



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2025 – 06:56 pm GMT

PDB ID : 9G7O
Title : Crystal structure of Janthinobacterium lividum PE-like toxin, Jlx
Authors : Masuyer, G.
Deposited on : 2024-07-22
Resolution : 1.75 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

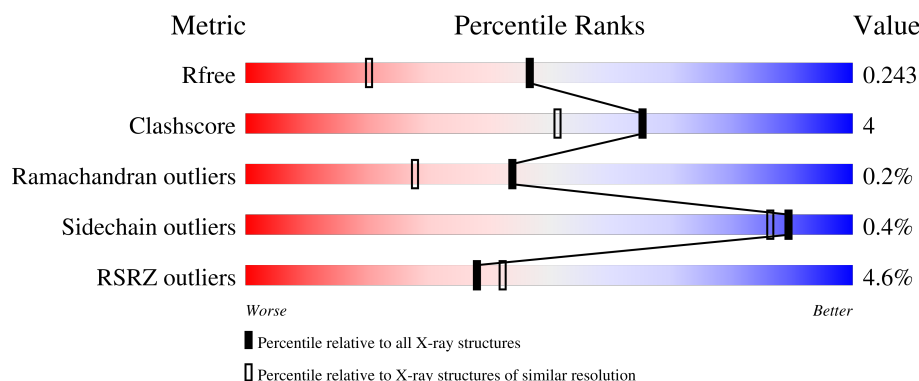
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	617	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>
1	B	617	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	C	617	<div> <div>5%</div> <div>93%</div> <div>6%</div> </div>
1	D	617	<div> <div>7%</div> <div>89%</div> <div>10%</div> </div>

2 Entry composition [i](#)

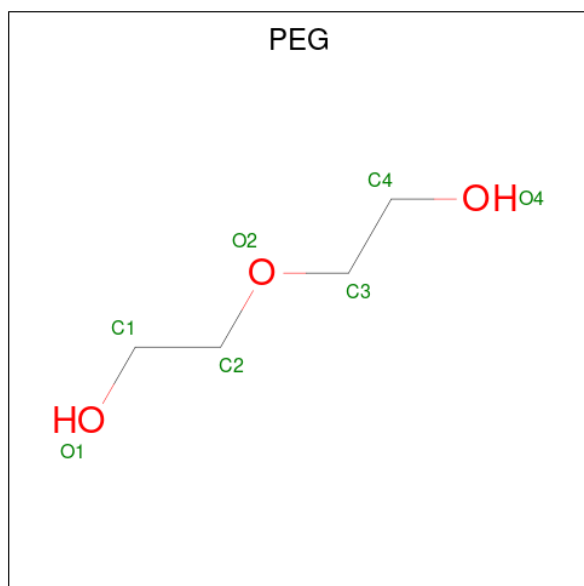
There are 7 unique types of molecules in this entry. The entry contains 39568 atoms, of which 18837 are hydrogens and 0 are deuteriums.

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 *Janthinobacterium lividum* PE-like toxin catalytically inactive mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	616	Total	C	H	N	O	S	129	2	0
			9475	3012	4693	848	907	15			
1	B	611	Total	C	H	N	O	S	126	0	0
			9369	2979	4643	838	895	14			
1	C	614	Total	C	H	N	O	S	128	0	0
			9408	2993	4660	841	900	14			
1	D	616	Total	C	H	N	O	S	129	1	0
			9458	3007	4684	847	906	14			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



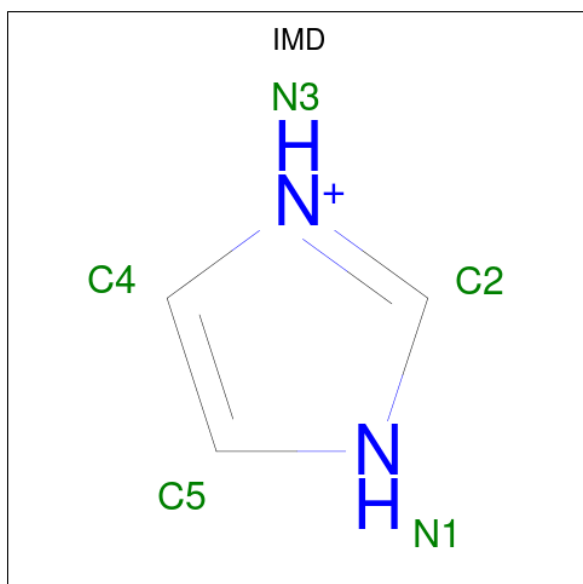
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			17	4	10	3		
2	A	1	Total	C	H	O	1	0
			17	4	10	3		

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

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

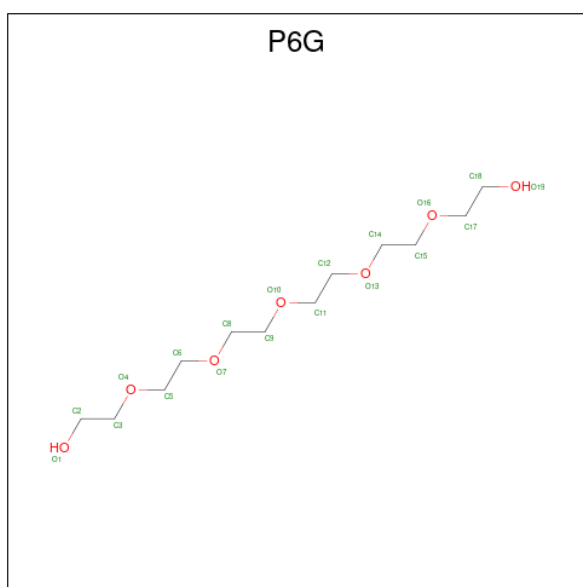


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			10	3	5	2		
3	A	1	Total	C	H	N	0	0
			10	3	5	2		
3	B	1	Total	C	H	N	0	0
			10	3	5	2		
3	C	1	Total	C	H	N	0	0
			10	3	5	2		
3	D	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $\text{C}_{12}\text{H}_{26}\text{O}_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 45	C 12	H 26	O 7	1	0
5	C	1	Total 45	C 12	H 26	O 7	1	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

