



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 10:19 AM EST

PDB ID : 7M06  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, Y110F mutant with R,R-bislysine bound at the allosteric site at 2.7 Angstrom  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2021-03-10  
Resolution : 2.70 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

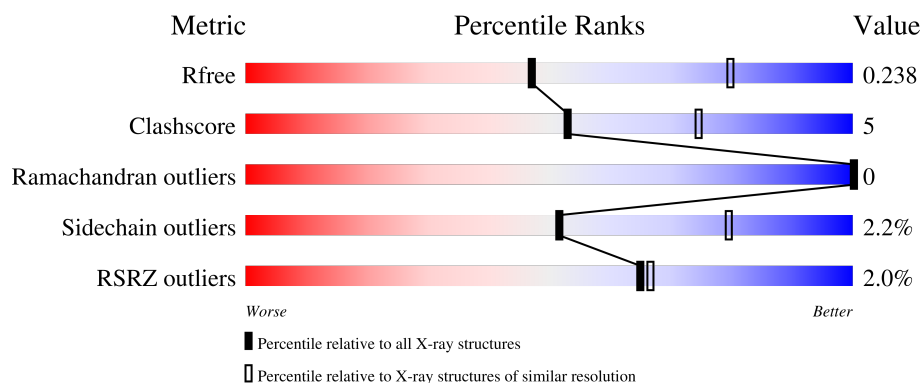
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	310	
1	B	310	
1	C	310	
1	D	310	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	3VN	B	301	-	-	-	X
4	3VN	C	301	-	-	-	X
5	PEG	D	304	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9256 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2271	1446	378	434	13			
1	B	296	Total	C	N	O	S	0	0	0
			2257	1435	375	434	13			
1	C	296	Total	C	N	O	S	0	0	0
			2256	1435	374	434	13			
1	D	297	Total	C	N	O	S	0	0	0
			2272	1446	378	435	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	110	PHE	TYR	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	110	PHE	TYR	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	110	PHE	TYR	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	110	PHE	TYR	engineered mutation	UNP Q9PPB4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

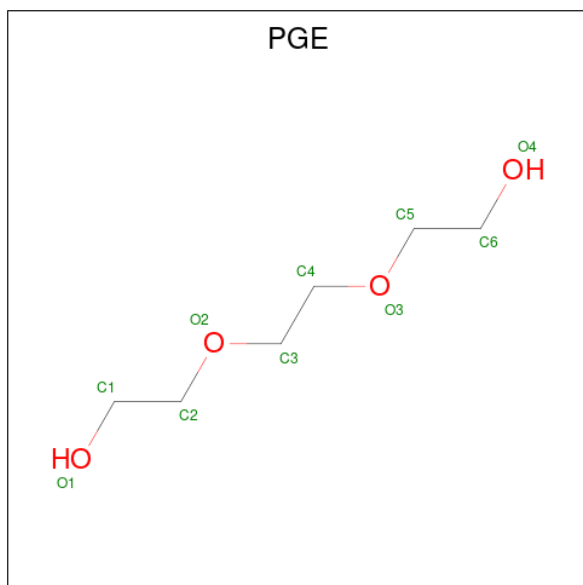
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	1	Total Mg 1 1	0	0
2	C	4	Total Mg 4 4	0	0

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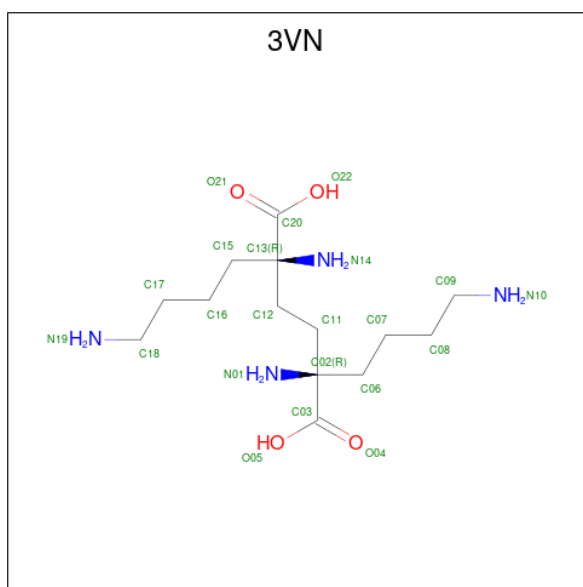
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ) (labeled as "Ligand of Interest" by depositor).



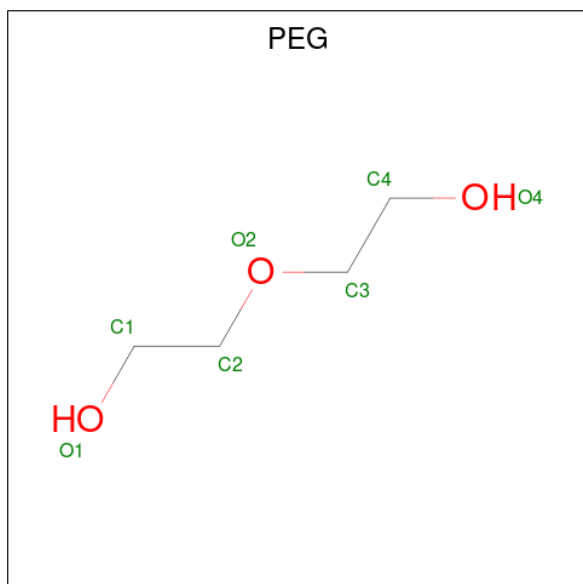
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	6	3		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula:  $C_{14}H_{30}N_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			22	14	4	4		
4	C	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ) (labeled as "Ligand of Interest" by depositor).



