	0

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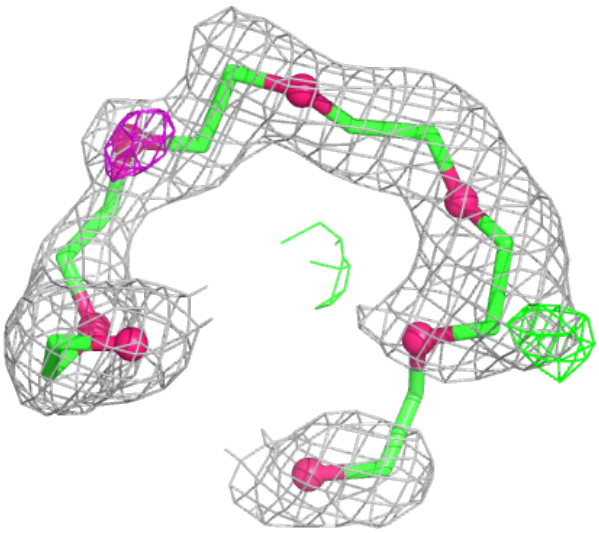
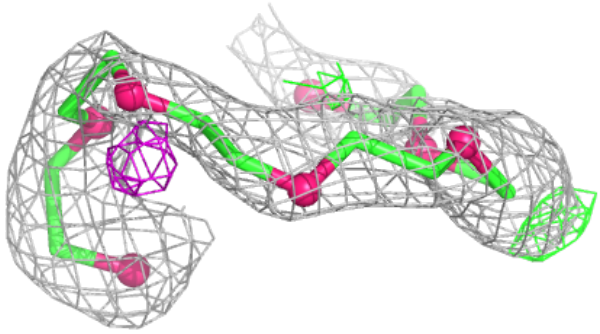
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	P6G	C	204	19/19	0.92	0.15	29,44,77,79	0
3	PEG	B	206	7/7	0.92	0.26	39,44,57,58	0
3	PEG	C	202	7/7	0.92	0.07	38,48,51,56	0
5	P6G	D	206	19/19	0.92	0.11	27,45,61,63	0
3	PEG	D	202	7/7	0.93	0.14	31,48,56,57	0

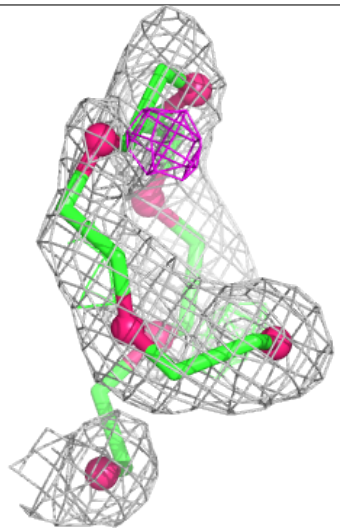
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G C 206:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

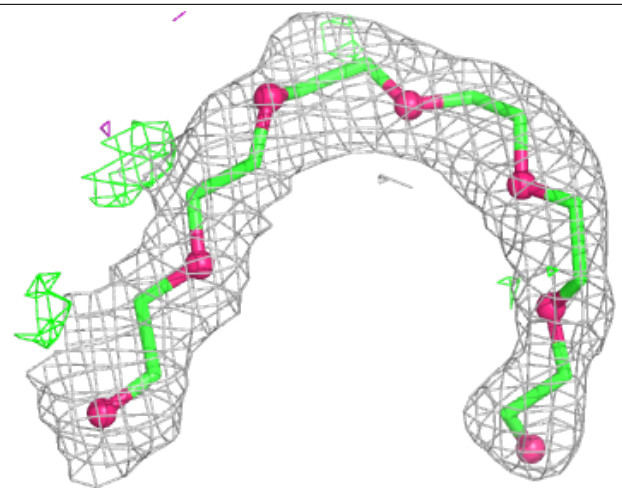


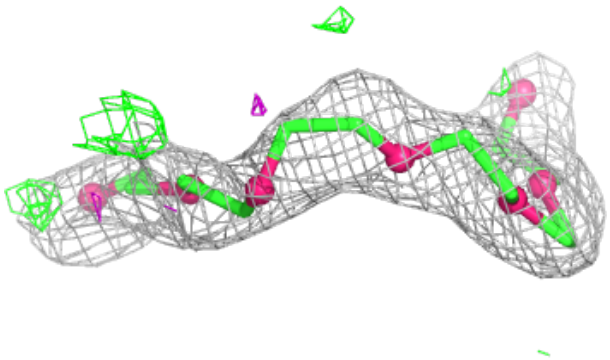




Electron density around P6G C 205:

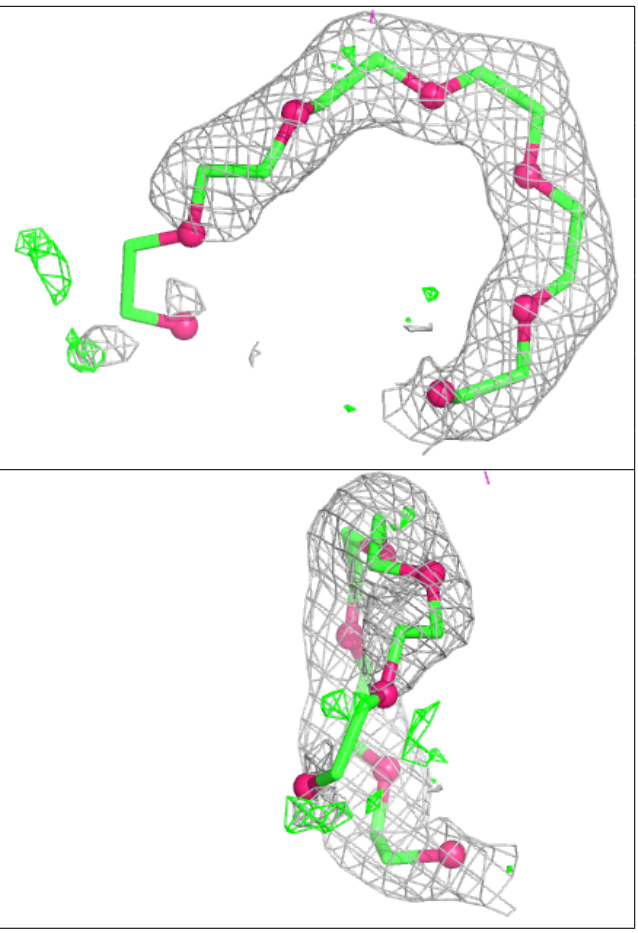
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

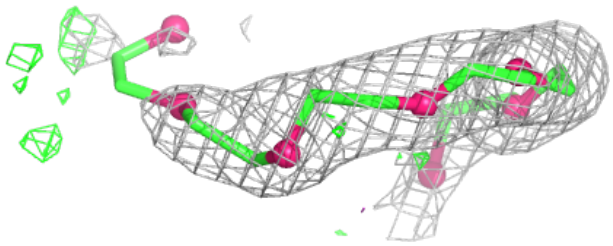




Electron density around P6G C 204:

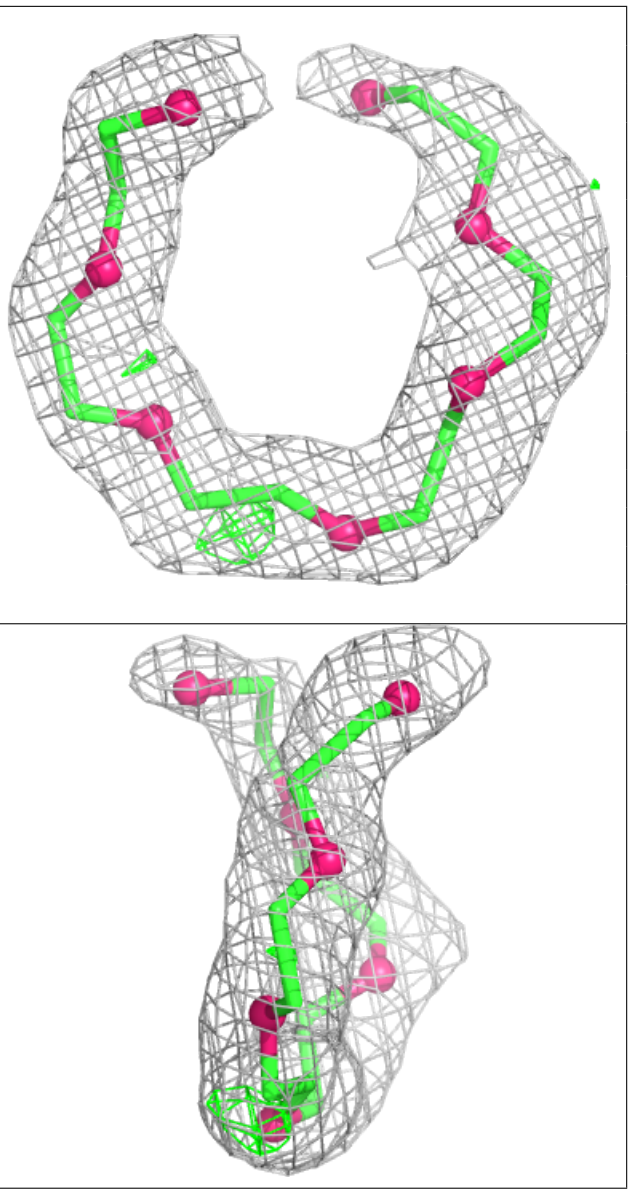
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around P6G D 206:

$2mF_o$-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.