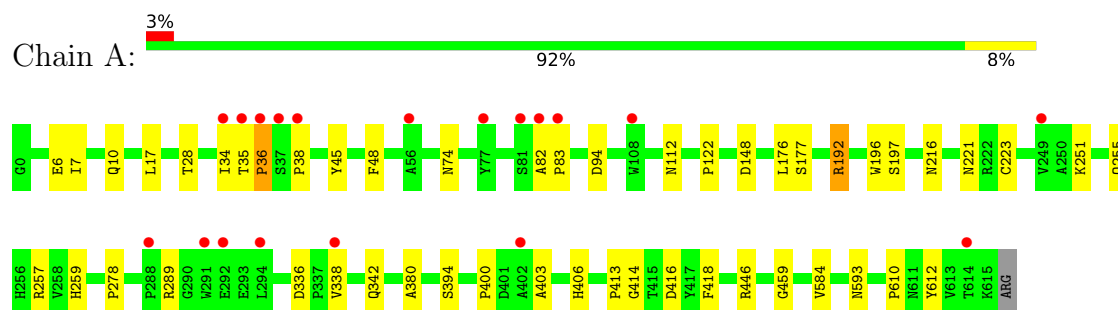
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	428	Total	O	0	0
			428	428		
7	B	385	Total	O	0	0
			385	385		
7	C	370	Total	O	0	0
			370	370		
7	D	390	Total	O	0	0
			390	390		

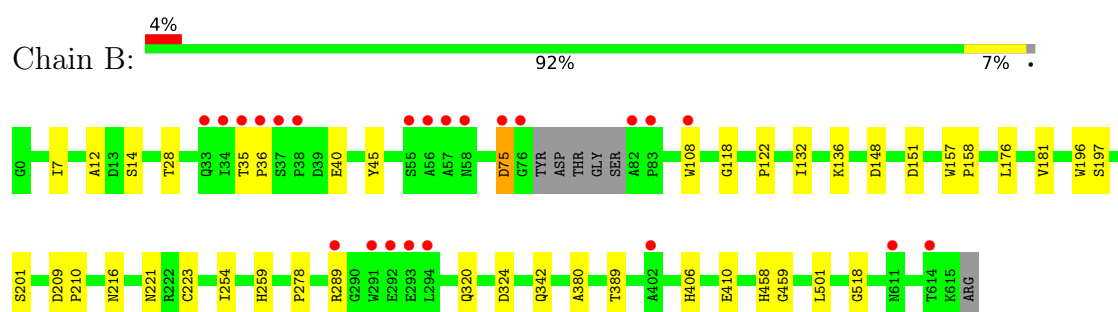
3 Residue-property plots [i](#)

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.

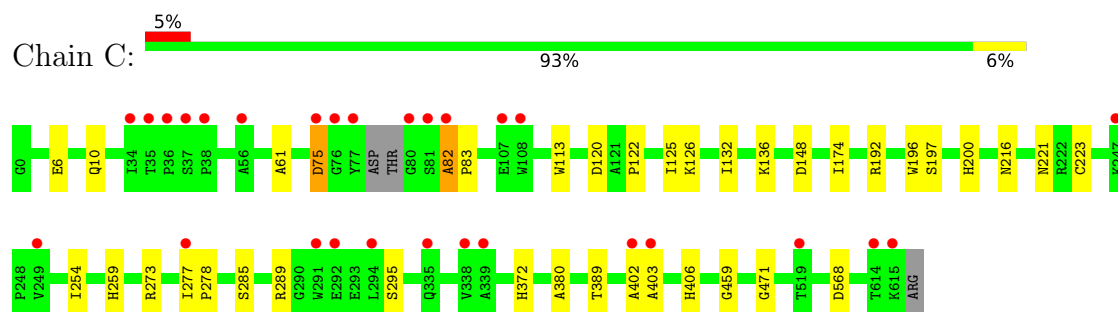
- Molecule 1: *Janthinobacterium lividum* PE-like toxin catalytically inactive mutant



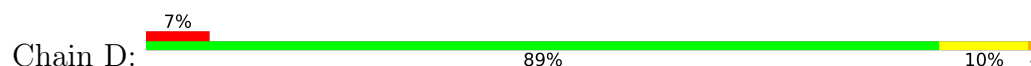
- Molecule 1: *Janthinobacterium lividum* PE-like toxin catalytically inactive mutant

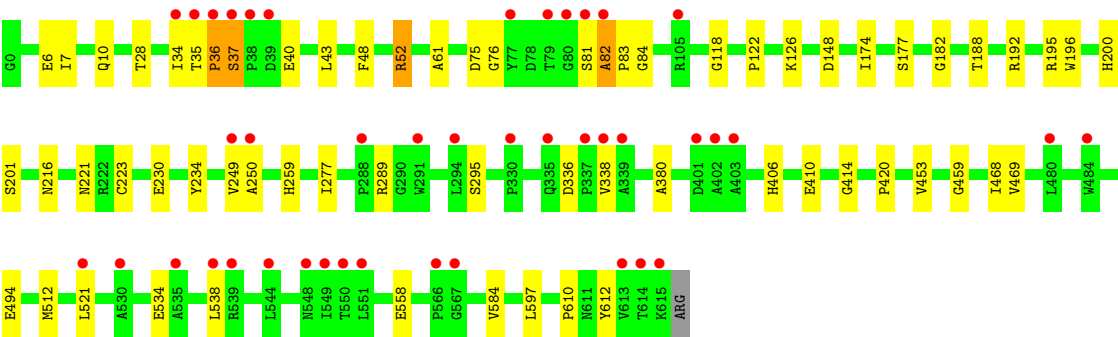


- Molecule 1: *Janthinobacterium lividum* PE-like toxin catalytically inactive mutant



- Molecule 1: *Janthinobacterium lividum* PE-like toxin catalytically inactive mutant





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.62Å 143.24Å 110.67Å 90.00° 119.35° 90.00°	Depositor
Resolution (Å)	115.60 – 1.75 115.60 – 1.75	Depositor EDS
% Data completeness (in resolution range)	61.1 (115.60-1.75) 61.1 (115.60-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.247 0.209 , 0.243	Depositor DCC
R_{free} test set	15312 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.046 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	39568	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % 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 1.5202e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, PEG, SO4, P6G, CL

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	0.64	0/4899	0.76	1/6674 (0.0%)
1	B	0.64	0/4841	0.76	0/6595
1	C	0.64	0/4864	0.75	0/6626
1	D	0.64	0/4891	0.77	0/6664
All	All	0.64	0/19495	0.76	1/26559 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	CG-CD-NE	5.31	122.95	111.80