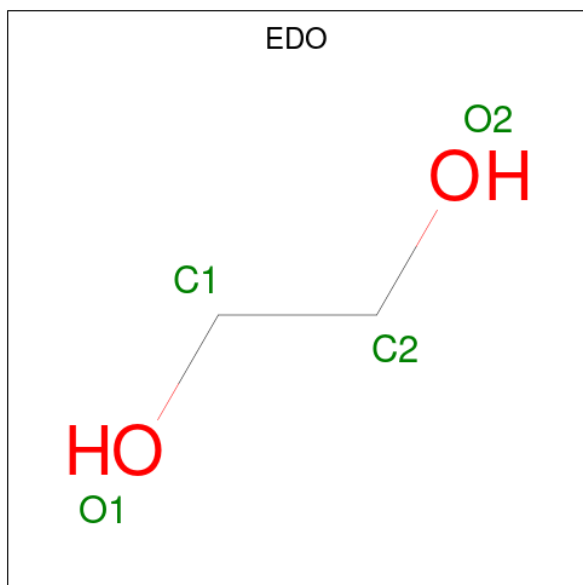
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			5	3	2		

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	21	Total	O	0	0
			21	21		
7	B	21	Total	O	0	0
			21	21		
7	C	27	Total	O	0	0
			27	27		
7	D	23	Total	O	0	0
			23	23		

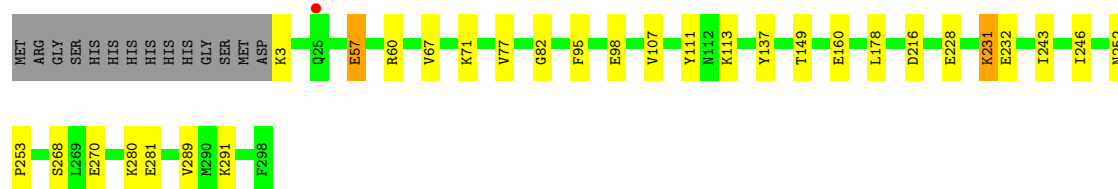


### 3 Residue-property plots [i](#)


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.

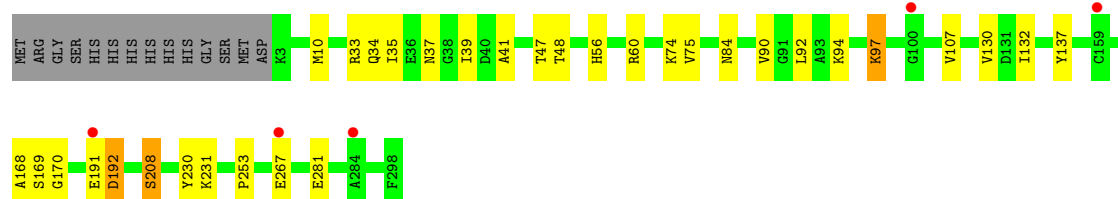
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A: 




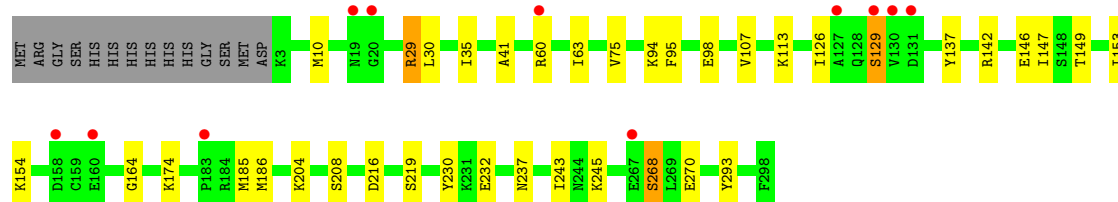
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B: 




- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

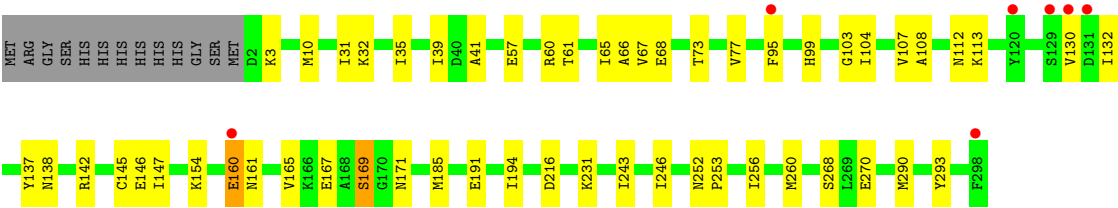
Chain C: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.03Å 84.29Å 200.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.15 – 2.70 43.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.15-2.70) 99.8 (43.15-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.194 , 0.242 0.194 , 0.238	Depositor DCC
$R_{free}$ test set	1717 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3VN, PEG, EDO, PGE, MG

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	0.48	0/2310	0.61	1/3123 (0.0%)
1	B	0.49	0/2296	0.58	0/3109
1	C	0.45	0/2295	0.60	0/3108
1	D	0.46	0/2311	0.57	0/3126
All	All	0.47	0/9212	0.59	1/12466 (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	98	GLU	CB-CA-C	5.13	120.67	110.40

