



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 12:11 PM EST

PDB ID : 7KOH  
Title : Crystal structure of antigen 43 from Escherichia coli EDL933  
Authors : Vo, J.L.; Paxman, J.J.; Heras, B.  
Deposited on : 2020-11-09  
Resolution : 2.98 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

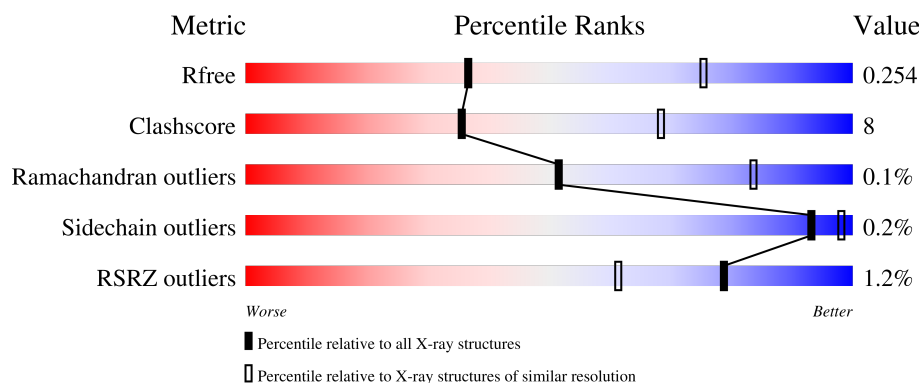
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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  $\geq 3$ , 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	565	<div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	B	565	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	C	565	<div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	D	565	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>

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	PEG	A	610	-	-	-	X
2	PEG	B	608	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16189 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 Antigen 43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			3860	2326	708	823	3			
1	B	544	Total	C	N	O	S	0	0	0
			3865	2329	709	824	3			
1	C	545	Total	C	N	O	S	0	0	0
			3874	2334	711	826	3			
1	D	544	Total	C	N	O	S	0	0	0
			3866	2330	709	824	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8X9L4
A	-1	ASN	-	expression tag	UNP Q8X9L4
A	0	ALA	-	expression tag	UNP Q8X9L4
B	-2	SER	-	expression tag	UNP Q8X9L4
B	-1	ASN	-	expression tag	UNP Q8X9L4
B	0	ALA	-	expression tag	UNP Q8X9L4
C	-2	SER	-	expression tag	UNP Q8X9L4
C	-1	ASN	-	expression tag	UNP Q8X9L4
C	0	ALA	-	expression tag	UNP Q8X9L4
D	-2	SER	-	expression tag	UNP Q8X9L4
D	-1	ASN	-	expression tag	UNP Q8X9L4
D	0	ALA	-	expression tag	UNP Q8X9L4

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



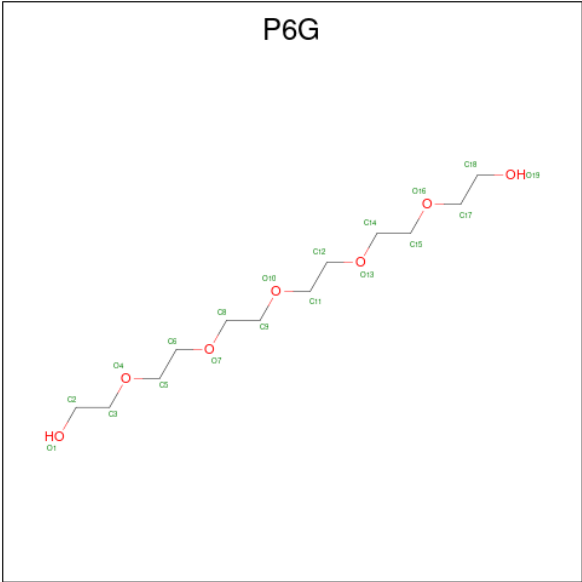
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

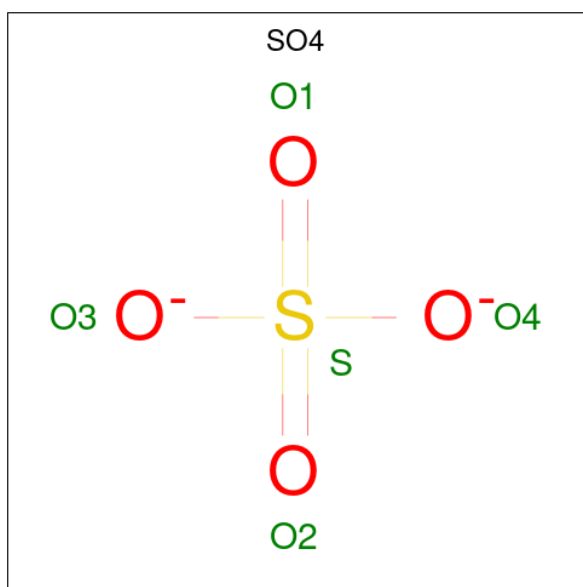
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		

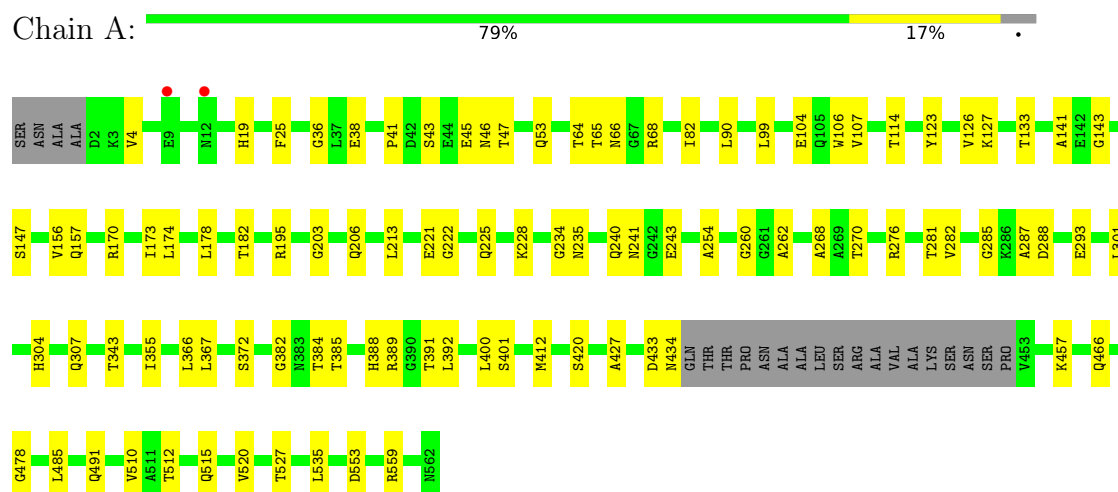
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		
8	B	78	Total	O	0	0
			78	78		
8	C	92	Total	O	0	0
			92	92		
8	D	73	Total	O	0	0
			73	73		

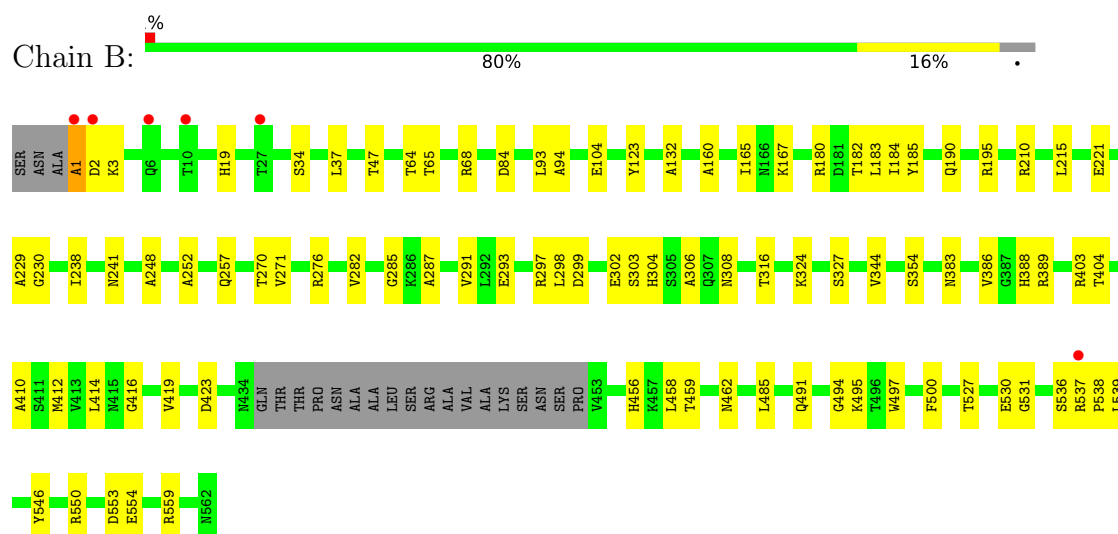
### 3 Residue-property plots [i](#)

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.

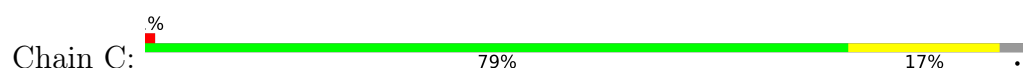
#### • Molecule 1: Antigen 43

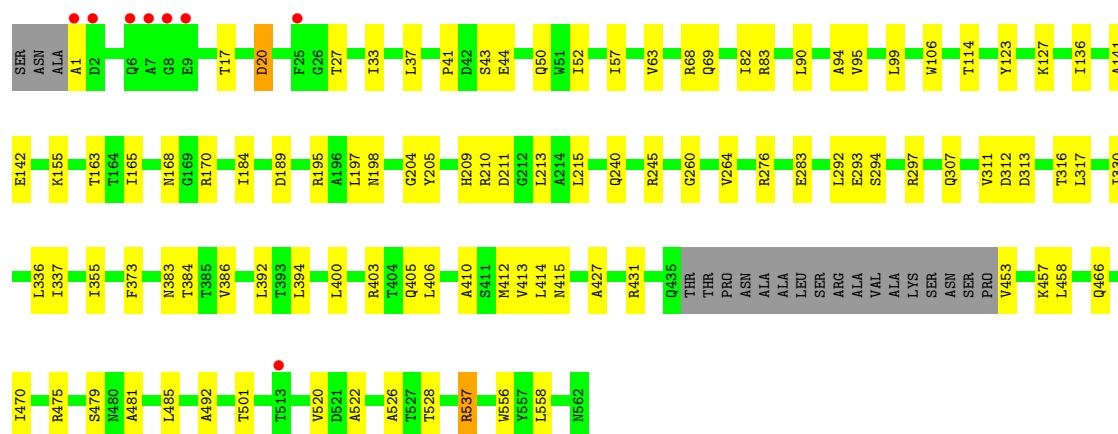


#### • Molecule 1: Antigen 43

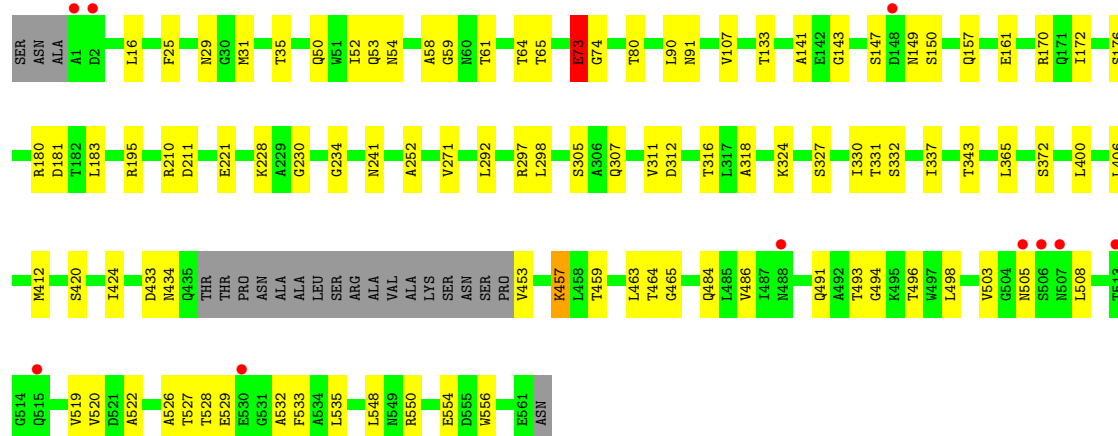
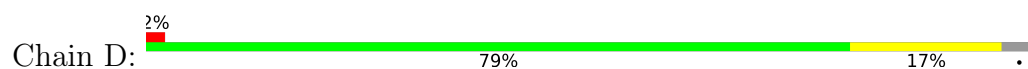


#### • Molecule 1: Antigen 43





### • Molecule 1: Antigen 43



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.55Å 178.66Å 246.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.98 50.83 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.78-2.98) 97.2 (50.83-2.98)	Depositor EDS
$R_{merge}$	0.48	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.206 , 0.254 0.205 , 0.254	Depositor DCC
$R_{free}$ test set	4223 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