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	4782	4693	4677	30	3
1	B	4726	4643	4628	28	0
1	C	4748	4660	4645	31	0
1	D	4774	4684	4669	49	3
2	A	14	20	20	2	0
2	B	14	20	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	14	20	20	0	0
2	D	14	20	20	0	0
3	A	10	10	10	2	0
3	B	5	5	5	3	0
3	C	5	5	5	1	0
3	D	5	5	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	B	19	26	26	0	0
5	C	19	26	26	0	0
6	B	5	0	0	1	0
7	A	428	0	0	1	0
7	B	385	0	0	5	0
7	C	370	0	0	5	0
7	D	390	0	0	4	1
All	All	20731	18837	18776	140	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (140) 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:D:82:ALA:HB3	1:D:83:PRO:HD3	1.42	1.01
1:C:82:ALA:HB3	1:C:83:PRO:HD3	1.42	1.00
1:A:82:ALA:HB3	1:A:83:PRO:HD3	1.51	0.92
1:C:82:ALA:CB	1:C:83:PRO:HD3	2.12	0.79
1:D:82:ALA:CB	1:D:83:PRO:HD3	2.17	0.74
1:D:75:ASP:HB2	7:D:838:HOH:O	1.89	0.73
4:D:704:CL:CL	7:D:987:HOH:O	2.45	0.71
1:D:336:ASP:OD1	1:D:338:VAL:HG12	1.91	0.71
1:C:568:ASP:O	7:C:801:HOH:O	2.09	0.71
1:B:459:GLY:H	3:B:704:IMD:H5	1.56	0.69
1:A:459:GLY:H	3:A:703:IMD:H2	1.56	0.68
1:C:75:ASP:HB2	7:C:804:HOH:O	1.95	0.65
1:D:380:ALA:O	1:D:406:HIS:HE1	1.81	0.64
1:A:336:ASP:OD1	1:A:338:VAL:HG12	1.97	0.64
1:B:289:ARG:NH2	7:B:801:HOH:O	2.31	0.63
1:D:34:ILE:HD11	1:D:43:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:MET:HE1	1:D:584:VAL:HG11	1.80	0.63
1:D:469:VAL:HG23	1:D:512:MET:CE	2.29	0.62
1:C:372:HIS:HE1	1:C:403:ALA:O	1.82	0.62
1:D:459:GLY:H	3:D:703:IMD:HN3	1.48	0.61
1:A:342:GLN:HG2	2:B:702:PEG:H42	1.81	0.61
1:D:52:ARG:HA	1:D:52:ARG:HE	1.65	0.61
1:C:277:ILE:HD12	1:C:295:SER:HA	1.84	0.60
1:A:380:ALA:O	1:A:406:HIS:HE1	1.84	0.59
1:A:35:THR:HB	1:A:36:PRO:HD3	1.83	0.59
1:A:216:ASN:HD22	1:A:221:ASN:HA	1.67	0.58
1:B:380:ALA:O	1:B:406:HIS:HE1	1.87	0.58
1:A:48:PHE:HB2	1:A:177:SER:HB2	1.85	0.58
1:B:35:THR:HB	1:B:36:PRO:HD3	1.87	0.57
1:C:277:ILE:CD1	1:C:295:SER:HA	2.35	0.57
1:C:372:HIS:CE1	1:C:403:ALA:O	2.58	0.57
1:A:216:ASN:HD21	1:A:223:CYS:HB2	1.70	0.56
1:D:126:LYS:HZ1	1:D:200:HIS:HD2	1.54	0.56
1:D:277:ILE:HD12	1:D:295:SER:HA	1.88	0.56
1:C:402:ALA:HB3	7:C:802:HOH:O	2.06	0.56
1:C:82:ALA:HB3	1:C:83:PRO:CD	2.26	0.56
1:D:216:ASN:HD22	1:D:221:ASN:HA	1.72	0.55
1:B:216:ASN:HD22	1:B:221:ASN:HA	1.71	0.55
1:A:10:GLN:NE2	7:A:808:HOH:O	2.39	0.54
1:D:148:ASP:OD2	1:D:259:HIS:HD2	1.89	0.54
2:B:702:PEG:H21	7:B:935:HOH:O	2.07	0.53
1:D:82:ALA:HB3	1:D:83:PRO:CD	2.27	0.53
1:D:469:VAL:HG23	1:D:512:MET:HE2	1.92	0.52
1:C:380:ALA:O	1:C:406:HIS:HE1	1.92	0.52
1:B:122:PRO:HD3	1:B:196:TRP:CD2	2.45	0.52
1:D:230:GLU:HB2	7:D:1027:HOH:O	2.10	0.52
1:C:148:ASP:OD2	1:C:259:HIS:HD2	1.92	0.51
1:C:82:ALA:CB	1:C:83:PRO:CD	2.86	0.51
1:C:402:ALA:CB	7:C:802:HOH:O	2.57	0.51
1:D:35:THR:N	1:D:36:PRO:CD	2.73	0.51
1:D:122:PRO:HD3	1:D:196:TRP:CD2	2.46	0.51
1:A:148:ASP:OD2	1:A:259:HIS:HD2	1.92	0.51
1:A:122:PRO:HD3	1:A:196:TRP:CD2	2.45	0.51
1:D:277:ILE:CD1	1:D:295:SER:HA	2.40	0.51
1:C:216:ASN:HB3	1:C:221:ASN:HD22	1.75	0.51
1:D:469:VAL:HG23	1:D:512:MET:HE3	1.92	0.50
1:B:320:GLN:NE2	1:B:324:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:SER:O	1:C:278:PRO:HB3	2.11	0.50
1:D:40:GLU:HG2	1:D:118:GLY:HA3	1.94	0.50
1:B:216:ASN:HD21	1:B:223:CYS:HB2	1.77	0.49
1:C:126:LYS:HZ1	1:C:200:HIS:HD2	1.60	0.49
1:D:216:ASN:HD21	1:D:223:CYS:HB2	1.77	0.49