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	2271	0	2312	19	3
1	B	2257	0	2275	23	0
1	C	2256	0	2270	24	0
1	D	2272	0	2303	38	3
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
2	D	2	0	0	0	0
3	A	9	0	11	1	0
3	B	10	0	14	1	0
3	C	10	0	14	3	0
3	D	10	0	14	3	0
4	B	22	0	28	2	0
4	C	22	0	28	0	0
5	B	5	0	5	0	0
5	D	7	0	10	0	0
6	D	4	0	6	0	0
7	A	21	0	0	3	0
7	B	21	0	0	0	0
7	C	27	0	0	1	0
7	D	23	0	0	3	0
All	All	9256	0	9290	100	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (100) 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:A:160:GLU:OE1	7:A:401:HOH:O	1.78	1.00
1:D:95:PHE:CE1	1:D:99:HIS:NE2	2.33	0.96
1:C:154:LYS:CE	3:C:306:PGE:H6	1.95	0.96
1:D:95:PHE:HE1	1:D:99:HIS:HE2	1.19	0.85
1:C:154:LYS:CE	3:C:306:PGE:C6	2.55	0.84
1:A:228:GLU:OE2	1:D:231:LYS:HE3	1.80	0.81
1:A:231:LYS:HE2	1:A:232:GLU:HG2	1.64	0.79
1:D:32:LYS:NZ	7:D:403:HOH:O	2.21	0.73
1:D:160:GLU:O	1:D:160:GLU:HG3	1.91	0.70
1:D:95:PHE:CE1	1:D:99:HIS:CD2	2.82	0.67
1:B:281:GLU:N	1:B:281:GLU:OE1	2.29	0.65
1:D:130:VAL:O	1:D:161:ASN:ND2	2.30	0.65
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.79	0.65
1:B:192:ASP:OD1	1:B:208:SER:HB2	1.99	0.62
1:D:154:LYS:HD2	3:D:303:PGE:H4	1.81	0.60
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.83	0.60
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.84	0.60
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.85	0.59
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.86	0.58
1:C:154:LYS:CE	3:C:306:PGE:H62	2.31	0.57
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.86	0.57
1:D:167:GLU:OE1	1:D:169:SER:HB3	2.03	0.57
1:A:149:THR:HG23	1:A:178:LEU:HD23	1.86	0.57
1:B:170:GLY:HA2	1:B:191:GLU:OE1	2.05	0.57
1:C:142:ARG:HG2	1:D:113:LYS:HE2	1.86	0.57
1:A:67:VAL:HA	1:A:77:VAL:HG21	1.88	0.56
1:D:95:PHE:CZ	1:D:99:HIS:CD2	2.95	0.55
1:D:154:LYS:NZ	3:D:303:PGE:H6	2.22	0.55
1:B:169:SER:N	1:B:191:GLU:OE2	2.41	0.54
1:C:60:ARG:HG3	1:C:95:PHE:CZ	2.42	0.54
1:C:94:LYS:O	1:C:98:GLU:HG3	2.08	0.53
1:C:268:SER:OG	1:C:270:GLU:HG3	2.07	0.53
1:B:35:ILE:HG12	1:B:75:VAL:HG21	1.90	0.53
1:B:56:HIS:HB3	1:B:60:ARG:NH2	2.23	0.52
1:B:168:ALA:C	1:B:191:GLU:OE2	2.48	0.52
1:D:165:VAL:HG12	1:D:185:MET:HE1	1.91	0.52
1:B:170:GLY:N	1:B:191:GLU:OE2	2.41	0.52
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.91	0.52
1:C:147:ILE:O	1:C:174:LYS:NZ	2.29	0.51
1:C:29:ARG:HG3	1:C:29:ARG:O	2.08	0.51
1:B:34:GLN:OE1	1:B:39:ILE:HG13	2.09	0.51
1:A:228:GLU:CD	1:D:231:LYS:HE3	2.31	0.51
1:C:63:ILE:HD12	1:C:95:PHE:HE2	1.75	0.51
1:B:230:TYR:CD2	1:C:230:TYR:HD2	2.28	0.50
1:D:67:VAL:HA	1:D:77:VAL:HG21	1.94	0.49
3:A:303:PGE:C6	1:B:84:ASN:HD21	2.25	0.49
1:A:111:TYR:OH	1:B:47:THR:OG1	2.30	0.49
1:B:74:LYS:O	1:B:74:LYS:HG3	2.12	0.48
1:D:113:LYS:HA	7:D:405:HOH:O	2.14	0.47
1:A:216:ASP:N	1:A:216:ASP:OD1	2.48	0.47
1:A:243:ILE:HD12	1:A:289:VAL:HG13	1.96	0.47
1:C:237:ASN:ND2	7:C:405:HOH:O	2.31	0.47
4:B:301:3VN:H14	4:B:301:3VN:H20	1.62	0.47
1:D:112:ASN:O	7:D:401:HOH:O	2.20	0.47
1:A:60:ARG:HB2	1:A:95:PHE:HZ	1.80	0.47
1:C:126:ILE:O	1:C:129:SER:HB3	2.15	0.46
3:B:303:PGE:H32	3:B:303:PGE:H12	1.70	0.46
1:D:104:ILE:HG23	1:D:132:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD21	4:B:301:3VN:H10	1.98	0.45
1:D:169:SER:OG	1:D:171:ASN:HB3	2.16	0.45
1:D:252:ASN:OD1	1:D:253:PRO:HA	2.16	0.45
1:B:94:LYS:HG2	1:B:130:VAL:HG22	1.99	0.44
1:D:103:GLY:HA2	1:D:132:ILE:HG12	1.99	0.44
1:B:168:ALA:HA	1:B:191:GLU:OE2	2.17	0.44
1:C:186:MET:SD	1:C:204:LYS:HG3	2.57	0.44
1:C:232:GLU:OE2	1:C:232:GLU:N	2.50	0.44
1:D:243:ILE:HB	1:D:293:TYR:CE1	2.53	0.44
1:D:35:ILE:HD13	1:D:73:THR:HG21	1.99	0.44
1:D:39:ILE:HD13	1:D:39:ILE:HA	1.92	0.44
1:D:31:ILE:HD13	1:D:66:ALA:HA	2.00	0.44
1:D:108:ALA:HB2	1:D:147:ILE:HD11	1.99	0.43
1:B:33:ARG:O	1:B:37:ASN:ND2	2.44	0.43
1:D:154:LYS:HZ3	3:D:303:PGE:H6	1.83	0.43
1:D:61:THR:O	1:D:65:ILE:HG13	2.18	0.43
1:D:191:GLU:HB3	1:D:194:ILE:HG12	1.99	0.43
1:A:268:SER:OG	1:A:270:GLU:HG3	2.19	0.43
1:B:97:LYS:HD2	1:B:130:VAL:HG13	2.00	0.43
1:C:243:ILE:HB	1:C:293:TYR:CE1	2.54	0.43
1:B:97:LYS:HG3	1:B:132:ILE:HG23	1.99	0.43
1:B:90:VAL:O	1:B:94:LYS:HG3	2.19	0.43
1:D:246:ILE:HA	1:D:246:ILE:HD12	1.79	0.43
1:D:216:ASP:OD1	1:D:216:ASP:N	2.52	0.42
1:D:268:SER:OG	1:D:270:GLU:HG3	2.19	0.42
1:D:138:ASN:HD21	1:D:146:GLU:HG3	1.83	0.42
1:C:164:GLY:HA2	1:C:185:MET:HG3	2.01	0.42
1:D:256:ILE:O	1:D:260:MET:HG2	2.20	0.42
1:A:82:GLY:O	7:A:402:HOH:O	2.22	0.42
1:A:246:ILE:HD13	1:A:246:ILE:HA	1.88	0.41
1:B:48:THR:HG23	1:B:253:PRO:HB3	2.02	0.41
1:C:149:THR:O	1:C:153:ILE:HG13	2.20	0.41
1:D:243:ILE:HA	1:D:246:ILE:HG22	2.02	0.41
1:A:3:LYS:HG2	1:A:160:GLU:O	2.20	0.41
1:C:216:ASP:OD1	1:C:216:ASP:N	2.53	0.41
1:A:71:LYS:O	1:A:71:LYS:HG3	2.20	0.41
1:A:252:ASN:OD1	1:A:253:PRO:HA	2.20	0.41
1:A:113:LYS:HA	7:A:406:HOH:O	2.20	0.41
1:C:245:LYS:HA	1:C:245:LYS:HD2	1.84	0.40
1:C:113:LYS:HD2	1:D:142:ARG:HG2	2.02	0.40
1:A:280:LYS:HG3	1:A:281:GLU:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:OE2	1:D:57:GLU:OE1[1_565]	1.27	0.93
1:A:57:GLU:CD	1:D:57:GLU:OE1[1_565]	1.65	0.55
1:A:57:GLU:OE1	1:D:57:GLU:OE1[1_565]	1.77	0.43