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

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	0.47	0/3896	0.69	0/5289
1	B	0.48	0/3901	0.71	2/5296 (0.0%)
1	C	0.51	2/3910 (0.1%)	0.78	4/5308 (0.1%)
1	D	0.52	2/3902 (0.1%)	0.75	2/5297 (0.0%)
All	All	0.49	4/15609 (0.0%)	0.73	8/21190 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLU	CD-OE1	8.32	1.34	1.25
1	C	44	GLU	CB-CG	6.59	1.64	1.52
1	D	457	LYS	CB-CG	5.42	1.67	1.52
1	C	44	GLU	CD-OE1	5.04	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	537	ARG	NE-CZ-NH1	-15.12	112.74	120.30
1	C	537	ARG	NE-CZ-NH2	14.46	127.53	120.30
1	D	73	GLU	CG-CD-OE1	-8.62	101.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	LYS	CD-CE-NZ	-7.03	95.53	111.70
1	C	431	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	B	485	LEU	CB-CG-CD2	-6.67	99.66	111.00
1	D	73	GLU	CA-CB-CG	6.48	127.65	113.40
1	C	431	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	ALA	Peptide
1	D	73	GLU	Sidechain

## 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	3860	0	3720	63	0
1	B	3865	0	3728	61	0
1	C	3874	0	3736	68	0
1	D	3866	0	3730	67	0
2	A	26	0	35	0	0
2	B	38	0	50	2	0
2	C	21	0	30	1	0
2	D	68	0	95	4	0
3	A	35	0	40	4	0
3	B	24	0	29	1	0
3	C	31	0	37	2	0
3	D	33	0	43	1	0
4	A	24	0	32	1	0
4	B	42	0	56	2	0
4	C	12	0	16	1	0
4	D	24	0	32	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	5	0	0	0	0
8	A	94	0	0	1	0
8	B	78	0	0	0	0
8	C	92	0	0	2	0
8	D	73	0	0	0	0
All	All	16189	0	15409	252	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (252) 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:495:LYS:HB3	4:B:613:GOL:H32	1.40	1.00
1:D:520:VAL:HG12	1:D:556:TRP:HB2	1.62	0.80
1:B:167:LYS:HD3	1:C:136:ILE:HD11	1.63	0.80
1:C:17:THR:O	1:C:20:ASP:HB2	1.80	0.80
1:A:19:HIS:HB3	1:A:47:THR:HG23	1.65	0.78
1:C:127:LYS:NZ	6:C:610:CL:CL	2.55	0.77
1:A:36:GLY:O	1:A:68:ARG:NH1	2.18	0.76
1:D:31:MET:HB2	1:D:61:THR:HG22	1.65	0.76
1:B:419:VAL:HG12	1:B:459:THR:HB	1.66	0.76
1:A:90:LEU:HD23	1:A:107:VAL:HG12	1.67	0.75
1:D:491:GLN:HG2	1:D:527:THR:HB	1.68	0.74
1:C:501:THR:HG22	1:C:537:ARG:NH2	2.04	0.73
1:B:64:THR:HG22	1:B:65:THR:H	1.54	0.72
1:C:165:ILE:HD12	1:C:184:ILE:HG12	1.72	0.72
1:C:412:MET:HE2	1:C:414:LEU:HD21	1.71	0.71
1:B:221:GLU:HG3	1:B:241:ASN:HB2	1.73	0.71
1:D:25:PHE:HE1	1:D:53:GLN:HG3	1.54	0.70
1:D:64:THR:HG22	1:D:65:THR:H	1.55	0.70
1:B:210:ARG:HE	1:B:230:GLY:HA3	1.56	0.70
1:A:114:THR:HG22	1:A:133:THR:HB	1.73	0.69
1:D:52:ILE:HD11	1:D:58:ALA:HB2	1.74	0.69
1:A:234:GLY:HA3	1:C:215:LEU:HD11	1.73	0.69
1:D:406:LEU:HD21	1:D:412:MET:HB2	1.73	0.69
1:D:25:PHE:CE1	1:D:53:GLN:HG3	2.28	0.69
1:B:404:THR:HG21	1:B:412:MET:HE1	1.73	0.68
1:C:453:VAL:HB	3:C:605:P6G:H62	1.76	0.68
1:C:141:ALA:HB2	1:C:170:ARG:HB2	1.77	0.67
1:C:95:VAL:HG23	1:C:114:THR:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ARG:HB2	1:C:481:ALA:HB3	1.77	0.66
1:A:104:GLU:HG2	1:A:123:TYR:HD2	1.61	0.65
1:C:297:ARG:HG3	1:C:316:THR:HB	1.77	0.65
1:B:165:ILE:HD12	1:B:184:ILE:HG12	1.80	0.64
1:A:276:ARG:NH1	1:A:293:GLU:OE1	2.31	0.64
1:A:515:GLN:O	1:A:559:ARG:NH1	2.31	0.63
1:B:308:ASN:H	1:B:327:SER:HB2	1.63	0.62
1:B:1:ALA:O	1:B:3:LYS:HD3	1.99	0.62
1:D:528:THR:O	1:D:550:ARG:NH1	2.33	0.62
1:B:302:GLU:O	1:B:303:SER:OG	2.18	0.62
1:C:123:TYR:OH	1:C:155:LYS:HE2	2.01	0.61
1:A:457:LYS:HD2	4:A:613:GOL:H31	1.85	0.59
1:A:156:VAL:HG22	1:A:173:ILE:HA	1.83	0.59
1:D:307:GLN:O	1:D:327:SER:HB3	2.02	0.59
1:C:414:LEU:HD11	1:C:458:LEU:HD22	1.83	0.59
1:B:195:ARG:HG3	1:D:195:ARG:HD3	1.85	0.58
1:B:491:GLN:HG3	1:B:527:THR:HG22	1.85	0.58
1:C:41:PRO:HB3	1:C:106:TRP:CZ2	2.38	0.58
1:D:54:ASN:HA	1:D:74:GLY:HA3	1.85	0.57
1:D:498:LEU:HD12	1:D:548:LEU:HD21	1.86	0.57
1:A:38:GLU:HG3	1:A:66:ASN:HB3	1.86	0.57
1:D:494:GLY:O	1:D:532:ALA:HA	2.05	0.57
1:B:383:ASN:ND2	2:B:609:PEG:H42	2.20	0.56
1:D:31:MET:HG3	1:D:50:GLN:NE2	2.21	0.56
1:A:240:GLN:HG3	1:A:260:GLY:HA3	1.87	0.56
1:B:84:ASP:OD1	1:C:83:ARG:NH2	2.39	0.55
1:B:215:LEU:HD11	1:D:234:GLY:HA3	1.87	0.55
1:C:400:LEU:HD11	1:C:412:MET:HE3	1.88	0.55
1:A:485:LEU:HD12	1:A:520:VAL:HG22	1.89	0.55
1:B:276:ARG:NH1	1:B:293:GLU:OE1	2.38	0.55
1:A:228:LYS:HZ1	3:A:607:P6G:H82	1.72	0.55
1:A:107:VAL:CG2	1:A:126:VAL:HA	2.37	0.54
1:D:522:ALA:HB1	1:D:526:ALA:HB3	1.89	0.54
1:B:495:LYS:NZ	1:B:531:GLY:HA3	2.22	0.54
1:C:142:GLU:HG3	1:C:168:ASN:HB3	1.90	0.54
1:B:500:PHE:C	1:B:537:ARG:HH21	2.10	0.54
1:B:383:ASN:HD21	2:B:609:PEG:H42	1.71	0.53
1:A:141:ALA:HB2	1:A:170:ARG:HB2	1.90	0.53
1:A:182:THR:HG22	8:A:715:HOH:O	2.07	0.53
1:B:497:TRP:HB3	1:B:536:SER:OG	2.09	0.53
1:B:537:ARG:HH22	1:B:539:LEU:HD13	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:ALA:O	1:D:554:GLU:HG3	2.08	0.53
1:D:61:THR:OG1	1:D:80:THR:HG22	2.08	0.53
1:D:52:ILE:CD1	1:D:58:ALA:HB2	2.39	0.53
1:C:394:LEU:HD21	1:C:400:LEU:HD21	1.90	0.53
1:D:31:MET:HG3	1:D:50:GLN:HE22	1.73	0.53
1:C:522:ALA:HB1	1:C:526:ALA:HB3	1.91	0.52
1:D:459:THR:HG23	1:D:486:VAL:HB	1.91	0.52
1:A:433:ASP:OD2	1:A:434:ASN:N	2.41	0.52
1:B:414:LEU:HD11	1:B:458:LEU:HD22	1.89	0.52
1:D:535:LEU:CD1	1:D:548:LEU:HB2	2.39	0.52
1:A:114:THR:HA	1:A:133:THR:O	2.09	0.52
1:A:221:GLU:HG3	1:A:241:ASN:HB2	1.92	0.52
1:B:500:PHE:O	1:B:537:ARG:NE	2.41	0.52
1:C:336:LEU:HD23	1:C:337:ILE:N	2.25	0.52
1:D:496:THR:HB	1:D:533:PHE:CD1	2.46	0.51
1:B:19:HIS:ND1	1:B:47:THR:HG23	2.26	0.51
1:C:384:THR:HG21	1:C:392:LEU:HD22	1.94	0.50
1:D:141:ALA:HB2	1:D:170:ARG:HB2	1.93	0.50
1:B:64:THR:HG22	1:B:65:THR:N	2.22	0.50
1:B:416:GLY:HA2	1:B:456:HIS:CD2	2.47	0.50
1:A:478:GLY:HA2	1:A:510:VAL:HG11	1.93	0.50
1:A:288:ASP:OD1	1:A:307:GLN:HG3	2.11	0.50
1:C:240:GLN:HG3	1:C:260:GLY:HA3	1.92	0.50
1:A:384:THR:HG21	1:A:392:LEU:HD22	1.92	0.50
1:C:292:LEU:HD12	1:C:297:ARG:N	2.27	0.50
1:A:143:GLY:HA3	1:A:147:SER:HB2	1.94	0.49
1:B:182:THR:HG21	1:B:190:GLN:HE22	1.77	0.49
1:D:292:LEU:HD11	1:D:298:LEU:HB3	1.95	0.49
1:D:252:ALA:O	1:D:271:VAL:HA	2.12	0.49
1:D:312:ASP:HA	1:D:331:THR:HB	1.95	0.49
1:D:331:THR:HG22	1:D:332:SER:O	2.12	0.49
1:A:427:ALA:HB2	1:A:466:GLN:HB2	1.94	0.49
1:A:268:ALA:HB2	1:A:301:LEU:HD12	1.95	0.49
1:C:33:ILE:HG12	1:C:50:GLN:HB2	1.95	0.48
1:B:546:TYR:HA	1:B:559:ARG:O	2.12	0.48
1:C:283:GLU:O	1:C:283:GLU:HG3	2.14	0.48
1:A:41:PRO:HB3	1:A:106:TRP:CZ2	2.49	0.48
1:D:150:SER:HA	1:D:172:ILE:HD12	1.95	0.48
1:D:498:LEU:HD12	1:D:548:LEU:CD2	2.44	0.48