1:B:201:SER:OG	1:B:410:GLU:OE2	2.20	0.48
1:C:285:SER:HB3	1:C:289:ARG:NH2	2.28	0.48
1:C:113:TRP:HA	1:C:126:LYS:O	2.13	0.48
1:A:197:SER:O	1:A:278:PRO:HB3	2.14	0.48
1:D:534:GLU:O	1:D:538:LEU:HG	2.13	0.48
1:A:257:ARG:NH2	1:A:403:ALA:O	2.33	0.48
1:C:406:HIS:HD2	7:C:901:HOH:O	1.96	0.48
1:A:413:PRO:HD2	1:A:416:ASP:OD2	2.15	0.47
1:B:148:ASP:OD2	1:B:259:HIS:HD2	1.96	0.47
1:A:17:LEU:HD11	1:A:176:LEU:HD12	1.97	0.47
1:A:414:GLY:HA3	1:A:584:VAL:O	2.15	0.47
1:A:82:ALA:CB	1:A:83:PRO:HD3	2.31	0.46
1:A:342:GLN:HA	2:B:702:PEG:H41	1.97	0.46
1:B:7:ILE:HB	1:B:28:THR:HG21	1.95	0.46
1:B:458:HIS:HA	3:B:704:IMD:H5	1.98	0.46
1:A:459:GLY:N	3:A:703:IMD:H2	2.27	0.46
1:B:40:GLU:HG2	1:B:118:GLY:HA3	1.99	0.45
1:B:197:SER:O	1:B:278:PRO:HB3	2.16	0.45
1:D:414:GLY:HA3	1:D:584:VAL:O	2.16	0.45
1:B:216:ASN:HB3	1:B:221:ASN:HD22	1.82	0.45
1:D:76:GLY:CA	1:D:81:SER:HB2	2.46	0.45
1:A:593:ASN:O	2:A:704:PEG:H41	2.16	0.45
1:D:61:ALA:HB1	1:D:174:ILE:HD11	1.99	0.45
1:D:84:GLY:HA2	7:D:1079:HOH:O	2.17	0.45
1:A:34:ILE:HG21	1:A:38:PRO:HB3	1.99	0.45
1:D:192:ARG:NH2	1:D:289:ARG:NH2	2.64	0.45
1:D:201:SER:OG	1:D:410:GLU:OE2	2.27	0.45
1:B:459:GLY:N	3:B:704:IMD:H5	2.28	0.45
1:A:192:ARG:NH2	1:A:289:ARG:NH2	2.65	0.45
2:A:704:PEG:H42	1:B:342:GLN:HA	2.00	0.44
1:D:122:PRO:HD3	1:D:196:TRP:CE2	2.52	0.44
1:B:254:ILE:HB	1:B:389:THR:HB	2.00	0.44
1:D:336:ASP:OD1	1:D:338:VAL:CG1	2.65	0.44
1:C:120:ASP:O	1:C:192:ARG:NE	2.45	0.43
1:C:216:ASN:HD21	1:C:223:CYS:HB2	1.82	0.43
1:C:61:ALA:HB1	1:C:174:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLY:HA3	1:D:234:TYR:CZ	2.53	0.43
1:A:418:PHE:O	1:A:446:ARG:NH1	2.51	0.43
1:D:216:ASN:ND2	1:D:221:ASN:HA	2.34	0.43
1:B:12:ALA:HA	7:B:1037:HOH:O	2.18	0.43
1:D:468:ILE:CG2	1:D:512:MET:HE1	2.48	0.43
1:B:75:ASP:HA	7:B:1099:HOH:O	2.19	0.43
1:B:14:SER:HA	1:B:176:LEU:O	2.19	0.42
1:A:45:TYR:O	1:A:112:ASN:HA	2.18	0.42
1:C:132:ILE:CG2	1:C:136:LYS:HA	2.49	0.42
1:D:34:ILE:CD1	1:D:43:LEU:HD21	2.47	0.42
1:D:469:VAL:CG2	1:D:512:MET:HE2	2.49	0.42
1:B:151:ASP:CG	6:B:706:SO4:O1	2.58	0.42
1:D:188:THR:HA	1:D:195:ARG:HD3	2.01	0.42
1:C:6:GLU:H	1:C:10:GLN:NE2	2.17	0.42
1:C:254:ILE:HB	1:C:389:THR:HB	2.01	0.42
1:D:35:THR:C	1:D:37:SER:H	2.23	0.42
1:B:216:ASN:ND2	1:B:221:ASN:HA	2.34	0.42
1:C:122:PRO:HD3	1:C:196:TRP:CD2	2.55	0.42
1:B:518:GLY:HA3	7:B:1167:HOH:O	2.20	0.42
1:D:61:ALA:CB	1:D:174:ILE:HD11	2.50	0.42
1:B:45:TYR:CD2	1:B:181:VAL:HG22	2.54	0.41
1:A:6:GLU:H	1:A:10:GLN:NE2	2.18	0.41
1:C:216:ASN:HB3	1:C:221:ASN:ND2	2.35	0.41
1:A:251:LYS:HE2	1:A:394:SER:OG	2.20	0.41
1:C:125:ILE:C	1:C:125:ILE:HD12	2.40	0.41
1:C:273:ARG:O	1:C:471:GLY:HA3	2.21	0.41
1:D:48:PHE:HB2	1:D:177:SER:HB2	2.02	0.41
1:D:249:VAL:HG23	1:D:250:ALA:N	2.35	0.41
1:B:209:ASP:N	1:B:210:PRO:CD	2.84	0.41
1:D:610:PRO:HG2	1:D:612:TYR:CE1	2.55	0.41
1:B:157:TRP:HA	1:B:158:PRO:HA	1.88	0.41
1:B:132:ILE:CG2	1:B:136:LYS:HA	2.51	0.41
1:C:459:GLY:H	3:C:704:IMD:HN3	1.68	0.41
1:D:7:ILE:HB	1:D:28:THR:HG21	2.01	0.41
1:D:216:ASN:HB3	1:D:221:ASN:HD22	1.84	0.41
1:A:610:PRO:HG2	1:A:612:TYR:CE1	2.56	0.41
1:D:82:ALA:CB	1:D:83:PRO:CD	2.91	0.40
1:D:453:VAL:HG21	1:D:521:LEU:HD21	2.04	0.40
1:D:494:GLU:HA	1:D:597:LEU:HD22	2.02	0.40
1:A:255:GLN:NE2	1:A:400:PRO:HD2	2.36	0.40
1:A:7:ILE:HB	1:A:28:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLU:H	1:D:10:GLN:NE2	2.20	0.40