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	B	294/310 (95%)	284 (97%)	10 (3%)	0	100	100
1	C	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	D	295/310 (95%)	290 (98%)	5 (2%)	0	100	100
All	All	1177/1240 (95%)	1150 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/261 (95%)	245 (99%)	3 (1%)	71	88
1	B	245/261 (94%)	240 (98%)	5 (2%)	55	81
1	C	244/261 (94%)	237 (97%)	7 (3%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	247/261 (95%)	240 (97%)	7 (3%)	43 73
All	All	984/1044 (94%)	962 (98%)	22 (2%)	52 79

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	231	LYS
1	A	291	LYS
1	B	97	LYS
1	B	192	ASP
1	B	208	SER
1	B	231	LYS
1	B	267	GLU
1	C	29	ARG
1	C	30	LEU
1	C	129	SER
1	C	146	GLU
1	C	208	SER
1	C	219	SER
1	C	268	SER
1	D	3	LYS
1	D	60	ARG
1	D	68	GLU
1	D	145	CYS
1	D	160	GLU
1	D	169	SER
1	D	290	MET

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

Mol	Chain	Res	Type
1	B	223	HIS
1	C	128	GLN
1	C	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z  > 2$
4	3VN	C	301	-	15,21,21	0.99	1 (6%)	12,28,28	2.85	6 (50%)
4	3VN	B	301	-	15,21,21	1.30	1 (6%)	12,28,28	1.70	3 (25%)
3	PGE	B	303	-	9,9,9	0.34	0	8,8,8	0.31	0
3	PGE	C	306	-	9,9,9	0.31	0	8,8,8	0.48	0
3	PGE	D	303	-	9,9,9	0.32	0	8,8,8	0.33	0
5	PEG	B	304	-	4,4,6	0.52	0	3,3,5	0.66	0
6	EDO	D	305	-	3,3,3	0.28	0	2,2,2	0.41	0
3	PGE	A	303	-	8,8,9	0.33	0	7,7,8	0.86	0
5	PEG	D	304	-	6,6,6	0.51	0	5,5,5	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3VN	C	301	-	-	10/19/31/31	-
4	3VN	B	301	-	-	7/19/31/31	-
3	PGE	B	303	-	-	5/7/7/7	-
3	PGE	C	306	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	D	303	-	-	4/7/7/7	-
5	PEG	B	304	-	-	1/2/2/4	-
6	EDO	D	305	-	-	1/1/1/1	-
3	PGE	A	303	-	-	2/6/6/7	-
5	PEG	D	304	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	3VN	C06-C02	3.39	1.58	1.55
4	C	301	3VN	C06-C02	2.47	1.57	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	3VN	C11-C12-C13	-5.44	105.59	115.19
4	C	301	3VN	C12-C11-C02	-4.35	107.52	115.19
4	C	301	3VN	C16-C15-C13	-3.99	108.13	115.20
4	B	301	3VN	C11-C12-C13	-3.68	108.69	115.19
4	C	301	3VN	C15-C16-C17	-3.47	102.85	113.19
4	C	301	3VN	C07-C06-C02	-2.83	110.17	115.20
4	B	301	3VN	C06-C02-C11	-2.27	107.15	111.94
4	B	301	3VN	C16-C15-C13	-2.20	111.29	115.20
4	C	301	3VN	C15-C13-C12	-2.07	107.57	111.94

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	3VN	N01-C02-C11-C12
4	B	301	3VN	C03-C02-C11-C12
4	B	301	3VN	C06-C02-C11-C12
4	C	301	3VN	C03-C02-C11-C12
4	C	301	3VN	C11-C12-C13-C20
3	C	306	PGE	O2-C3-C4-O3
4	B	301	3VN	C02-C06-C07-C08
4	C	301	3VN	C02-C06-C07-C08
4	C	301	3VN	C11-C12-C13-N14
4	C	301	3VN	C11-C12-C13-C15
3	C	306	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
5	B	304	PEG	O2-C3-C4-O4
5	D	304	PEG	O2-C3-C4-O4
3	B	303	PGE	C1-C2-O2-C3
3	B	303	PGE	O2-C3-C4-O3
4	B	301	3VN	C15-C16-C17-C18
4	C	301	3VN	C06-C02-C11-C12
3	B	303	PGE	O1-C1-C2-O2
4	C	301	3VN	N01-C02-C11-C12
4	B	301	3VN	C16-C17-C18-N19
6	D	305	EDO	O1-C1-C2-O2
3	D	303	PGE	O2-C3-C4-O3
4	C	301	3VN	C16-C17-C18-N19
4	B	301	3VN	C13-C15-C16-C17
3	D	303	PGE	O1-C1-C2-O2
5	D	304	PEG	C4-C3-O2-C2
5	D	304	PEG	C1-C2-O2-C3
3	A	303	PGE	O2-C3-C4-O3
3	A	303	PGE	C1-C2-O2-C3
4	C	301	3VN	C13-C15-C16-C17
3	D	303	PGE	C3-C4-O3-C5
4	C	301	3VN	C07-C08-C09-N10
3	B	303	PGE	C3-C4-O3-C5
3	C	306	PGE	C6-C5-O3-C4
3	D	303	PGE	C1-C2-O2-C3
5	D	304	PEG	O1-C1-C2-O2
3	B	303	PGE	O3-C5-C6-O4