1:C:355:ILE:HD13	1:C:373:PHE:HE1	1.78	0.48
1:D:90:LEU:HD23	1:D:107:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:HG2	1:C:195:ARG:HD3	1.96	0.47
1:A:281:THR:O	1:A:287:ALA:HA	2.14	0.47
1:B:229:ALA:HB2	1:B:248:ALA:O	2.14	0.47
1:A:82:ILE:HB	1:A:99:LEU:HD23	1.95	0.47
1:B:537:ARG:NH1	1:B:538:PRO:O	2.47	0.47
1:B:93:LEU:HD12	1:B:94:ALA:N	2.30	0.47
1:D:311:VAL:HB	1:D:330:ILE:HG12	1.96	0.47
1:B:287:ALA:O	1:B:306:ALA:HA	2.15	0.47
1:C:90:LEU:HD13	1:C:94:ALA:HB2	1.97	0.47
1:C:501:THR:HG22	1:C:537:ARG:HH21	1.75	0.47
1:B:500:PHE:O	1:B:537:ARG:NH2	2.43	0.47
3:B:611:P6G:H52	3:B:611:P6G:H22	1.53	0.47
1:C:184:ILE:HG22	1:C:204:GLY:HA3	1.95	0.47
1:C:1:ALA:O	1:C:20:ASP:OD2	2.33	0.47
1:B:423:ASP:OD1	1:B:462:ASN:HB2	2.15	0.46
1:C:197:LEU:HG	1:C:198:ASN:ND2	2.30	0.46
1:B:104:GLU:HG2	1:B:123:TYR:HD2	1.80	0.46
1:C:276:ARG:HA	2:C:602:PEG:H31	1.97	0.46
1:D:143:GLY:HA3	1:D:147:SER:HB2	1.98	0.46
1:D:16:LEU:HD23	1:D:35:THR:HG22	1.96	0.46
1:D:453:VAL:HG11	1:D:503:VAL:HG11	1.97	0.46
1:A:343:THR:HA	1:A:355:ILE:O	2.15	0.46
1:B:497:TRP:CZ2	4:B:613:GOL:H2	2.51	0.46
1:C:311:VAL:HG11	1:C:317:LEU:HB2	1.96	0.46
1:C:355:ILE:HD13	1:C:373:PHE:CE1	2.50	0.46
1:C:311:VAL:HG22	1:C:330:ILE:HA	1.98	0.46
1:A:512:THR:HG21	1:A:559:ARG:HA	1.98	0.46
1:D:465:GLY:O	1:D:494:GLY:HA3	2.15	0.46
1:A:127:LYS:HE2	1:A:127:LYS:HA	1.97	0.46
1:D:505:ASN:OD1	1:D:508:LEU:HB2	2.16	0.46
1:A:46:ASN:HB3	1:A:68:ARG:NH1	2.30	0.45
1:B:183:LEU:HD21	1:B:185:TYR:CZ	2.51	0.45
1:D:210:ARG:HG3	1:D:230:GLY:HA3	1.98	0.45
1:A:553:ASP:OD1	1:A:553:ASP:N	2.49	0.45
1:D:91:ASN:HD21	2:D:601:PEG:H32	1.81	0.45
1:A:400:LEU:HB2	1:A:420:SER:HB2	1.99	0.45
1:B:297:ARG:HA	1:B:316:THR:O	2.16	0.45
1:B:495:LYS:HZ2	1:B:531:GLY:HA3	1.80	0.45
1:D:297:ARG:HA	1:D:316:THR:O	2.16	0.45
1:A:367:LEU:HD12	1:A:372:SER:N	2.32	0.45
1:A:4:VAL:HG13	1:A:4:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:VAL:HG12	1:C:415:ASN:HD21	1.81	0.45
1:C:457:LYS:HE3	4:C:609:GOL:H11	1.98	0.45
1:A:228:LYS:NZ	3:A:607:P6G:H52	2.32	0.45
1:D:149:ASN:O	1:D:172:ILE:HD11	2.16	0.45
1:B:383:ASN:HA	1:B:403:ARG:O	2.17	0.45
1:B:491:GLN:HG3	1:B:527:THR:CG2	2.47	0.45
1:D:180:ARG:O	1:D:181:ASP:HB2	2.17	0.45
1:D:550:ARG:NH2	1:D:554:GLU:OE1	2.50	0.45
1:A:157:GLN:CG	1:A:174:LEU:HD12	2.47	0.45
1:C:413:VAL:HG12	1:C:415:ASN:ND2	2.32	0.45
1:D:424:ILE:O	1:D:463:LEU:HD12	2.17	0.45
1:A:392:LEU:O	1:A:412:MET:HA	2.17	0.44
1:B:386:VAL:HG12	1:B:410:ALA:HB1	1.99	0.44
1:B:550:ARG:NH2	1:B:554:GLU:OE1	2.50	0.44
1:C:427:ALA:HB2	1:C:466:GLN:HB2	1.99	0.44
1:B:494:GLY:O	1:B:495:LYS:HD3	2.17	0.44
1:C:400:LEU:HD11	1:C:412:MET:CE	2.47	0.44
1:D:228:LYS:HE3	2:D:603:PEG:H21	2.00	0.44
1:D:433:ASP:OD1	1:D:434:ASN:N	2.39	0.44
1:D:519:VAL:HG21	1:D:548:LEU:HD11	2.00	0.44
1:D:520:VAL:CG1	1:D:556:TRP:HB2	2.40	0.44
1:B:285:GLY:CA	1:B:304:HIS:ND1	2.81	0.44
1:A:491:GLN:HG3	1:A:527:THR:OG1	2.18	0.44
1:B:37:LEU:HB2	1:B:68:ARG:HB2	1.98	0.44
1:D:505:ASN:OD1	1:D:508:LEU:N	2.51	0.44
1:A:43:SER:HB2	1:A:45:GLU:HG2	1.99	0.44
1:A:270:THR:HA	1:A:282:VAL:O	2.17	0.44
1:D:183:LEU:HB2	2:D:614:PEG:H32	1.99	0.44
1:C:210:ARG:NH1	8:C:702:HOH:O	2.51	0.44
1:C:276:ARG:NH1	1:C:293:GLU:OE2	2.51	0.44
1:C:470:ILE:CD1	1:C:485:LEU:HD11	2.47	0.44
1:D:29:ASN:HA	1:D:59:GLY:O	2.18	0.44
1:A:243:GLU:HB2	1:A:262:ALA:HB3	1.99	0.43
1:C:209:HIS:HE1	3:C:601:P6G:H22	1.83	0.43
1:C:406:LEU:HD21	1:C:412:MET:HB2	2.00	0.43
1:B:34:SER:O	1:B:34:SER:OG	2.29	0.43
1:C:520:VAL:HB	1:C:556:TRP:HB2	1.99	0.43
1:B:285:GLY:HA3	1:B:304:HIS:ND1	2.32	0.43
1:C:37:LEU:HB2	1:C:68:ARG:HB2	2.00	0.43
1:D:457:LYS:HD3	1:D:484:GLN:HB3	1.99	0.43
2:D:607:PEG:H42	2:D:607:PEG:H21	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLY:O	1:A:304:HIS:HB3	2.18	0.43
1:A:366:LEU:HA	1:A:385:THR:O	2.19	0.43
1:A:388:HIS:NE2	1:A:389:ARG:HG3	2.34	0.43
1:B:270:THR:HA	1:B:282:VAL:O	2.19	0.43
1:D:522:ALA:CB	1:D:554:GLU:HB2	2.49	0.43
1:B:195:ARG:NH1	1:D:211:ASP:O	2.52	0.43
1:C:52:ILE:HD12	1:C:52:ILE:H	1.84	0.43
1:A:178:LEU:HD22	1:C:211:ASP:HB3	2.00	0.43
1:D:464:THR:HG23	1:D:493:THR:OG1	2.19	0.43
3:D:610:P6G:H32	3:D:610:P6G:H62	1.67	0.43
1:B:132:ALA:O	1:B:160:ALA:HA	2.18	0.42
1:C:195:ARG:HA	1:C:213:LEU:O	2.18	0.42
1:D:221:GLU:HG3	1:D:241:ASN:HB2	2.01	0.42
1:D:535:LEU:HD11	1:D:548:LEU:HB2	2.00	0.42
1:A:107:VAL:HG23	1:A:126:VAL:HA	1.99	0.42
1:A:228:LYS:HE2	3:A:607:P6G:H82	2.01	0.42
1:A:203:GLY:HA2	1:A:222:GLY:C	2.40	0.42
1:A:25:PHE:CZ	1:A:53:GLN:HG3	2.54	0.42
1:C:386:VAL:HG12	1:C:410:ALA:HB1	2.01	0.42
1:A:195:ARG:HD3	1:C:195:ARG:HB3	2.02	0.42
1:B:238:ILE:HD12	1:B:257:GLN:HG3	2.02	0.42
1:C:405:GLN:C	1:C:406:LEU:HD12	2.40	0.42
1:A:64:THR:OG1	1:A:65:THR:N	2.53	0.42
1:B:298:LEU:HD12	1:B:299:ASP:N	2.35	0.42
1:B:344:VAL:O	1:B:354:SER:HA	2.20	0.42
1:B:530:GLU:CD	1:B:530:GLU:H	2.23	0.42
1:C:82:ILE:HB	1:C:99:LEU:HD22	2.01	0.42
1:D:400:LEU:HB2	1:D:420:SER:HB2	2.01	0.42
1:A:206:GLN:OE1	1:A:225:GLN:NE2	2.45	0.41
1:A:213:LEU:HD22	1:C:195:ARG:HB2	2.02	0.41
1:C:492:ALA:HB3	1:C:528:THR:HG22	2.02	0.41
1:B:388:HIS:CE1	1:B:389:ARG:HG3	2.55	0.41
1:B:252:ALA:O	1:B:271:VAL:HA	2.20	0.41
1:C:189:ASP:HB3	1:C:205:TYR:HB2	2.03	0.41
1:A:382:GLY:HA2	1:A:401:SER:O	2.21	0.41
1:B:553:ASP:O	1:B:554:GLU:HB2	2.19	0.41
1:D:318:ALA:HA	1:D:337:ILE:O	2.21	0.41
1:D:365:LEU:HA	1:D:365:LEU:HD23	1.81	0.41
1:A:195:ARG:HB3	1:C:213:LEU:HD22	2.03	0.41
1:A:372:SER:HA	1:A:391:THR:O	2.21	0.41
1:A:235:ASN:HA	1:A:254:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:HB	8:C:703:HOH:O	2.21	0.41
1:C:475:ARG:NH2	1:C:479:SER:OG	2.53	0.41
1:D:324:LYS:HA	1:D:343:THR:O	2.21	0.41
1:B:291:VAL:HG12	1:B:293:GLU:HG3	2.03	0.40
1:C:245:ARG:HA	1:C:264:VAL:O	2.21	0.40
1:C:558:LEU:HD23	1:C:558:LEU:HA	1.93	0.40
1:C:27:THR:HG23	1:C:57:ILE:HG23	2.03	0.40
1:D:157:GLN:HG2	1:D:176:SER:OG	2.21	0.40
1:D:305:SER:HA	1:D:324:LYS:O	2.22	0.40
1:D:337:ILE:HA	1:D:372:SER:O	2.20	0.40
1:D:529:GLU:HB2	1:D:532:ALA:HB2	2.03	0.40
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.85	0.40
1:B:180:ARG:HH21	1:B:180:ARG:HD2	1.70	0.40
1:C:312:ASP:OD1	1:C:313:ASP:N	2.42	0.40
1:C:383:ASN:HA	1:C:403:ARG:O	2.20	0.40
1:C:63:VAL:HG21	1:C:69:GLN:HB2	2.04	0.40
1:D:133:THR:HA	1:D:161:GLU:O	2.22	0.40
1:A:41:PRO:HB3	1:A:106:TRP:CH2	2.56	0.40
3:A:605:P6G:H82	3:A:605:P6G:H51	1.44	0.40