All (4) 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:35:THR:HG23	1:D:420:PRO:HG2[4_546]	0.75	0.85
7:D:820:HOH:O	7:D:820:HOH:O[2_556]	1.57	0.63
1:A:35:THR:CG2	1:D:420:PRO:HG2[4_546]	1.35	0.25
1:A:35:THR:CG2	1:D:420:PRO:CG[4_546]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	616/617 (100%)	599 (97%)	16 (3%)	1 (0%)	44	28
1	B	607/617 (98%)	590 (97%)	17 (3%)	0	100	100
1	C	610/617 (99%)	595 (98%)	14 (2%)	1 (0%)	44	28
1	D	615/617 (100%)	595 (97%)	17 (3%)	3 (0%)	25	11
All	All	2448/2468 (99%)	2379 (97%)	64 (3%)	5 (0%)	44	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	82	ALA
1	A	36	PRO
1	D	37	SER
1	D	82	ALA
1	D	36	PRO

5.3.2 Protein sidechains ⓘ

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	507/506 (100%)	505 (100%)	2 (0%)	89	86
1	B	501/506 (99%)	498 (99%)	3 (1%)	84	78
1	C	503/506 (99%)	502 (100%)	1 (0%)	92	90
1	D	506/506 (100%)	504 (100%)	2 (0%)	89	86
All	All	2017/2024 (100%)	2009 (100%)	8 (0%)	89	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	94	ASP
1	B	75	ASP
1	B	108	TRP
1	B	501	LEU
1	C	75	ASP
1	D	52	ARG
1	D	558	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	33	GLN
1	A	112	ASN
1	A	190	HIS
1	A	200	HIS
1	A	216	ASN
1	A	244	ASN
1	A	259	HIS
1	A	327	HIS
1	A	406	HIS
1	B	10	GLN

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	112	ASN
1	B	200	HIS
1	B	216	ASN
1	B	221	ASN
1	B	244	ASN
1	B	259	HIS
1	B	406	HIS
1	C	10	GLN
1	C	33	GLN
1	C	112	ASN
1	C	200	HIS
1	C	216	ASN
1	C	221	ASN
1	C	244	ASN
1	C	259	HIS
1	C	287	GLN
1	C	327	HIS
1	C	372	HIS
1	C	406	HIS
1	D	10	GLN
1	D	33	GLN
1	D	74	ASN
1	D	112	ASN
1	D	200	HIS
1	D	216	ASN
1	D	221	ASN
1	D	244	ASN
1	D	259	HIS
1	D	406	HIS
1	D	611	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	D	701	-	6,6,6	0.23	0	5,5,5	0.20	0
3	IMD	D	703	-	3,5,5	0.27	0	4,5,5	0.69	0
5	P6G	C	701	-	18,18,18	0.22	0	17,17,17	0.10	0
3	IMD	A	703	-	3,5,5	0.28	0	4,5,5	0.68	0
5	P6G	B	701	-	18,18,18	0.17	0	17,17,17	0.20	0
2	PEG	D	702	-	6,6,6	0.13	0	5,5,5	0.13	0
2	PEG	C	703	-	6,6,6	0.12	0	5,5,5	0.10	0
2	PEG	C	702	-	6,6,6	0.18	0	5,5,5	0.16	0
2	PEG	B	703	-	6,6,6	0.15	0	5,5,5	0.12	0
2	PEG	A	704	-	6,6,6	0.22	0	5,5,5	0.26	0
3	IMD	A	702	-	3,5,5	0.28	0	4,5,5	0.67	0
3	IMD	C	704	-	3,5,5	0.26	0	4,5,5	0.72	0
2	PEG	A	701	-	6,6,6	0.17	0	5,5,5	0.10	0
3	IMD	B	704	-	3,5,5	0.44	0	4,5,5	0.71	0
2	PEG	B	702	-	6,6,6	0.17	0	5,5,5	0.17	0
6	SO4	B	706	-	4,4,4	0.37	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	D	701	-	-	2/4/4/4	-
3	IMD	D	703	-	-	-	0/1/1/1
5	P6G	C	701	-	-	3/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	A	703	-	-	-	0/1/1/1
5	P6G	B	701	-	-	9/16/16/16	-
2	PEG	D	702	-	-	1/4/4/4	-
2	PEG	C	703	-	-	2/4/4/4	-
2	PEG	C	702	-	-	2/4/4/4	-
2	PEG	B	703	-	-	3/4/4/4	-
2	PEG	A	704	-	-	3/4/4/4	-
3	IMD	A	702	-	-	-	0/1/1/1
3	IMD	C	704	-	-	-	0/1/1/1
2	PEG	A	701	-	-	0/4/4/4	-
3	IMD	B	704	-	-	-	0/1/1/1
2	PEG	B	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	704	PEG	O2-C3-C4-O4
2	C	702	PEG	O2-C3-C4-O4
5	B	701	P6G	O1-C2-C3-O4
2	A	704	PEG	O1-C1-C2-O2
2	C	703	PEG	O1-C1-C2-O2
2	D	702	PEG	O2-C3-C4-O4
5	B	701	P6G	O16-C17-C18-O19
2	B	703	PEG	O1-C1-C2-O2
2	D	701	PEG	O2-C3-C4-O4
2	B	702	PEG	O1-C1-C2-O2
2	B	702	PEG	O2-C3-C4-O4
5	B	701	P6G	O4-C5-C6-O7
2	B	703	PEG	O2-C3-C4-O4
5	B	701	P6G	C15-C14-O13-C12
5	B	701	P6G	C8-C9-O10-C11
5	B	701	P6G	C11-C12-O13-C14
5	C	701	P6G	C8-C9-O10-C11
5	B	701	P6G	C5-C6-O7-C8
2	A	704	PEG	C1-C2-O2-C3
5	B	701	P6G	C12-C11-O10-C9