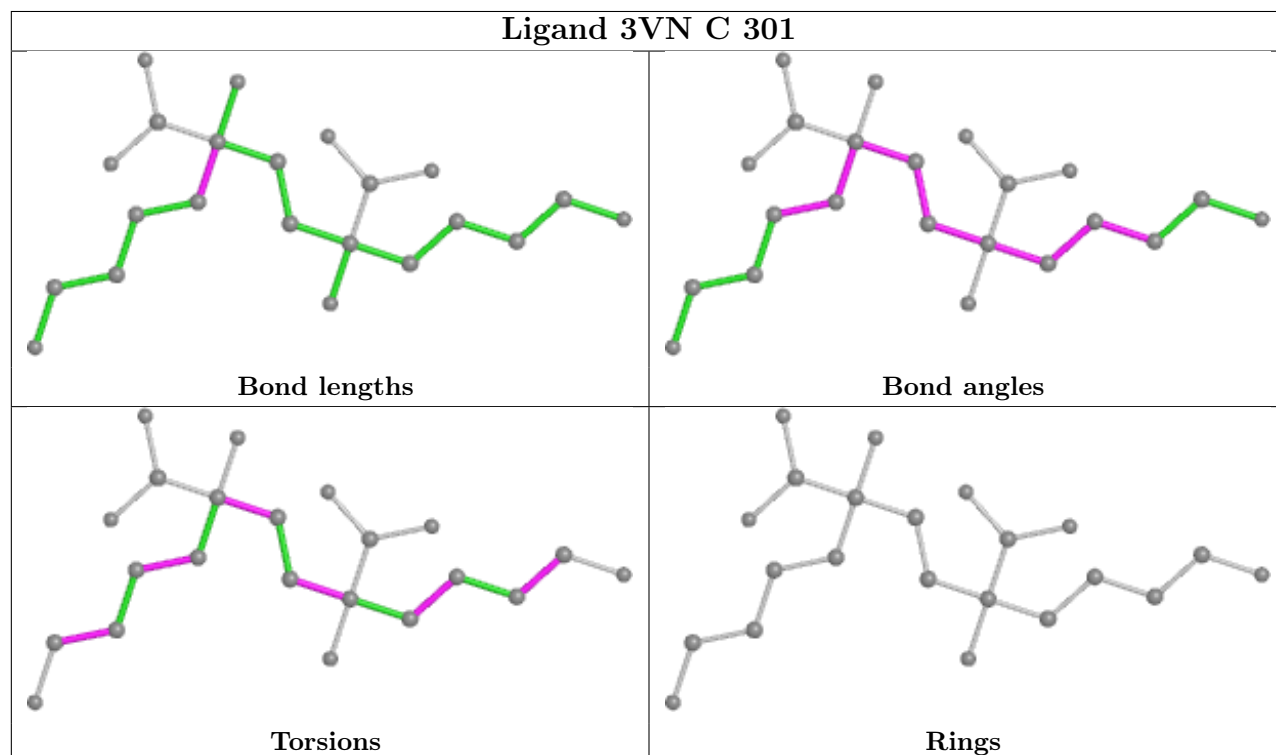
There are no ring outliers.