There are no symmetry-related clashes.

## 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	539/565 (95%)	516 (96%)	23 (4%)	0	100	100
1	B	540/565 (96%)	514 (95%)	25 (5%)	1 (0%)	47	80
1	C	541/565 (96%)	516 (95%)	23 (4%)	2 (0%)	34	70
1	D	540/565 (96%)	512 (95%)	28 (5%)	0	100	100
All	All	2160/2260 (96%)	2058 (95%)	99 (5%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	SER
1	B	2	ASP
1	C	43	SER

### 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	400/416 (96%)	400 (100%)	0	100	100
1	B	400/416 (96%)	400 (100%)	0	100	100
1	C	401/416 (96%)	399 (100%)	2 (0%)	88	95
1	D	400/416 (96%)	399 (100%)	1 (0%)	92	97
All	All	1601/1664 (96%)	1598 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	ASP
1	C	307	GLN
1	D	73	GLU

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	19	HIS
1	B	456	HIS
1	C	60	ASN
1	C	149	ASN
1	C	562	ASN
1	D	388	HIS
1	D	480	ASN
1	D	549	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 4 are monoatomic - leaving 60 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	C	603	-	6,6,6	0.60	0	5,5,5	0.73	0
4	GOL	D	615	-	5,5,5	1.48	1 (20%)	5,5,5	0.62	0
2	PEG	B	601	-	6,6,6	0.52	0	5,5,5	0.50	0
2	PEG	D	604	-	6,6,6	0.49	0	5,5,5	0.37	0
3	P6G	D	610	-	9,9,18	1.00	0	8,8,17	0.51	0
3	P6G	A	609	-	6,6,18	0.72	0	5,5,17	0.24	0
2	PEG	B	603	-	3,3,6	0.52	0	2,2,5	0.06	0
2	PEG	C	602	-	6,6,6	0.53	0	5,5,5	0.46	0
4	GOL	B	613	-	5,5,5	1.49	1 (20%)	5,5,5	0.86	0
3	P6G	C	606	-	6,6,18	0.85	0	5,5,17	0.32	0
4	GOL	B	615	-	5,5,5	1.14	0	5,5,5	0.86	0
4	GOL	D	617	-	5,5,5	1.26	0	5,5,5	0.75	0
2	PEG	D	614	-	6,6,6	0.48	0	5,5,5	0.45	0
4	GOL	A	613	-	5,5,5	1.15	1 (20%)	5,5,5	0.72	0
7	SO4	D	619	-	4,4,4	0.13	0	6,6,6	0.34	0
2	PEG	D	608	-	3,3,6	0.49	0	2,2,5	0.33	0
2	PEG	B	602	-	6,6,6	0.48	0	5,5,5	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	616	-	5,5,5	1.09	0	5,5,5	0.87	0
4	GOL	A	614	-	5,5,5	1.11	0	5,5,5	0.73	0
3	P6G	D	602	-	6,6,18	0.89	0	5,5,17	0.41	0
2	PEG	B	606	-	3,3,6	0.50	0	2,2,5	0.20	0
2	PEG	D	611	-	3,3,6	0.47	0	2,2,5	0.36	0
2	PEG	C	607	-	6,6,6	0.54	0	5,5,5	0.43	0
3	P6G	A	604	-	6,6,18	0.65	0	5,5,17	0.52	0
3	P6G	A	608	-	6,6,18	0.55	0	5,5,17	0.66	0
2	PEG	A	602	-	6,6,6	0.52	0	5,5,5	0.15	0
3	P6G	B	610	-	6,6,18	0.89	0	5,5,17	0.41	0
2	PEG	B	604	-	3,3,6	0.48	0	2,2,5	0.36	0
2	PEG	D	609	-	3,3,6	0.47	0	2,2,5	0.17	0
3	P6G	A	607	-	6,6,18	0.51	0	5,5,17	0.50	0
2	PEG	A	603	-	6,6,6	0.50	0	5,5,5	0.34	0
2	PEG	D	606	-	6,6,6	0.57	0	5,5,5	0.60	0
4	GOL	C	608	-	5,5,5	0.84	0	5,5,5	0.83	0
4	GOL	B	618	-	5,5,5	1.37	1 (20%)	5,5,5	0.59	0
4	GOL	D	618	-	5,5,5	1.12	0	5,5,5	0.69	0
2	PEG	B	609	-	3,3,6	0.49	0	2,2,5	0.32	0
4	GOL	A	611	-	5,5,5	1.43	1 (20%)	5,5,5	0.94	0
4	GOL	A	612	-	5,5,5	0.97	0	5,5,5	0.79	0
3	P6G	C	601	-	9,9,18	1.10	0	8,8,17	0.33	0
4	GOL	D	616	-	5,5,5	1.33	0	5,5,5	0.72	0
3	P6G	A	605	-	6,6,18	0.72	0	5,5,17	0.39	0
3	P6G	C	605	-	6,6,18	0.68	0	5,5,17	0.40	0
4	GOL	B	614	-	5,5,5	1.32	1 (20%)	5,5,5	0.92	0
2	PEG	B	605	-	3,3,6	0.52	0	2,2,5	0.07	0
4	GOL	B	612	-	5,5,5	1.37	0	5,5,5	0.47	0
4	GOL	C	609	-	5,5,5	1.18	0	5,5,5	0.60	0
4	GOL	B	617	-	5,5,5	1.09	0	5,5,5	0.88	0
2	PEG	A	610	-	3,3,6	0.55	0	2,2,5	0.17	0
2	PEG	D	605	-	6,6,6	0.57	0	5,5,5	0.61	0
3	P6G	C	604	-	6,6,18	0.88	0	5,5,17	0.28	0
3	P6G	B	611	-	9,9,18	0.71	0	8,8,17	0.41	0
2	PEG	A	601	-	3,3,6	0.49	0	2,2,5	0.08	0
3	P6G	B	607	-	6,6,18	0.87	0	5,5,17	0.36	0
2	PEG	D	607	-	6,6,6	0.48	0	5,5,5	0.30	0
3	P6G	D	612	-	15,15,18	0.94	0	14,14,17	0.54	0
2	PEG	D	603	-	6,6,6	0.49	0	5,5,5	0.50	0
2	PEG	B	608	-	3,3,6	0.54	0	2,2,5	0.06	0
2	PEG	D	613	-	6,6,6	0.56	0	5,5,5	0.55	0
2	PEG	D	601	-	6,6,6	0.55	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	A	606	-	3,3,6	0.52	0	2,2,5	0.22	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	C	603	-	-	1/4/4/4	-
4	GOL	D	615	-	-	0/4/4/4	-
2	PEG	B	601	-	-	2/4/4/4	-
2	PEG	D	604	-	-	2/4/4/4	-
3	P6G	D	610	-	-	3/7/7/16	-
3	P6G	A	609	-	-	3/4/4/16	-
2	PEG	B	603	-	-	1/1/1/4	-
2	PEG	C	602	-	-	2/4/4/4	-
4	GOL	B	613	-	-	4/4/4/4	-
3	P6G	C	606	-	-	1/4/4/16	-
4	GOL	B	615	-	-	2/4/4/4	-
4	GOL	D	617	-	-	3/4/4/4	-
2	PEG	D	614	-	-	2/4/4/4	-
4	GOL	A	613	-	-	2/4/4/4	-
2	PEG	D	608	-	-	1/1/1/4	-
2	PEG	B	602	-	-	1/4/4/4	-
4	GOL	B	616	-	-	2/4/4/4	-
4	GOL	A	614	-	-	2/4/4/4	-
3	P6G	D	602	-	-	1/4/4/16	-
2	PEG	B	606	-	-	0/1/1/4	-
2	PEG	D	611	-	-	1/1/1/4	-
2	PEG	C	607	-	-	3/4/4/4	-
3	P6G	A	604	-	-	3/4/4/16	-
3	P6G	A	608	-	-	4/4/4/16	-
2	PEG	A	602	-	-	2/4/4/4	-
3	P6G	B	610	-	-	2/4/4/16	-
2	PEG	B	604	-	-	1/1/1/4	-
2	PEG	D	609	-	-	1/1/1/4	-
3	P6G	A	607	-	-	2/4/4/16	-
2	PEG	A	603	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	D	606	-	-	2/4/4/4	-
4	GOL	C	608	-	-	2/4/4/4	-
4	GOL	B	618	-	-	2/4/4/4	-
4	GOL	D	618	-	-	2/4/4/4	-
2	PEG	B	609	-	-	0/1/1/4	-
4	GOL	A	611	-	-	4/4/4/4	-
4	GOL	A	612	-	-	4/4/4/4	-
3	P6G	C	601	-	-	2/7/7/16	-
4	GOL	D	616	-	-	4/4/4/4	-
3	P6G	A	605	-	-	2/4/4/16	-
3	P6G	C	605	-	-	1/4/4/16	-
4	GOL	B	614	-	-	2/4/4/4	-
2	PEG	B	605	-	-	1/1/1/4	-
4	GOL	B	612	-	-	0/4/4/4	-
4	GOL	C	609	-	-	4/4/4/4	-
4	GOL	B	617	-	-	2/4/4/4	-
2	PEG	A	610	-	-	1/1/1/4	-
2	PEG	D	605	-	-	3/4/4/4	-
3	P6G	C	604	-	-	1/4/4/16	-
3	P6G	B	611	-	-	5/7/7/16	-
2	PEG	A	601	-	-	1/1/1/4	-
3	P6G	B	607	-	-	3/4/4/16	-
2	PEG	D	607	-	-	3/4/4/4	-
3	P6G	D	612	-	-	8/13/13/16	-
2	PEG	D	603	-	-	4/4/4/4	-
2	PEG	B	608	-	-	0/1/1/4	-
2	PEG	D	613	-	-	4/4/4/4	-
2	PEG	D	601	-	-	2/4/4/4	-
2	PEG	A	606	-	-	1/1/1/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	613	GOL	C3-C2	2.70	1.62	1.51
4	A	611	GOL	C3-C2	2.50	1.62	1.51
4	D	615	GOL	C3-C2	2.23	1.60	1.51
4	B	614	GOL	C3-C2	2.23	1.60	1.51
4	A	613	GOL	C1-C2	2.06	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	618	GOL	C3-C2	2.03	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	611	GOL	O1-C1-C2-C3
4	A	612	GOL	O1-C1-C2-C3
4	A	612	GOL	C1-C2-C3-O3
4	A	613	GOL	O1-C1-C2-C3
4	A	614	GOL	C1-C2-C3-O3
4	A	614	GOL	O2-C2-C3-O3
4	B	613	GOL	O1-C1-C2-C3
4	B	613	GOL	C1-C2-C3-O3
4	B	614	GOL	O1-C1-C2-C3
4	B	615	GOL	C1-C2-C3-O3
4	B	617	GOL	C1-C2-C3-O3
4	B	618	GOL	C1-C2-C3-O3
4	B	618	GOL	O2-C2-C3-O3
4	D	616	GOL	C1-C2-C3-O3
4	D	617	GOL	O1-C1-C2-O2
4	D	617	GOL	O1-C1-C2-C3
4	D	618	GOL	O1-C1-C2-C3
3	B	611	P6G	C5-C6-O7-C8
2	D	601	PEG	C4-C3-O2-C2
2	D	614	PEG	C4-C3-O2-C2
2	D	607	PEG	C4-C3-O2-C2
2	D	607	PEG	O2-C3-C4-O4
3	A	605	P6G	C5-C6-O7-C8
3	B	611	P6G	C2-C3-O4-C5
2	C	607	PEG	O2-C3-C4-O4
3	B	607	P6G	O4-C5-C6-O7
3	B	607	P6G	O7-C8-C9-O10
3	C	604	P6G	O4-C5-C6-O7
3	D	612	P6G	O4-C5-C6-O7
4	A	612	GOL	O1-C1-C2-O2
4	B	615	GOL	O2-C2-C3-O3
4	C	609	GOL	O1-C1-C2-O2
3	D	612	P6G	O10-C11-C12-O13
2	D	603	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	611	P6G	O1-C2-C3-O4
3	B	611	P6G	O7-C8-C9-O10
3	C	601	P6G	O1-C2-C3-O4
3	D	612	P6G	O1-C2-C3-O4
2	A	602	PEG	O1-C1-C2-O2
2	C	602	PEG	O2-C3-C4-O4
3	B	610	P6G	O4-C5-C6-O7
3	D	602	P6G	O1-C2-C3-O4
4	B	616	GOL	C1-C2-C3-O3
4	C	609	GOL	O1-C1-C2-C3
4	C	609	GOL	C1-C2-C3-O3
2	A	603	PEG	O1-C1-C2-O2
2	B	601	PEG	O2-C3-C4-O4
2	D	606	PEG	O1-C1-C2-O2
2	D	607	PEG	O1-C1-C2-O2
2	D	614	PEG	O1-C1-C2-O2
3	C	601	P6G	O7-C8-C9-O10
4	A	612	GOL	O2-C2-C3-O3
4	A	613	GOL	O1-C1-C2-O2
4	B	613	GOL	O2-C2-C3-O3
4	B	616	GOL	O2-C2-C3-O3
4	C	609	GOL	O2-C2-C3-O3
4	D	616	GOL	O2-C2-C3-O3
4	D	618	GOL	O1-C1-C2-O2
3	B	610	P6G	O7-C8-C9-O10
2	B	603	PEG	O2-C3-C4-O4
2	B	604	PEG	O2-C3-C4-O4
2	D	609	PEG	O2-C3-C4-O4
3	A	605	P6G	O4-C5-C6-O7
2	D	601	PEG	O2-C3-C4-O4
2	D	603	PEG	O2-C3-C4-O4
2	D	604	PEG	O2-C3-C4-O4
2	D	605	PEG	O1-C1-C2-O2
2	D	613	PEG	O1-C1-C2-O2
3	A	604	P6G	O4-C5-C6-O7
3	A	607	P6G	O4-C5-C6-O7
3	D	610	P6G	O1-C2-C3-O4
4	A	611	GOL	O1-C1-C2-O2
4	B	613	GOL	O1-C1-C2-O2
4	B	614	GOL	O1-C1-C2-O2
4	B	617	GOL	O2-C2-C3-O3
3	D	612	P6G	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
4	C	608	GOL	O1-C1-C2-O2
4	C	608	GOL	O2-C2-C3-O3
2	B	601	PEG	C4-C3-O2-C2
3	D	612	P6G	C5-C6-O7-C8
3	D	610	P6G	C6-C5-O4-C3
2	A	610	PEG	O2-C3-C4-O4
3	A	608	P6G	O4-C5-C6-O7
3	A	609	P6G	O4-C5-C6-O7
2	D	605	PEG	C1-C2-O2-C3
3	D	612	P6G	C12-C11-O10-C9
2	D	605	PEG	C4-C3-O2-C2
3	D	612	P6G	C6-C5-O4-C3
2	D	613	PEG	C1-C2-O2-C3
3	C	606	P6G	C9-C8-O7-C6
3	D	612	P6G	C9-C8-O7-C6
3	A	608	P6G	C5-C6-O7-C8
3	A	609	P6G	C9-C8-O7-C6
4	D	616	GOL	O1-C1-C2-O2
4	D	617	GOL	O2-C2-C3-O3
2	D	604	PEG	O1-C1-C2-O2
3	A	608	P6G	C9-C8-O7-C6
4	A	611	GOL	C1-C2-C3-O3
4	D	616	GOL	O1-C1-C2-C3
2	D	603	PEG	C4-C3-O2-C2
3	A	607	P6G	C5-C6-O7-C8
2	A	602	PEG	O2-C3-C4-O4
2	C	602	PEG	O1-C1-C2-O2
2	D	611	PEG	O2-C3-C4-O4
2	B	602	PEG	C4-C3-O2-C2
2	C	607	PEG	C1-C2-O2-C3
3	A	604	P6G	C9-C8-O7-C6
3	A	609	P6G	C5-C6-O7-C8
3	A	608	P6G	O7-C8-C9-O10
2	C	603	PEG	O2-C3-C4-O4
2	D	613	PEG	O2-C3-C4-O4
3	A	604	P6G	C5-C6-O7-C8
2	A	601	PEG	O2-C3-C4-O4
3	C	605	P6G	C5-C6-O7-C8
2	D	606	PEG	O2-C3-C4-O4
2	A	606	PEG	O2-C3-C4-O4
2	D	608	PEG	O2-C3-C4-O4
4	A	611	GOL	O2-C2-C3-O3