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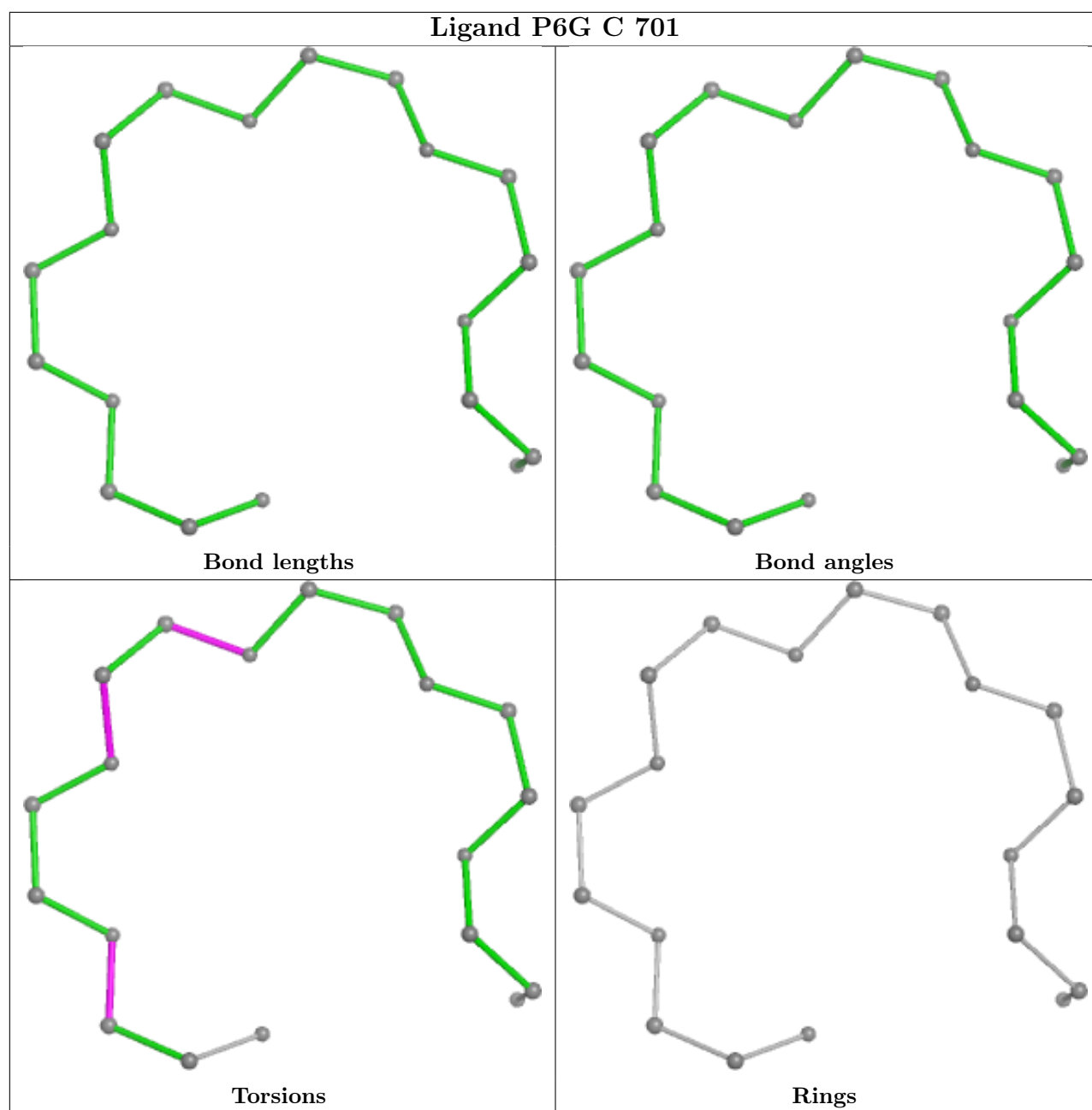
Mol	Chain	Res	Type	Atoms
5	C	701	P6G	C9-C8-O7-C6
5	C	701	P6G	C2-C3-O4-C5
2	C	703	PEG	C4-C3-O2-C2
2	B	703	PEG	C4-C3-O2-C2
2	D	701	PEG	C4-C3-O2-C2
5	B	701	P6G	C9-C8-O7-C6
2	C	702	PEG	C1-C2-O2-C3