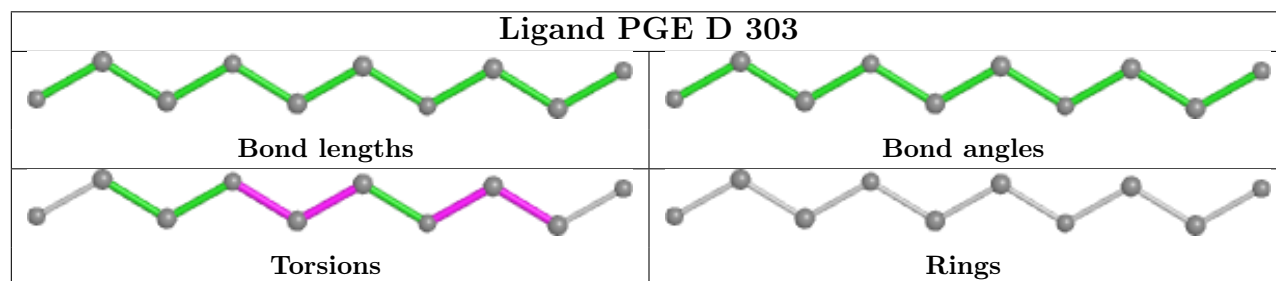
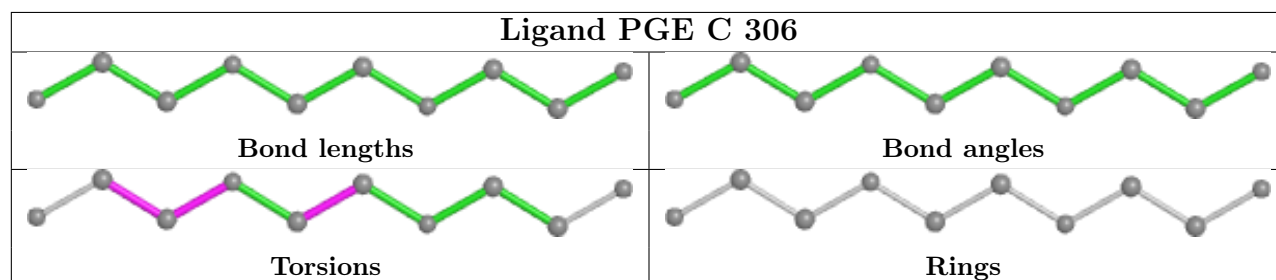
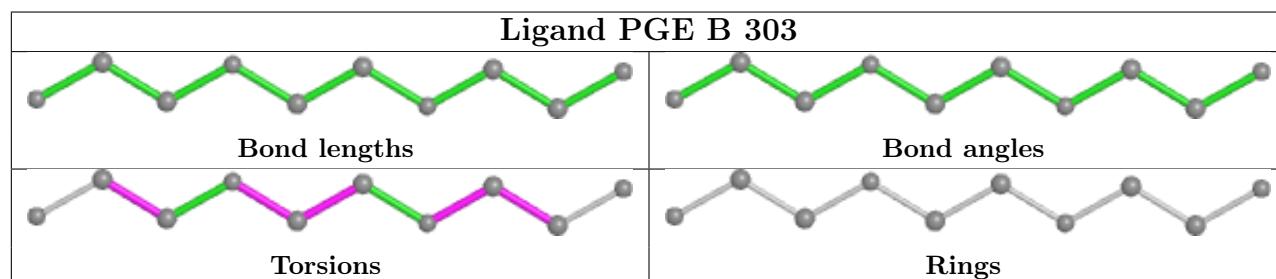
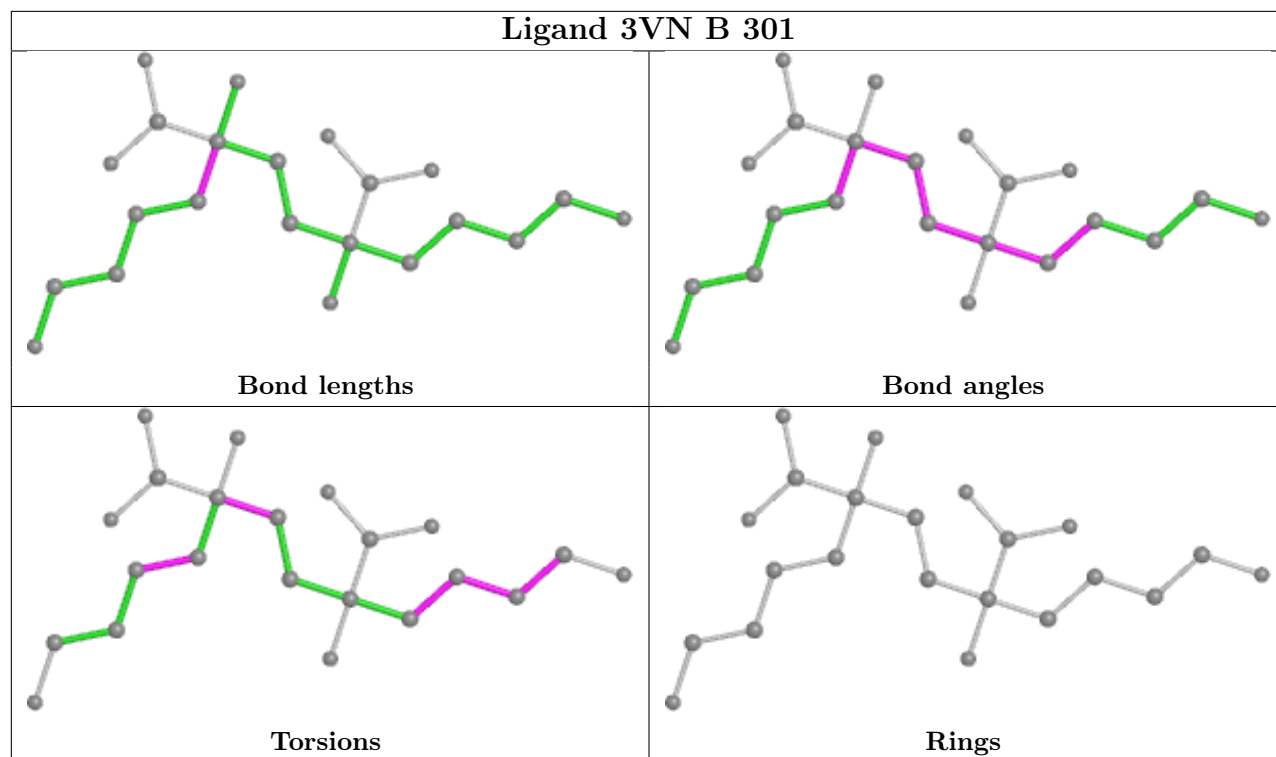
5 monomers are involved in 10 short contacts:

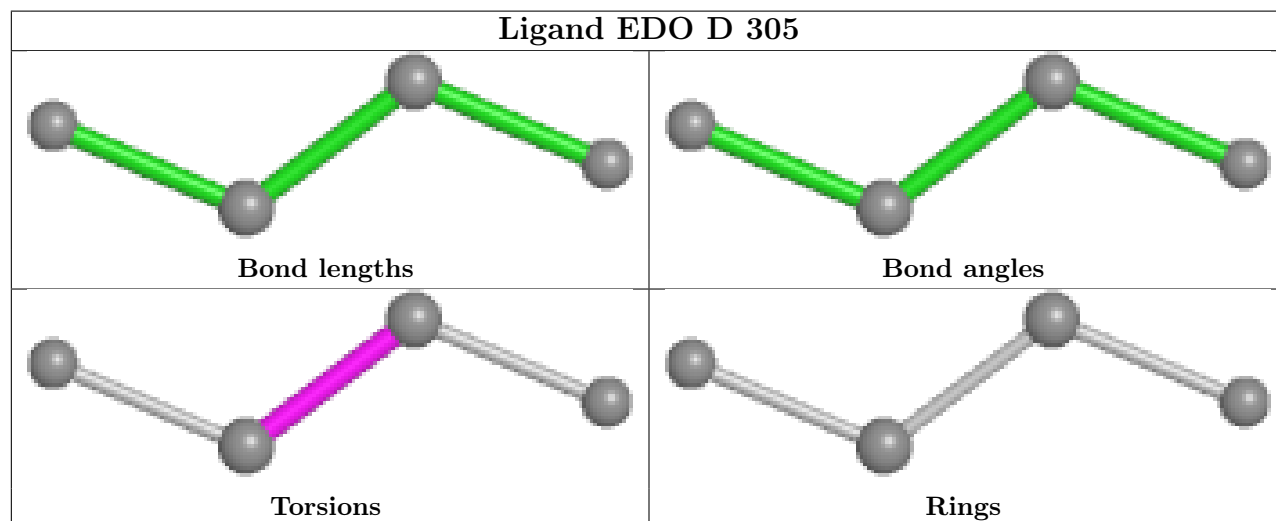
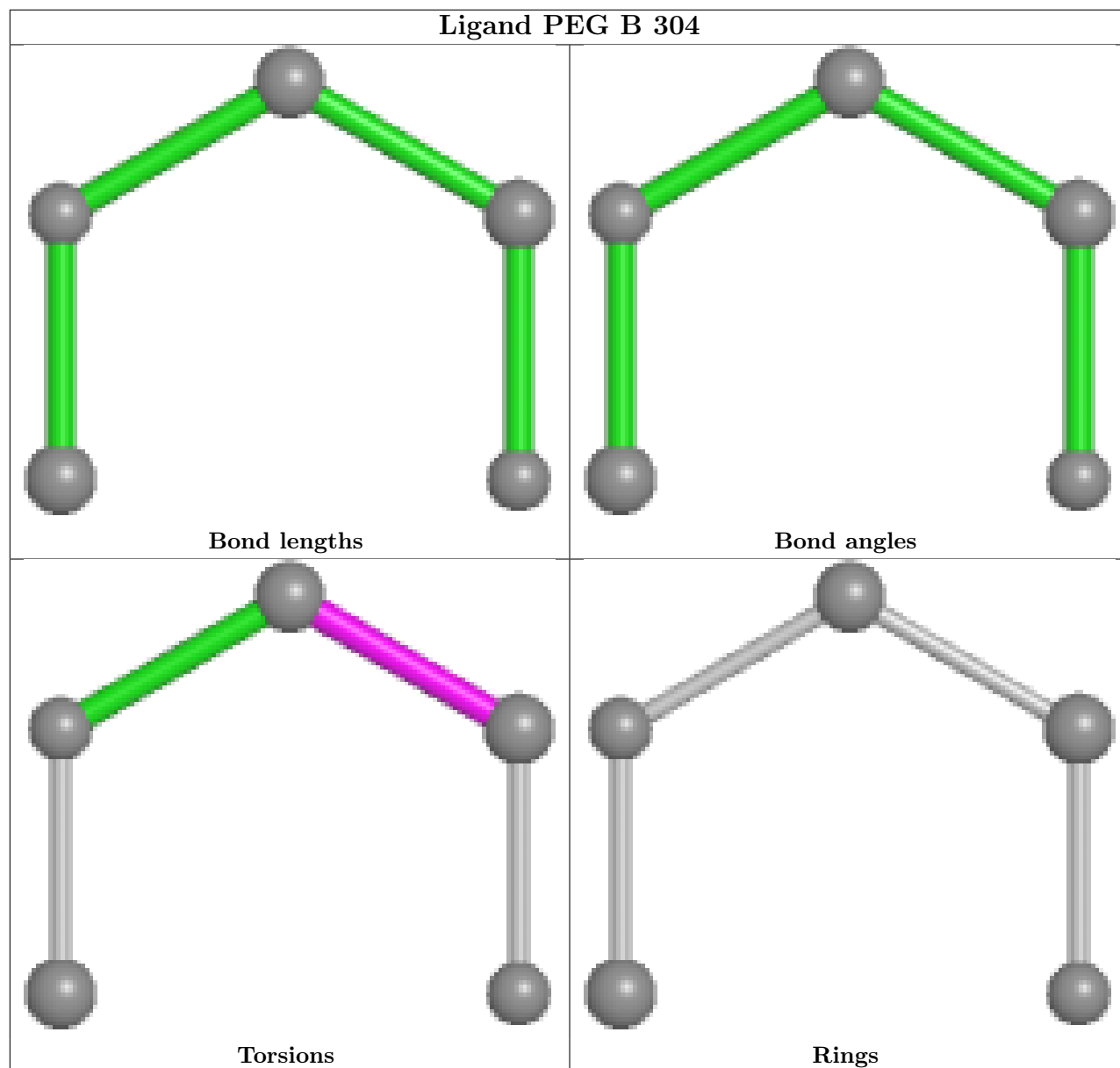
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	3VN	2	0
3	B	303	PGE	1	0
3	C	306	PGE	3	0
3	D	303	PGE	3	0
3	A	303	PGE	1	0

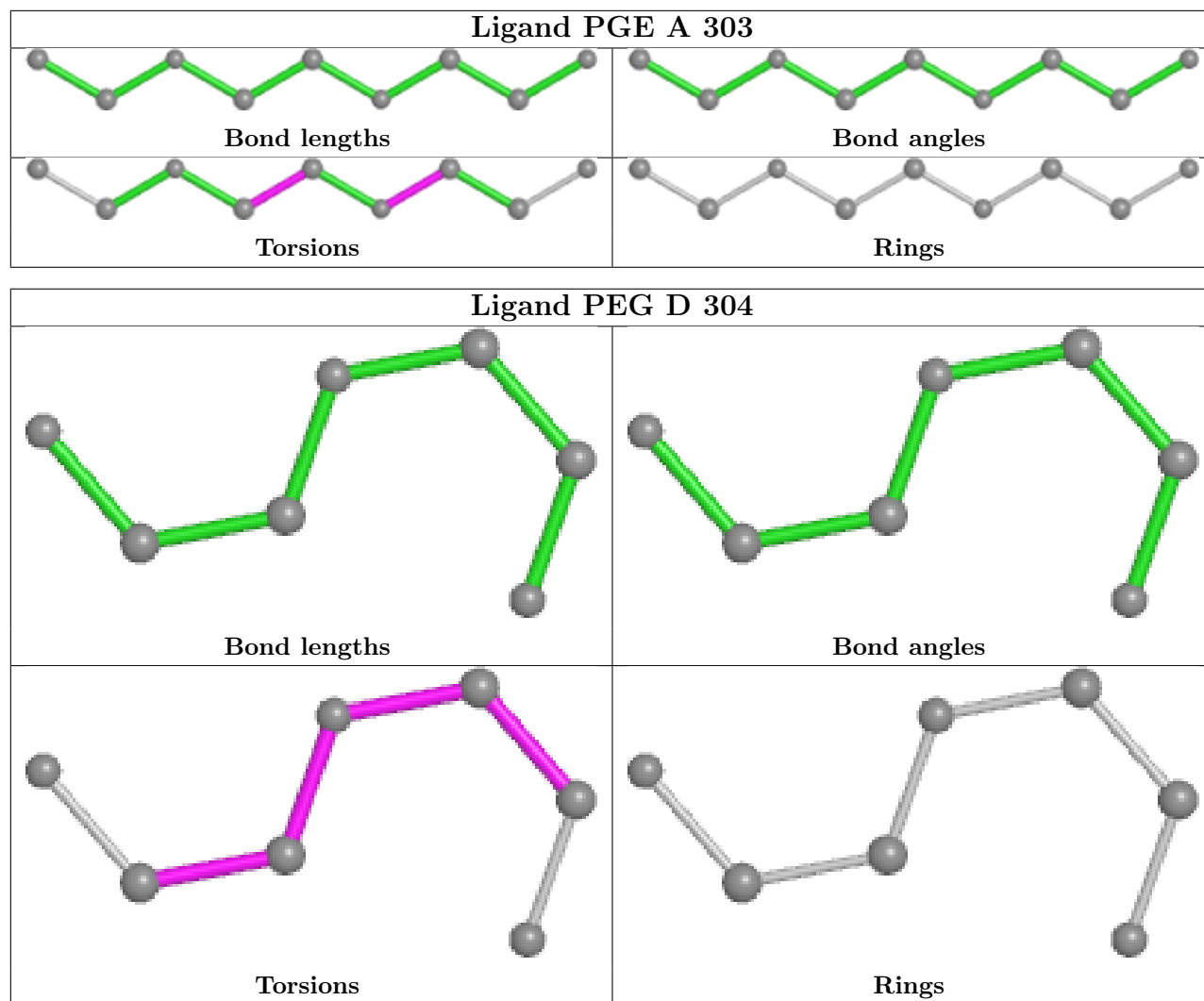
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	296/310 (95%)	0.05	1 (0%) 94 95	34, 46, 68, 85	0
1	B	296/310 (95%)	0.07	5 (1%) 70 72	32, 44, 60, 83	0
1	C	296/310 (95%)	0.21	11 (3%) 41 41	34, 44, 65, 81	0
1	D	297/310 (95%)	0.11	7 (2%) 59 60	32, 44, 65, 89	0
All	All	1185/1240 (95%)	0.11	24 (2%) 65 67	32, 44, 65, 89	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	ASP	4.1
1	C	60	ARG	3.7
1	D	129	SER	3.4
1	B	267	GLU	3.2
1	D	298	PHE	3.1
1	C	127	ALA	3.0
1	A	25	GLN	2.9
1	C	129	SER	2.8
1	C	20	GLY	2.7
1	C	183	PRO	2.7
1	C	158	ASP	2.5
1	C	160	GLU	2.5
1	D	131	ASP	2.5
1	D	160	GLU	2.3
1	B	191	GLU	2.2
1	D	95	PHE	2.2
1	C	19	ASN	2.2
1	B	100	GLY	2.1
1	D	130	VAL	2.1
1	B	159	CYS	2.1
1	D	120	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	267	GLU	2.1
1	B	284	ALA	2.1
1	C	130	VAL	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, 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.