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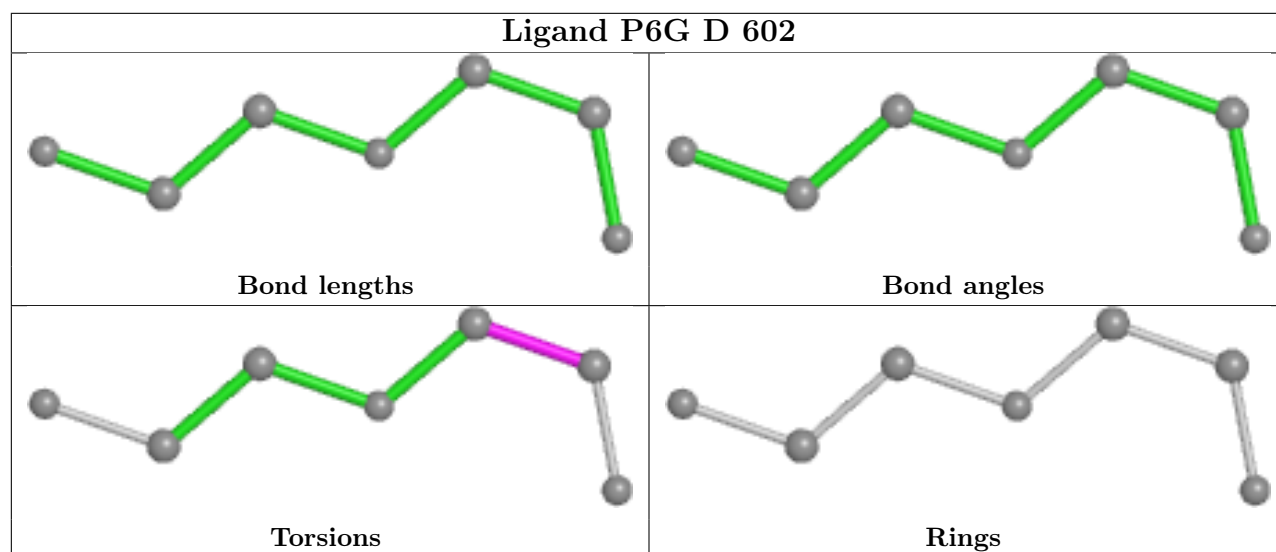
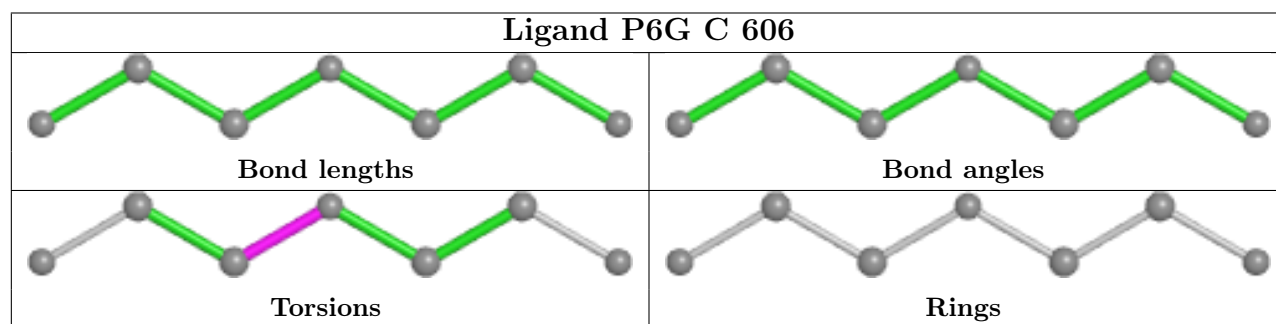
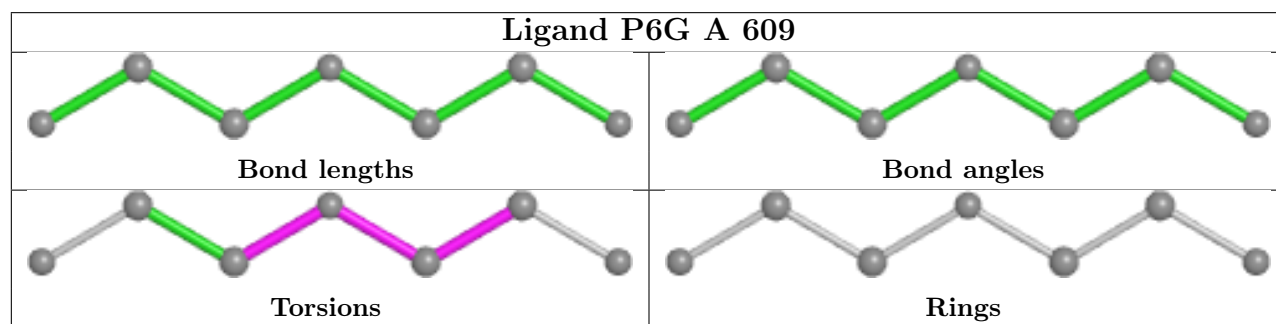
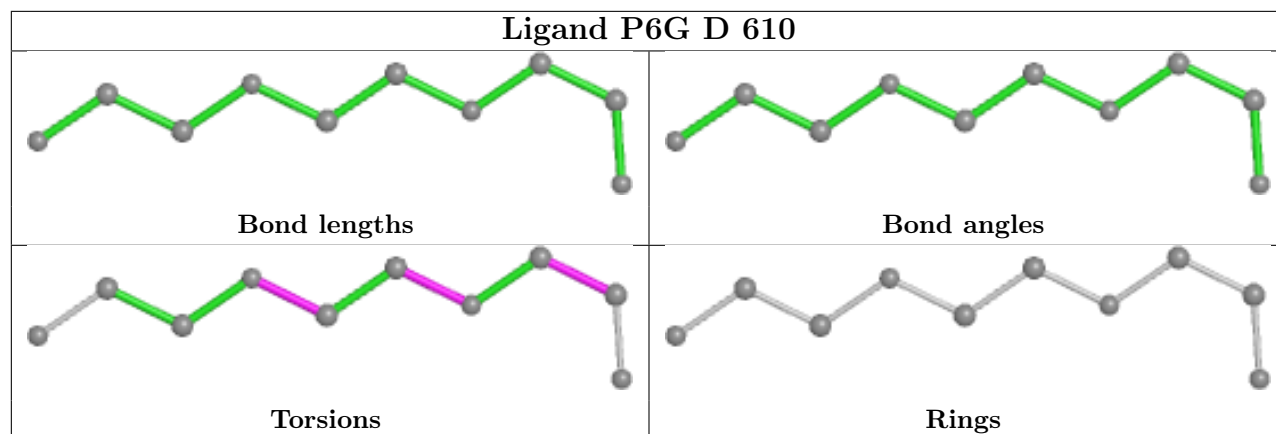
Mol	Chain	Res	Type	Atoms
3	B	607	P6G	C9-C8-O7-C6
3	B	611	P6G	O4-C5-C6-O7
3	D	610	P6G	C5-C6-O7-C8
2	D	613	PEG	C4-C3-O2-C2
2	D	603	PEG	C1-C2-O2-C3
2	A	603	PEG	O2-C3-C4-O4
2	C	607	PEG	O1-C1-C2-O2
2	B	605	PEG	O2-C3-C4-O4

There are no ring outliers.

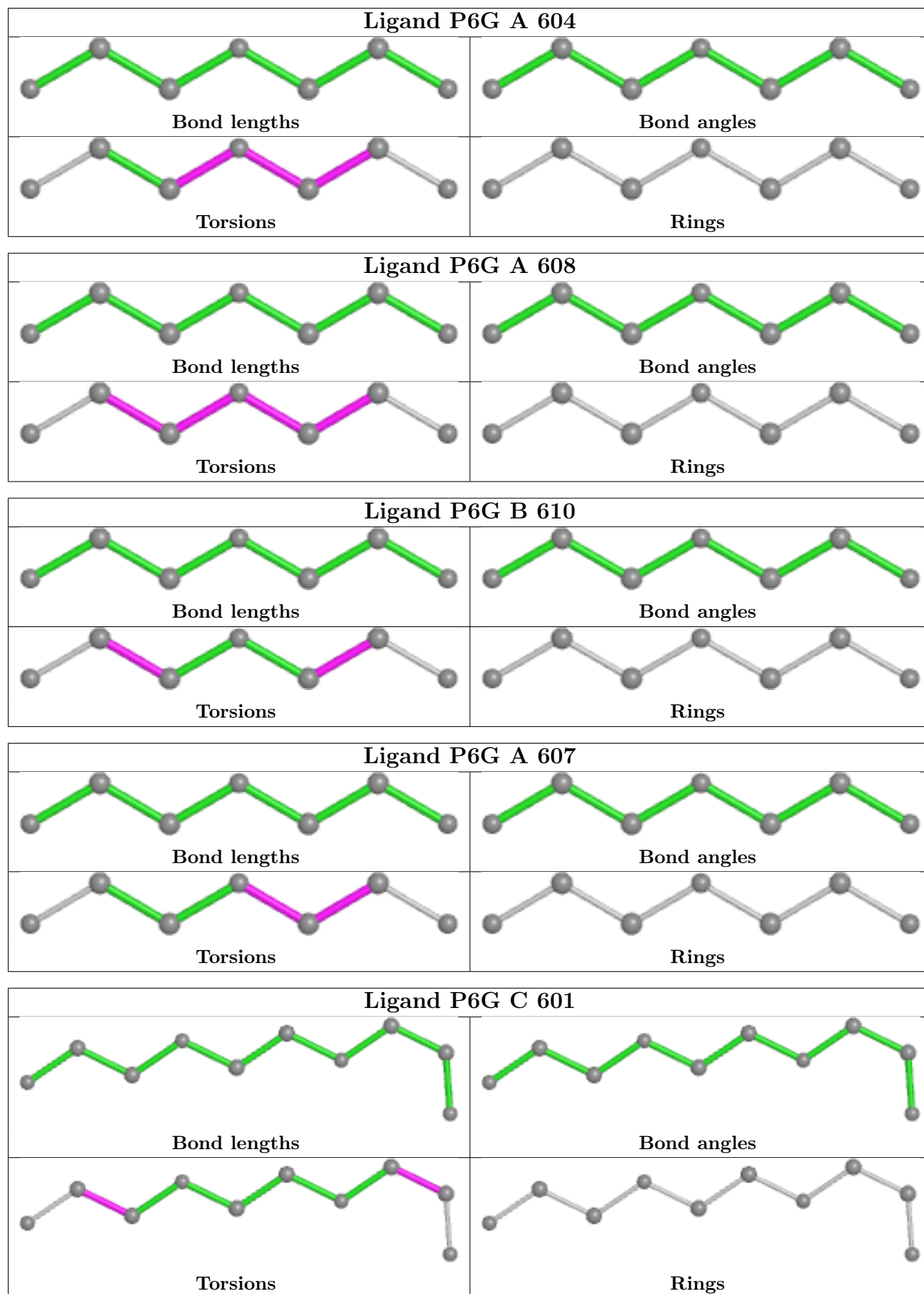
15 monomers are involved in 19 short contacts:

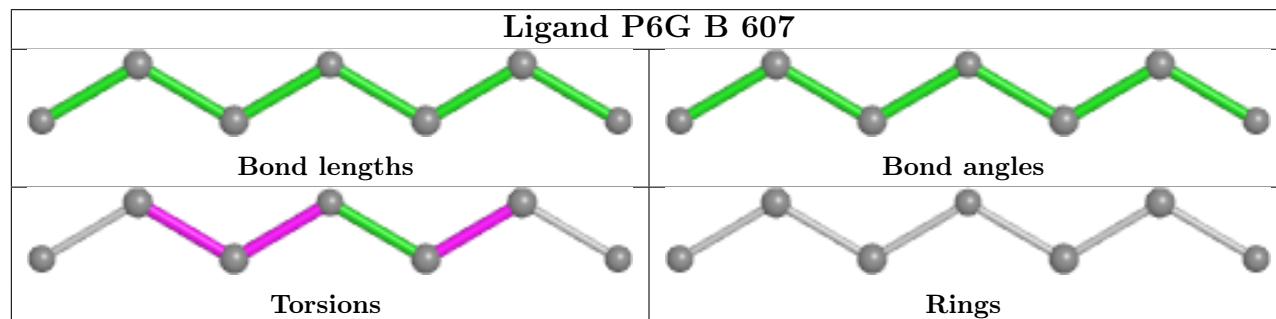
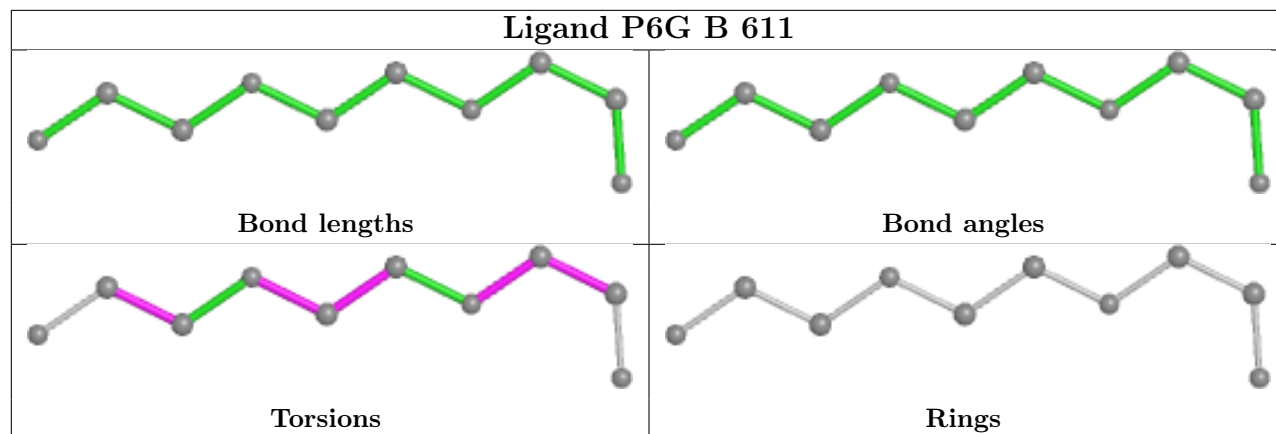
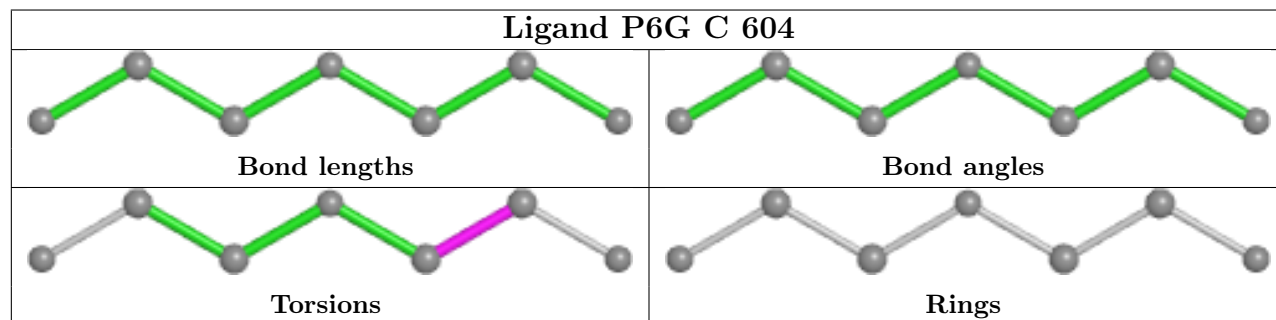
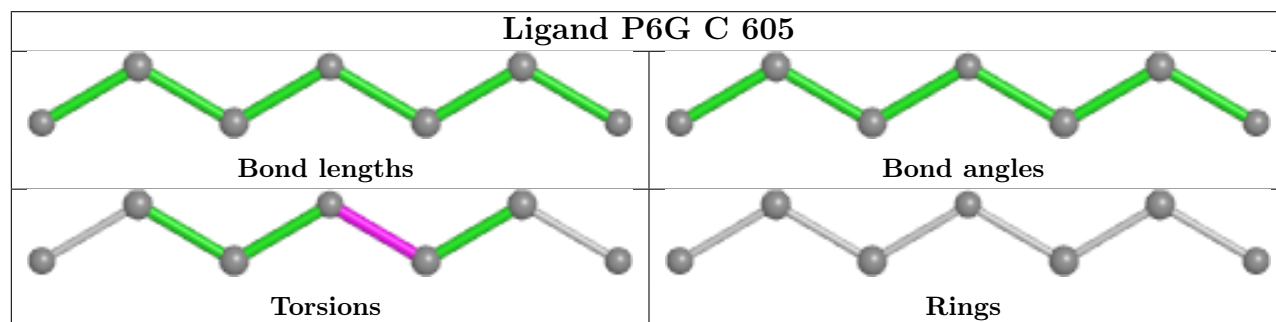
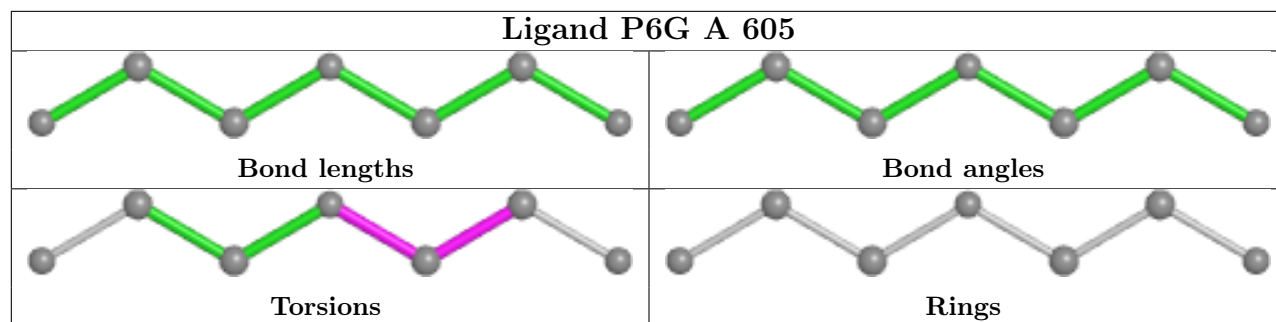
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	610	P6G	1	0
2	C	602	PEG	1	0
4	B	613	GOL	2	0
2	D	614	PEG	1	0
4	A	613	GOL	1	0
3	A	607	P6G	3	0
2	B	609	PEG	2	0
3	C	601	P6G	1	0
3	A	605	P6G	1	0
3	C	605	P6G	1	0
4	C	609	GOL	1	0
3	B	611	P6G	1	0
2	D	607	PEG	1	0
2	D	603	PEG	1	0
2	D	601	PEG	1	0

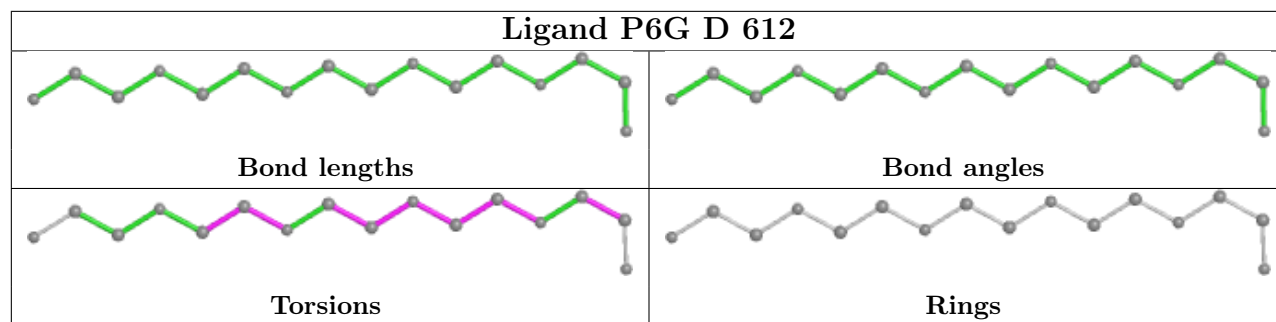
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	543/565 (96%)	-0.01	2 (0%) 92 83	26, 41, 80, 114	0
1	B	544/565 (96%)	-0.02	6 (1%) 80 63	25, 43, 70, 114	0
1	C	545/565 (96%)	-0.06	8 (1%) 73 54	25, 41, 71, 114	0
1	D	544/565 (96%)	0.01	10 (1%) 68 48	23, 41, 85, 149	0
All	All	2176/2260 (96%)	-0.02	26 (1%) 79 61	23, 41, 79, 149	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	506	SER	5.3
1	C	1	ALA	5.1
1	D	1	ALA	4.5
1	D	507	ASN	4.2
1	C	2	ASP	3.5
1	C	7	ALA	2.9
1	B	2	ASP	2.8
1	B	1	ALA	2.6
1	D	505	ASN	2.5
1	D	513	THR	2.4
1	C	9	GLU	2.4
1	D	515	GLN	2.3
1	C	513	THR	2.3
1	D	530	GLU	2.3
1	B	27	THR	2.3
1	C	6	GLN	2.3
1	C	25	PHE	2.2
1	A	12	ASN	2.2
1	B	10	THR	2.2
1	A	9	GLU	2.2
1	D	148	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	488	ASN	2.2
1	C	8	GLY	2.1
1	B	537	ARG	2.1
1	B	6	GLN	2.1
1	D	2	ASP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PEG	A	610	4/7	0.62	0.40	59,62,62,65	0
2	PEG	B	608	4/7	0.64	0.49	67,72,72,76	0
4	GOL	B	613	6/6	0.79	0.29	47,56,61,63	0
3	P6G	B	610	7/19	0.80	0.29	56,58,65,67	0
4	GOL	B	614	6/6	0.81	0.27	47,59,65,65	0
2	PEG	D	605	7/7	0.82	0.30	54,56,60,67	0
3	P6G	D	610	10/19	0.82	0.27	42,63,70,76	0
2	PEG	C	603	7/7	0.83	0.27	50,51,60,66	0
2	PEG	B	604	4/7	0.83	0.29	55,59,62,63	0
4	GOL	B	615	6/6	0.83	0.32	47,58,60,63	0
4	GOL	D	618	6/6	0.83	0.28	49,56,60,63	0
2	PEG	B	609	4/7	0.84	0.35	63,68,75,77	0
3	P6G	A	604	7/19	0.84	0.26	58,64,72,73	0
4	GOL	D	615	6/6	0.84	0.24	47,56,59,63	0
3	P6G	A	605	7/19	0.84	0.33	56,58,63,64	0
4	GOL	B	617	6/6	0.85	0.54	48,55,58,63	0
3	P6G	A	608	7/19	0.85	0.21	56,61,64,71	0
2	PEG	D	607	7/7	0.85	0.26	47,55,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	P6G	D	602	7/19	0.86	0.17	50,67,73,77	0
2	PEG	D	606	7/7	0.86	0.18	56,61,68,70	0
4	GOL	B	618	6/6	0.86	0.35	48,54,62,63	0
2	PEG	D	601	7/7	0.86	0.29	41,56,65,67	0
2	PEG	A	602	7/7	0.86	0.28	45,49,53,53	0
3	P6G	B	607	7/19	0.87	0.43	62,69,74,75	0
2	PEG	B	603	4/7	0.87	0.16	47,50,52,53	0
3	P6G	C	601	10/19	0.87	0.30	40,63,67,70	0
2	PEG	D	604	7/7	0.87	0.20	46,48,52,53	0
5	MG	A	615	1/1	0.87	0.17	35,35,35,35	0
2	PEG	C	607	7/7	0.88	0.25	47,49,57,59	0
2	PEG	C	602	7/7	0.88	0.23	47,53,65,66	0
2	PEG	B	602	7/7	0.88	0.22	58,61,64,64	0
2	PEG	D	613	7/7	0.88	0.21	41,46,54,54	0
5	MG	D	620	1/1	0.88	0.12	36,36,36,36	0
3	P6G	D	612	16/19	0.89	0.21	53,62,67,72	0
4	GOL	B	616	6/6	0.89	0.27	55,61,67,68	0
2	PEG	B	606	4/7	0.90	0.21	49,50,53,56	0
4	GOL	C	608	6/6	0.90	0.24	49,56,63,63	0
4	GOL	C	609	6/6	0.90	0.17	51,56,58,63	0
2	PEG	D	608	4/7	0.90	0.18	41,45,50,53	0
2	PEG	B	601	7/7	0.90	0.24	50,55,59,61	0
4	GOL	A	611	6/6	0.90	0.24	47,57,59,63	0
4	GOL	A	614	6/6	0.90	0.17	47,53,58,63	0
3	P6G	C	605	7/19	0.91	0.27	57,62,63,64	0
5	MG	C	611	1/1	0.91	0.25	36,36,36,36	0
2	PEG	A	606	4/7	0.91	0.15	56,59,65,68	0
6	CL	C	610	1/1	0.91	0.11	50,50,50,50	0
4	GOL	D	616	6/6	0.92	0.23	47,51,56,63	0
4	GOL	B	612	6/6	0.92	0.22	47,51,56,63	0
2	PEG	D	603	7/7	0.92	0.26	41,48,53,54	0
2	PEG	A	603	7/7	0.92	0.20	43,49,52,53	0
3	P6G	C	606	7/19	0.92	0.18	56,62,64,64	0
2	PEG	A	601	4/7	0.92	0.24	46,50,52,53	0
3	P6G	C	604	7/19	0.93	0.26	56,58,64,65	0
3	P6G	A	607	7/19	0.93	0.15	56,60,63,64	0
4	GOL	D	617	6/6	0.93	0.27	47,56,63,65	0
4	GOL	A	612	6/6	0.93	0.21	74,76,78,83	0
4	GOL	A	613	6/6	0.93	0.26	52,57,59,63	0
2	PEG	D	609	4/7	0.93	0.19	41,45,46,53	0
3	P6G	B	611	10/19	0.93	0.22	41,59,63,64	0
3	P6G	A	609	7/19	0.93	0.21	56,58,63,64	0

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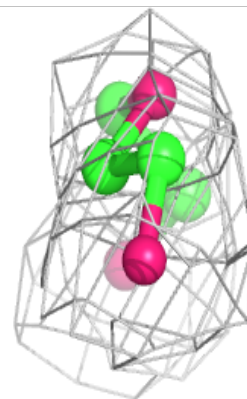
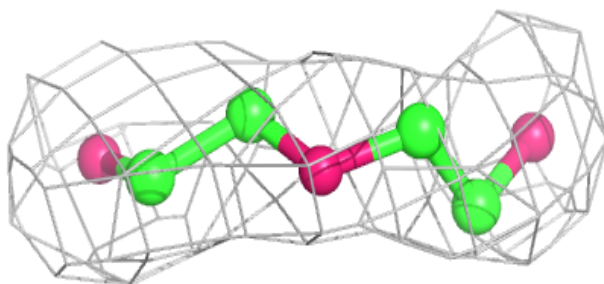
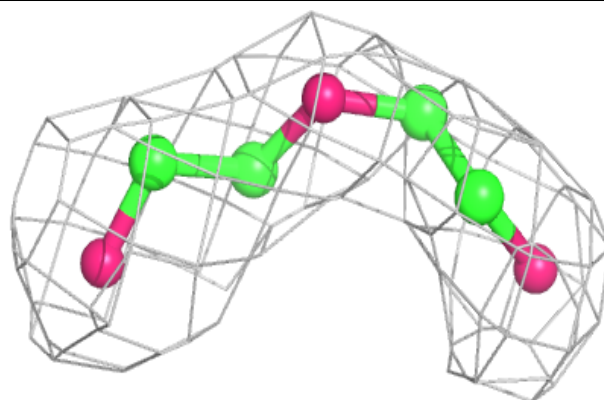
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	D	611	4/7	0.95	0.35	43,44,46,53	0
2	PEG	D	614	7/7	0.95	0.18	41,45,52,53	0
7	SO4	D	619	5/5	0.95	0.18	61,66,88,114	0
2	PEG	B	605	4/7	0.97	0.12	41,45,46,53	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.