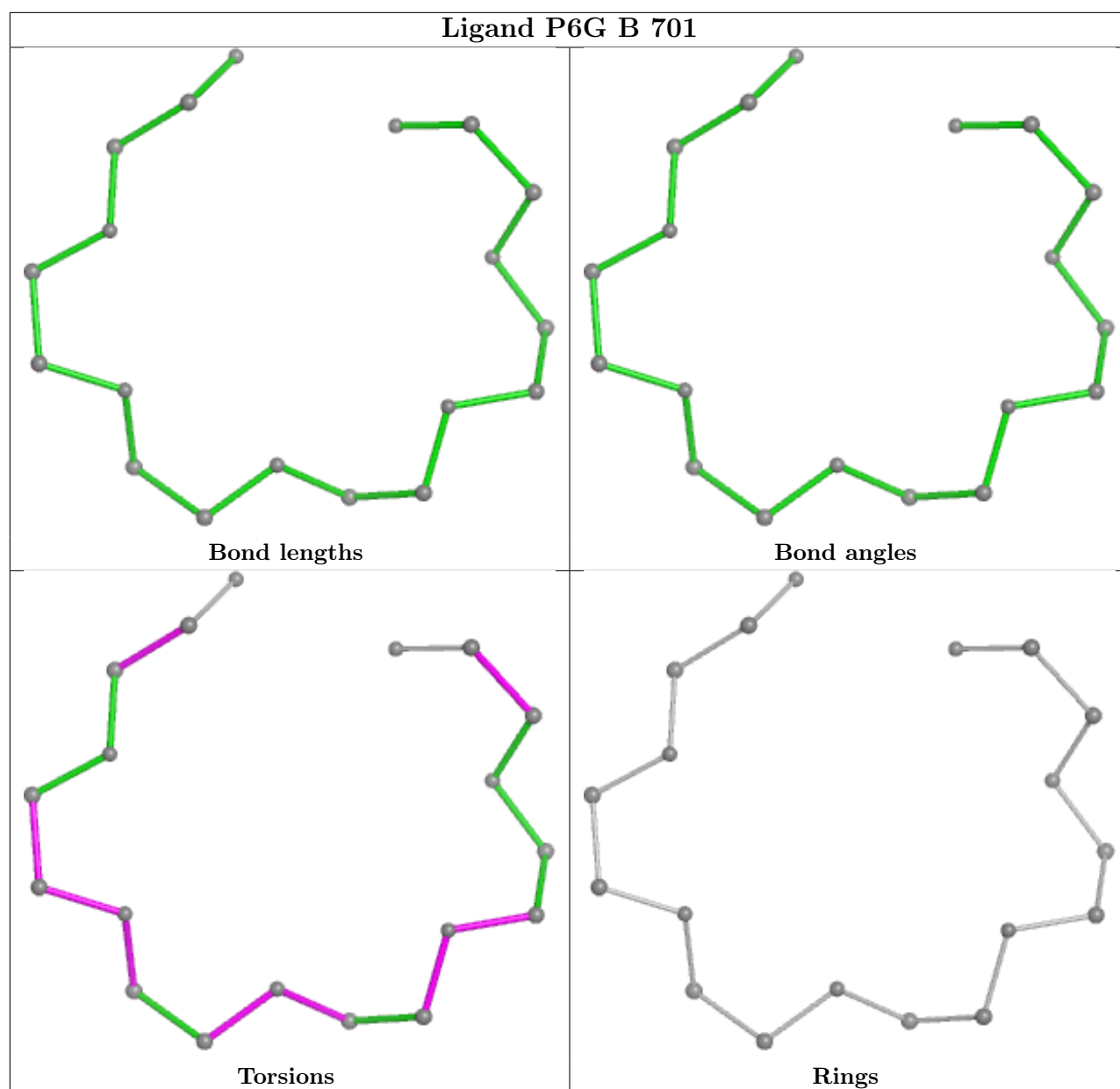
There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	IMD	1	0
3	A	703	IMD	2	0
2	A	704	PEG	2	0
3	C	704	IMD	1	0
3	B	704	IMD	3	0
2	B	702	PEG	3	0
6	B	706	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	616/617 (99%)	0.11	19 (3%)	51	59	16, 28, 53, 104	2 (0%)
1	B	611/617 (99%)	0.20	23 (3%)	44	51	17, 30, 55, 96	0
1	C	614/617 (99%)	0.26	28 (4%)	38	42	17, 30, 55, 104	0
1	D	616/617 (99%)	0.25	42 (6%)	25	28	14, 29, 57, 111	1 (0%)
All	All	2457/2468 (99%)	0.20	112 (4%)	38	42	14, 29, 55, 111	3 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	TYR	6.9
1	A	36	PRO	5.9
1	B	57	ALA	5.7
1	D	34	ILE	5.6
1	C	34	ILE	5.5
1	D	35	THR	5.4
1	D	249	VAL	5.3
1	B	82	ALA	5.2
1	C	36	PRO	5.0
1	D	82	ALA	5.0
1	B	76	GLY	4.9
1	A	82	ALA	4.8
1	D	38	PRO	4.7
1	B	294	LEU	4.7
1	A	34	ILE	4.6
1	D	36	PRO	4.4
1	B	56	ALA	4.3
1	A	35	THR	4.3
1	B	35	THR	4.3
1	C	35	THR	4.2
1	C	37	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	36	PRO	4.2
1	C	80	GLY	4.1
1	A	38	PRO	4.0
1	D	402	ALA	4.0
1	C	38	PRO	3.9
1	C	82	ALA	3.9
1	A	338	VAL	3.9
1	D	338	VAL	3.9
1	B	34	ILE	3.8
1	C	294	LEU	3.7
1	A	291	TRP	3.6
1	B	291	TRP	3.6
1	B	293	GLU	3.6
1	A	37	SER	3.5
1	B	58	ASN	3.5
1	C	291	TRP	3.5
1	C	402	ALA	3.4
1	B	402	ALA	3.4
1	D	614	THR	3.2
1	D	544	LEU	3.2
1	D	250	ALA	3.2
1	C	81	SER	3.1
1	B	38	PRO	3.0
1	A	108	TRP	3.0
1	D	291	TRP	3.0
1	B	83	PRO	3.0
1	A	402	ALA	3.0
1	D	551	LEU	3.0
1	A	249	VAL	3.0
1	D	613	VAL	3.0
1	D	37	SER	2.9
1	D	81	SER	2.9
1	D	530	ALA	2.9
1	A	81	SER	2.9
1	D	535	ALA	2.9
1	C	247	LYS	2.9
1	C	615	LYS	2.8
1	D	403	ALA	2.8
1	C	56	ALA	2.8
1	C	403	ALA	2.8
1	C	292	GLU	2.8
1	B	289	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	294	LEU	2.7
1	D	330	PRO	2.6
1	D	39	ASP	2.6
1	D	550	THR	2.6
1	C	339	ALA	2.6
1	B	614	THR	2.6
1	C	338	VAL	2.6
1	D	294	LEU	2.5
1	B	611	ASN	2.5
1	A	77	TYR	2.5
1	D	77	TYR	2.5
1	A	83	PRO	2.5
1	C	519	THR	2.5
1	C	249	VAL	2.5
1	C	277	ILE	2.4
1	A	288	PRO	2.4
1	C	108	TRP	2.4
1	B	55	SER	2.4
1	D	335	GLN	2.4
1	D	339	ALA	2.3
1	D	521	LEU	2.3
1	D	337	PRO	2.3
1	C	76	GLY	2.3
1	C	614	THR	2.3
1	B	108	TRP	2.2
1	D	484	TRP	2.2
1	C	75	ASP	2.2
1	D	567	GLY	2.2
1	A	56	ALA	2.2
1	A	292	GLU	2.2
1	D	105	ARG	2.2
1	D	566	PRO	2.2
1	C	335	GLN	2.2
1	D	548	ASN	2.2
1	D	80	GLY	2.2
1	D	480	LEU	2.1
1	D	538	LEU	2.1
1	D	539	ARG	2.1
1	B	37	SER	2.1
1	D	615	LYS	2.1
1	B	75	ASP	2.1
1	D	79	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	288	PRO	2.1
1	D	549	ILE	2.1
1	A	614	THR	2.0
1	B	292	GLU	2.0
1	C	107	GLU	2.0
1	B	33	GLN	2.0
1	D	401	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IMD	A	702	5/5	0.76	0.22	53,55,57,58	0
6	SO4	B	706	5/5	0.78	0.14	77,77,80,84	0
3	IMD	B	704	5/5	0.80	0.20	43,48,51,52	0
2	PEG	D	701	7/7	0.82	0.15	41,45,47,47	1
2	PEG	A	701	7/7	0.83	0.19	52,57,59,59	1
3	IMD	A	703	5/5	0.84	0.16	40,43,44,45	0
2	PEG	B	703	7/7	0.85	0.14	46,50,52,53	1
2	PEG	D	702	7/7	0.85	0.18	58,64,72,72	1
2	PEG	C	703	7/7	0.87	0.14	56,58,59,60	1
3	IMD	D	703	5/5	0.88	0.13	37,40,42,42	0
5	P6G	B	701	19/19	0.89	0.14	56,59,67,67	1
5	P6G	C	701	19/19	0.89	0.15	53,63,83,84	1
2	PEG	C	702	7/7	0.89	0.12	44,46,48,49	1
2	PEG	A	704	7/7	0.90	0.10	32,36,50,50	1
2	PEG	B	702	7/7	0.91	0.09	41,42,43,44	1
3	IMD	C	704	5/5	0.91	0.11	38,40,41,41	0