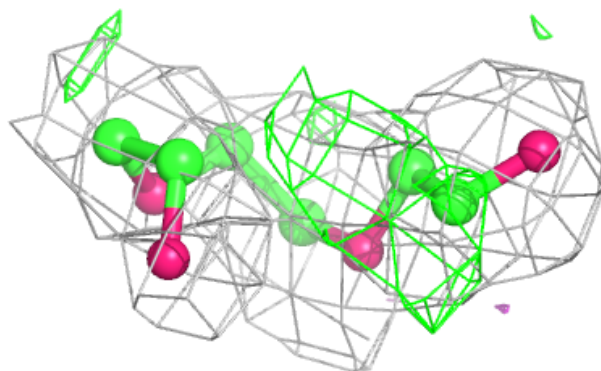
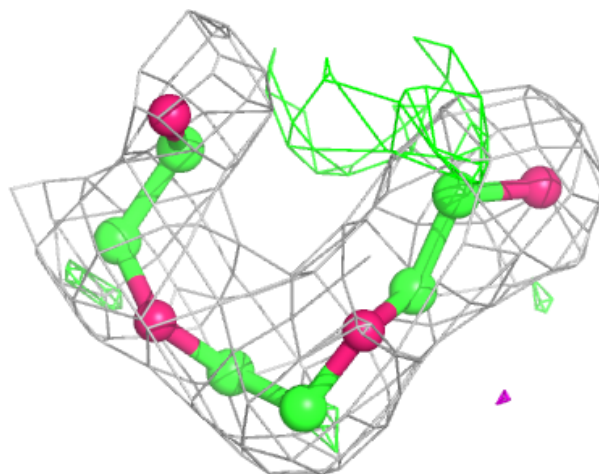
**Electron density around P6G B 610:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P6G D 610:**

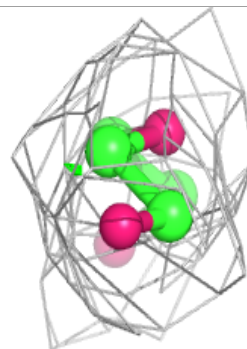
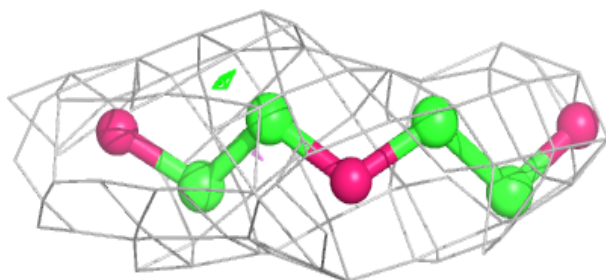
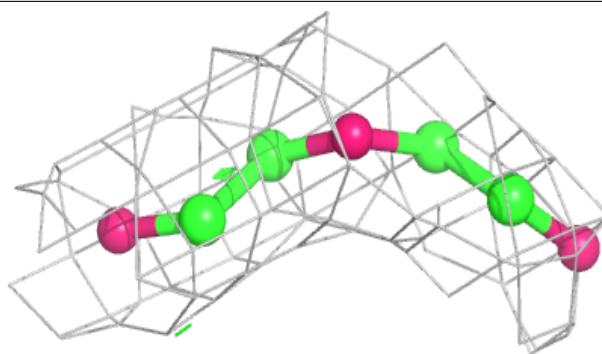
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



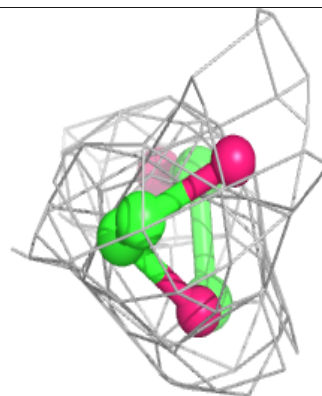
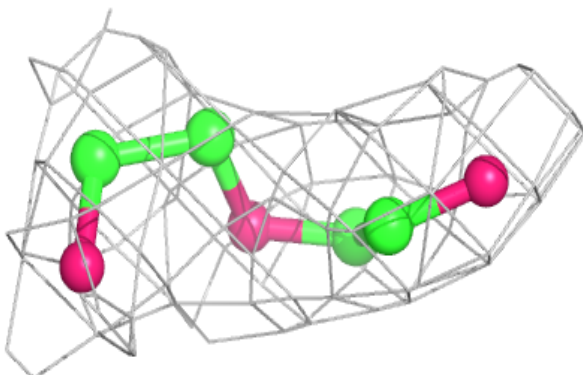
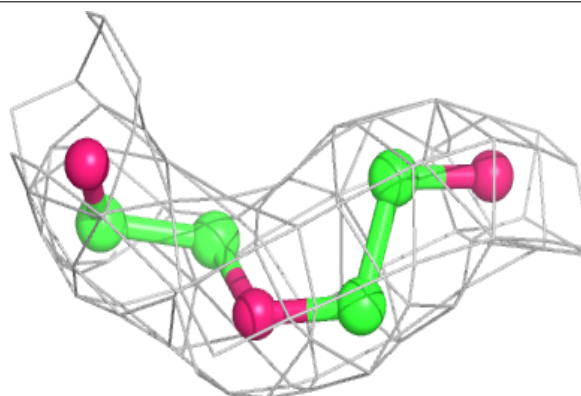


**Electron density around P6G A 604:**

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

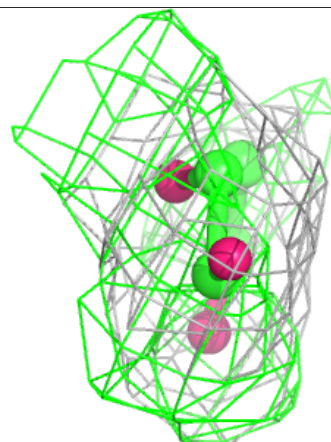
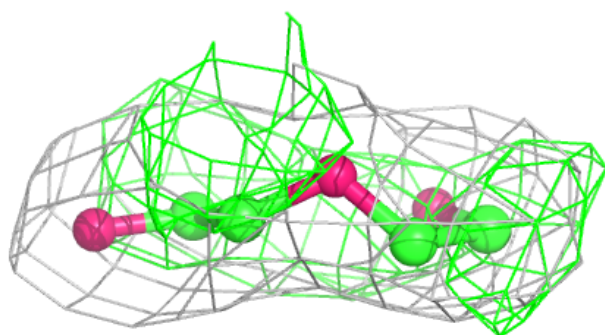
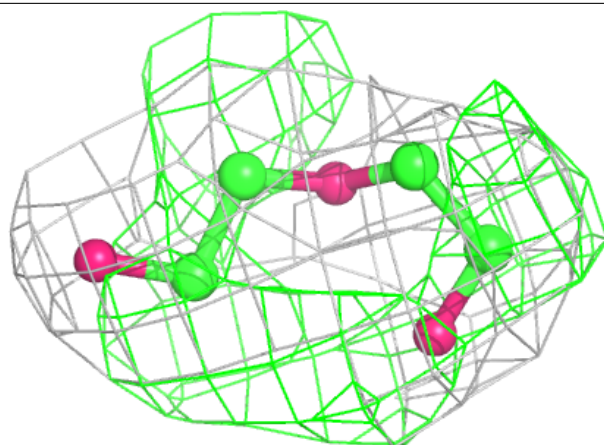
**Electron density around P6G A 605:**

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

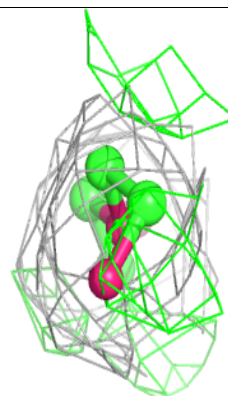
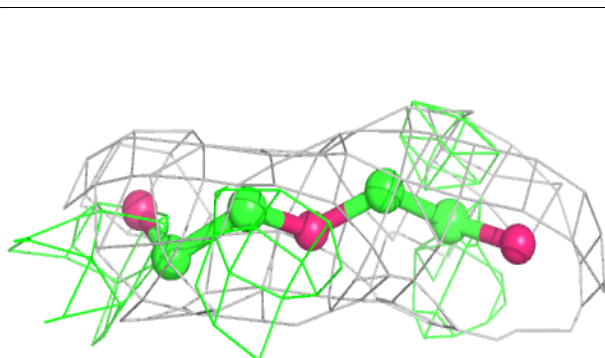
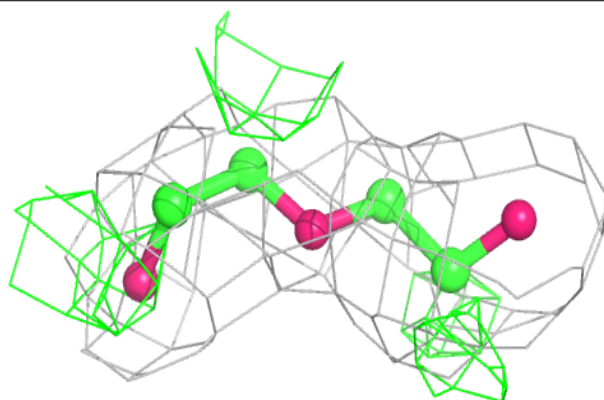


**Electron density around P6G A 608:**

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

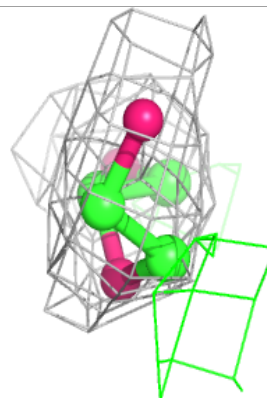
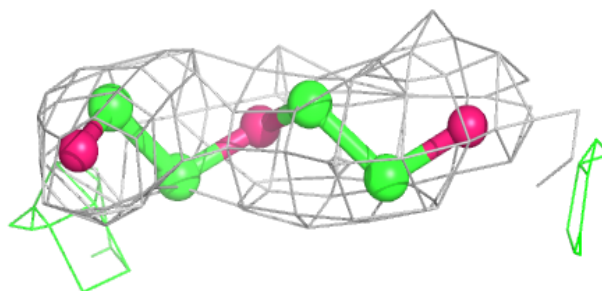
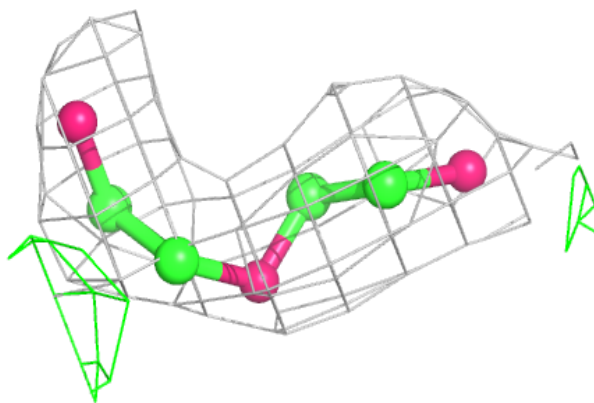
**Electron density around P6G D 602:**

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

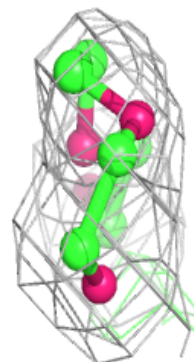
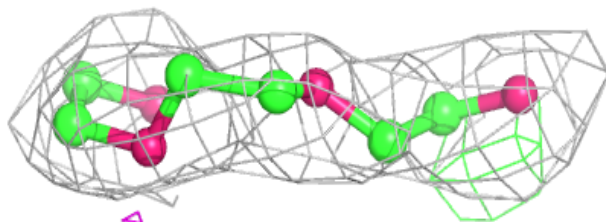
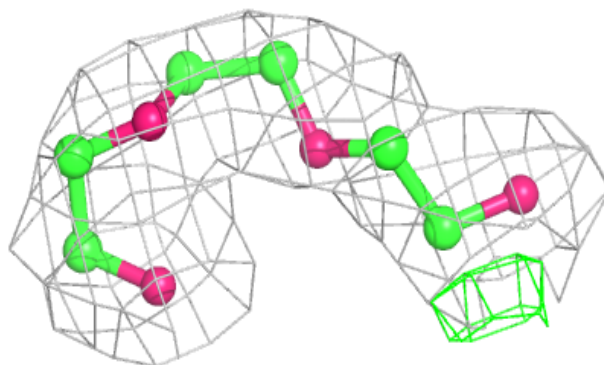


**Electron density around P6G B 607:**

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

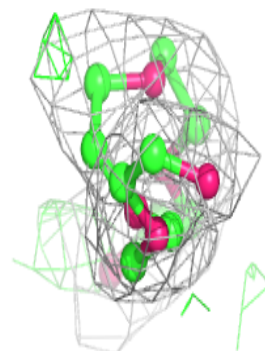
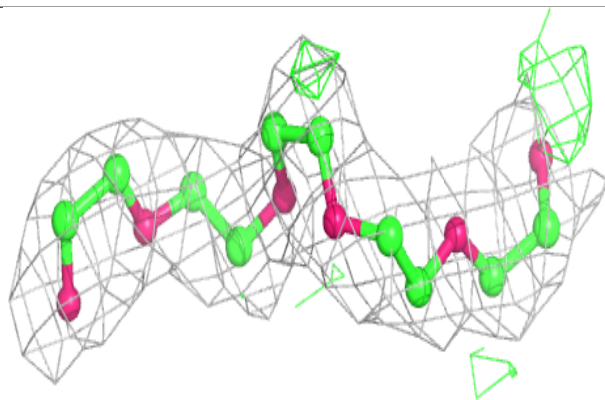
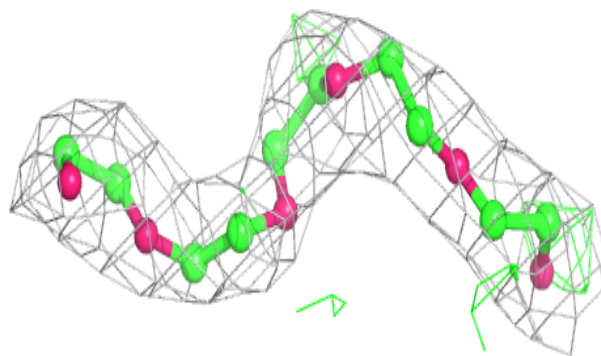
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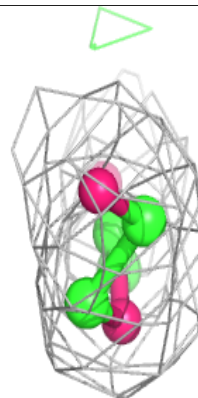
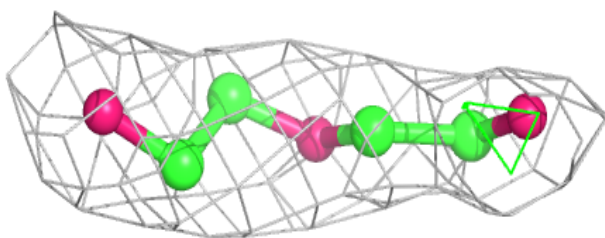
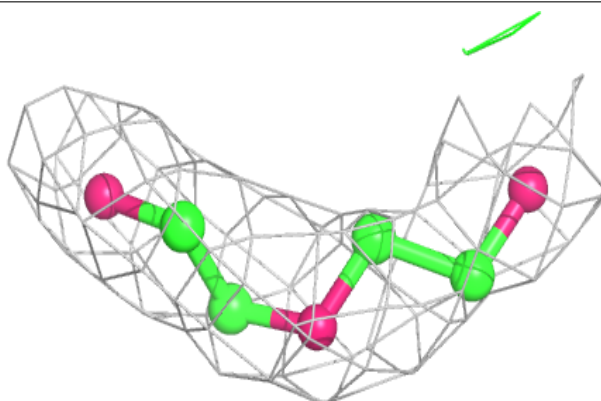


**Electron density around P6G D 612:**

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

**Electron density around P6G C 605:**

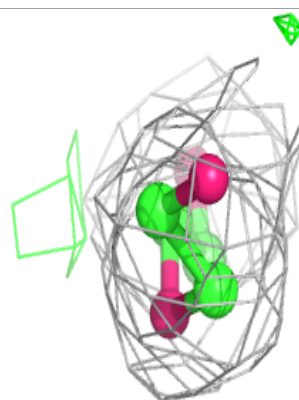
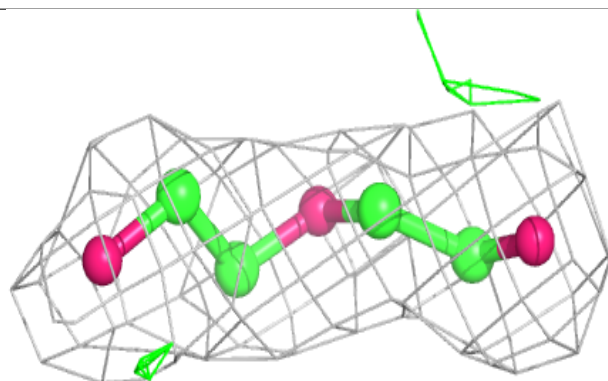
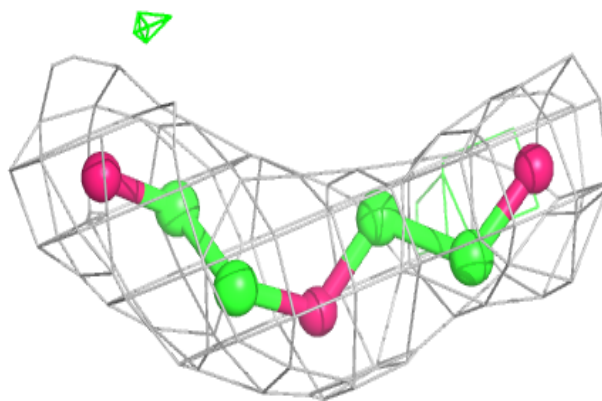
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



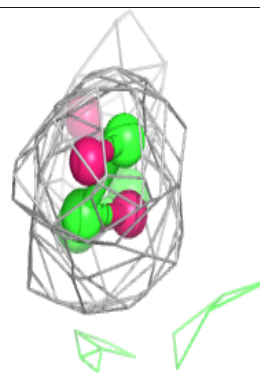
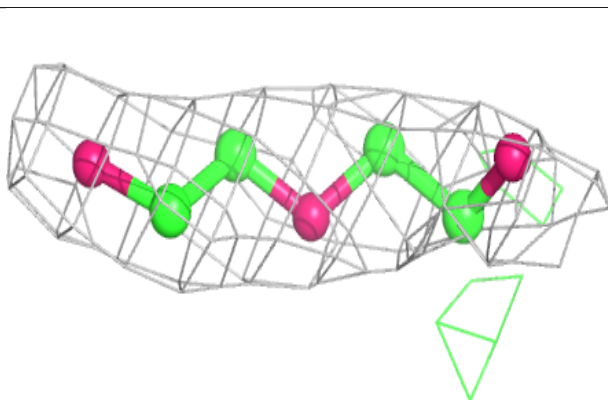
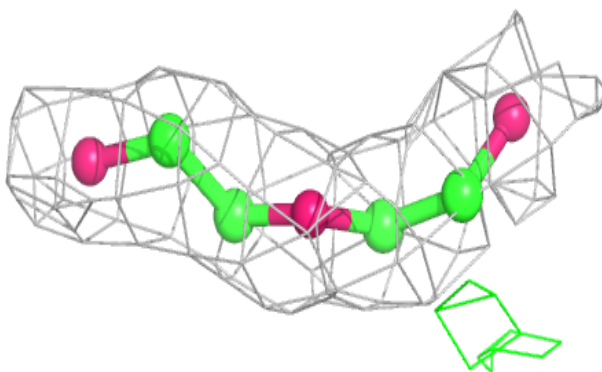


**Electron density around P6G C 606:**

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

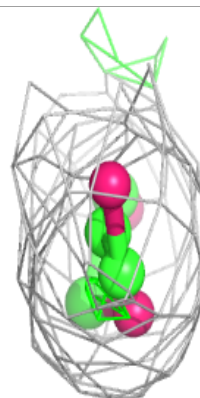
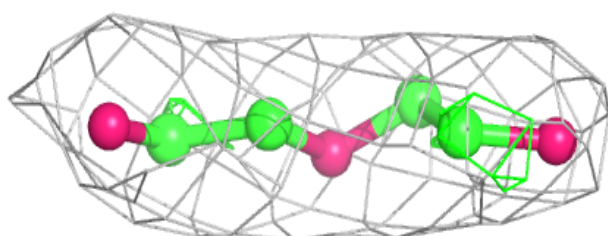
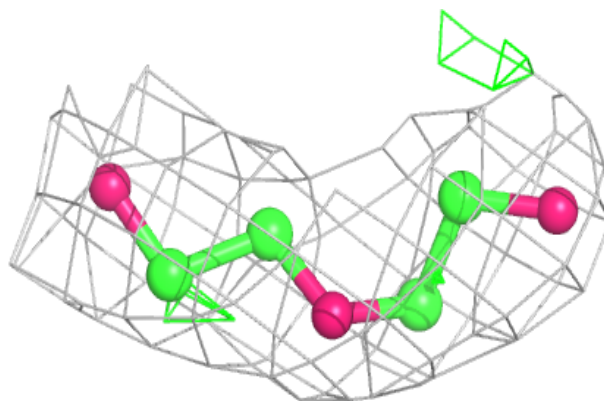
**Electron density around P6G C 604:**

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and green (positive)

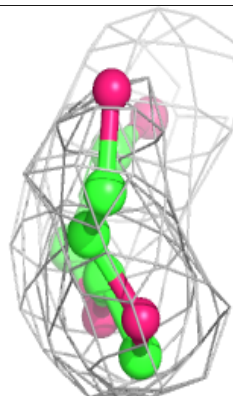
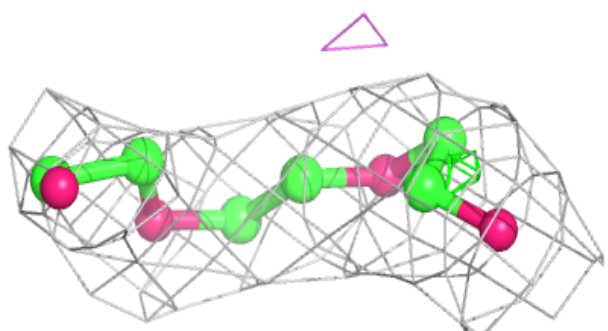
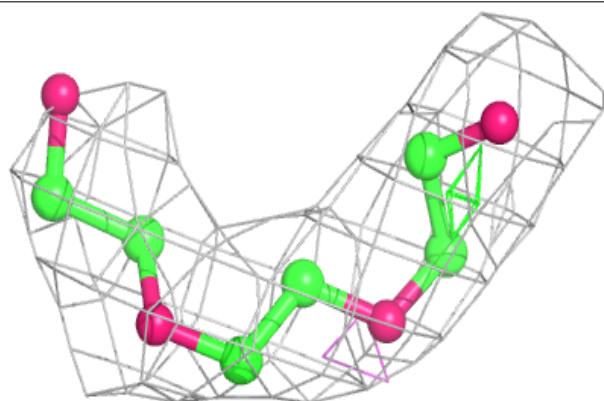


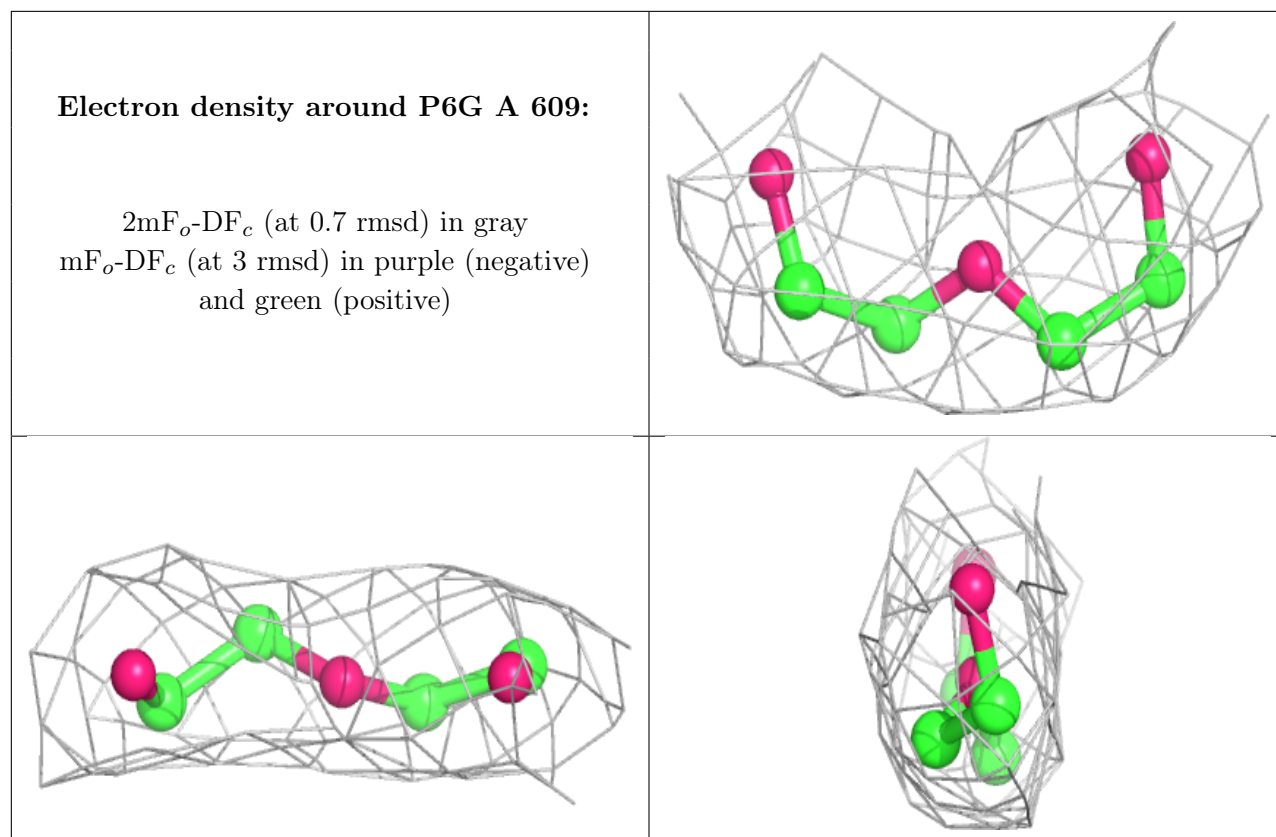
**Electron density around P6G A 607:**

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

**Electron density around P6G B 611:**

$2mF_o-DF_c$  (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.