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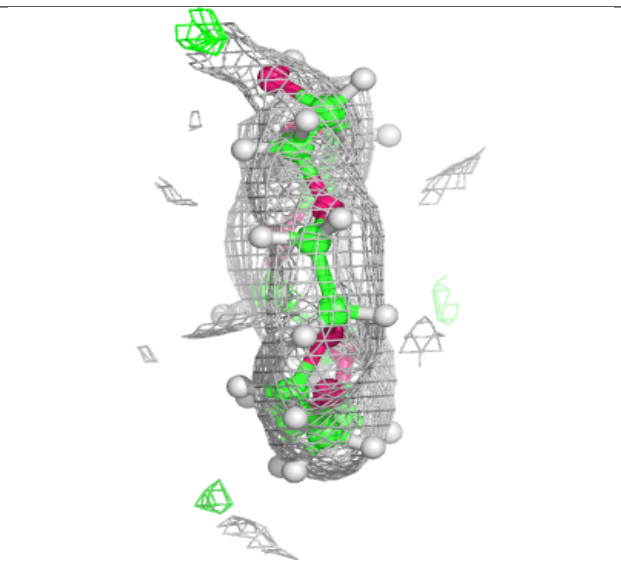
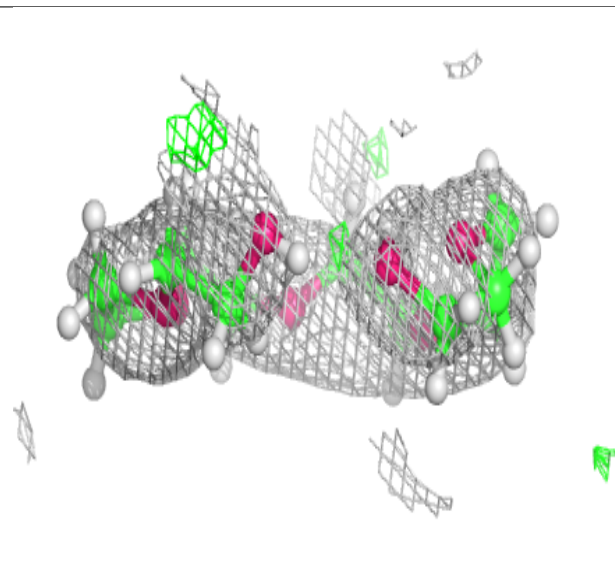
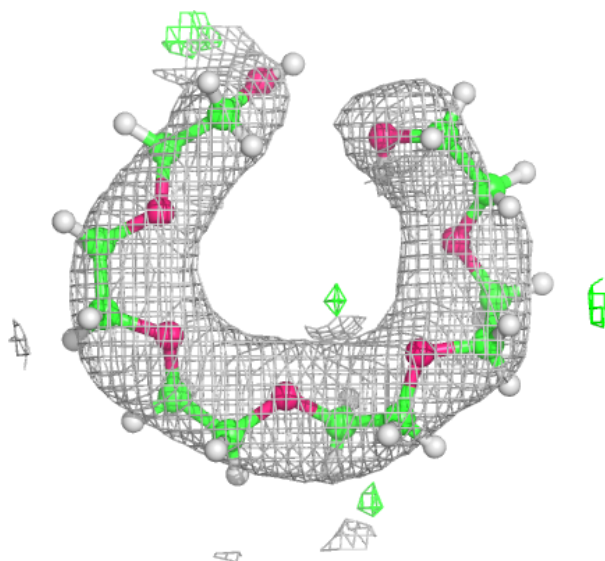
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	D	704	1/1	0.94	0.08	48,48,48,48	0
4	CL	C	705	1/1	0.94	0.09	49,49,49,49	0
4	CL	B	705	1/1	0.96	0.07	48,48,48,48	0
4	CL	A	705	1/1	0.96	0.07	46,46,46,46	0

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.

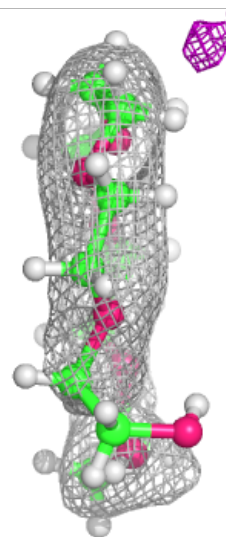
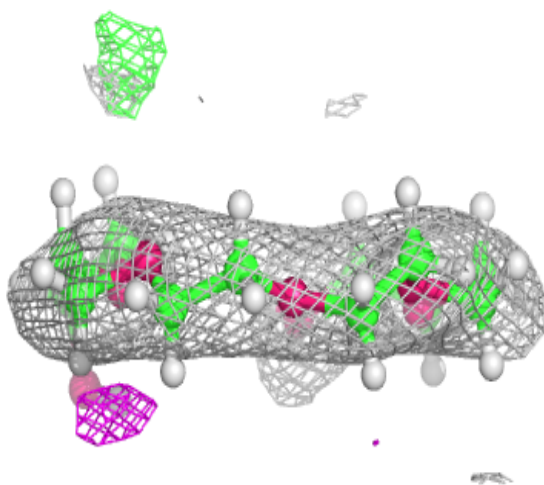
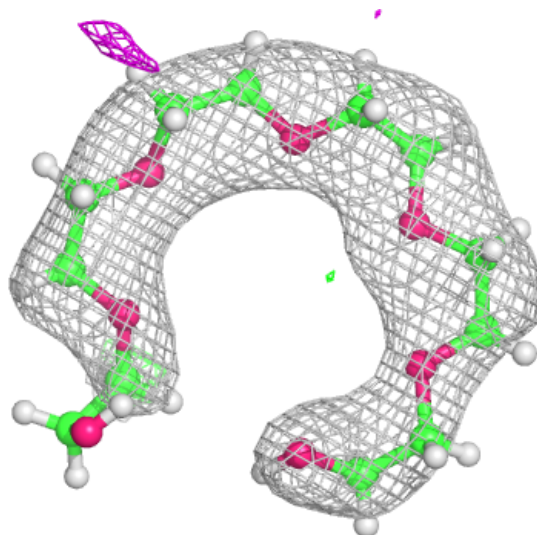
Electron density around P6G B 701:

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 701:

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.