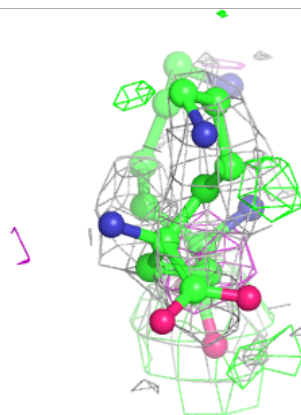
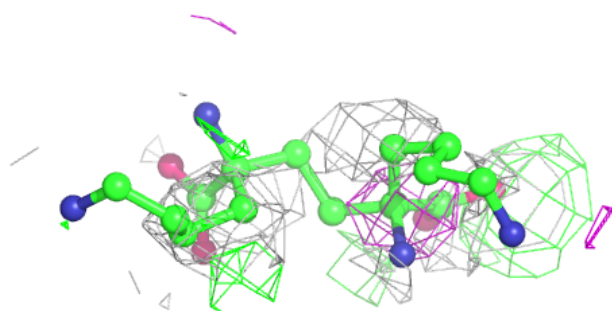
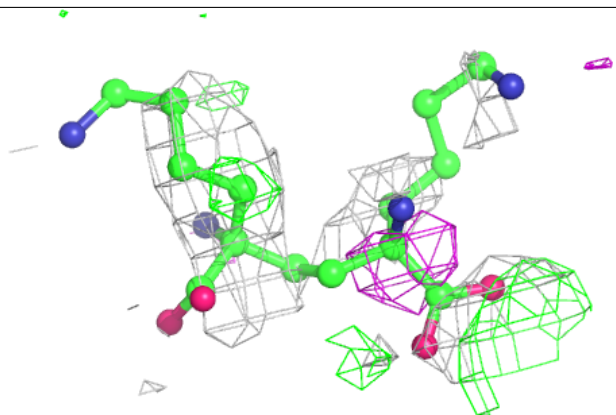
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	3VN	B	301	22/22	0.26	0.62	93,103,110,110	0
4	3VN	C	301	22/22	0.31	0.67	122,127,128,129	0
5	PEG	D	304	7/7	0.65	0.43	41,42,46,47	0
5	PEG	B	304	5/7	0.74	0.40	44,45,49,51	0
3	PGE	A	303	9/10	0.77	0.35	52,54,55,55	0
3	PGE	B	303	10/10	0.85	0.23	62,63,64,64	0
2	MG	A	302	1/1	0.87	0.35	50,50,50,50	0
2	MG	D	301	1/1	0.89	0.39	41,41,41,41	0
2	MG	D	302	1/1	0.89	0.58	53,53,53,53	0
2	MG	B	302	1/1	0.90	0.19	45,45,45,45	0
6	EDO	D	305	4/4	0.91	0.38	20,20,20,20	0
3	PGE	D	303	10/10	0.93	0.20	61,63,65,65	0
2	MG	A	301	1/1	0.93	0.37	40,40,40,40	0
3	PGE	C	306	10/10	0.93	0.23	50,54,58,58	0
2	MG	C	305	1/1	0.95	0.15	51,51,51,51	0
2	MG	C	302	1/1	0.95	0.49	30,30,30,30	0
2	MG	C	303	1/1	0.96	0.25	37,37,37,37	0
2	MG	C	304	1/1	0.96	0.28	39,39,39,39	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.

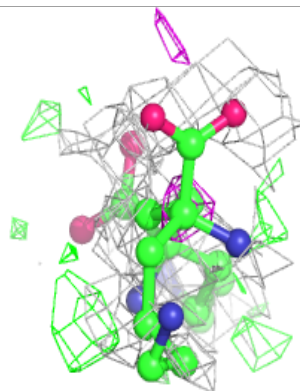
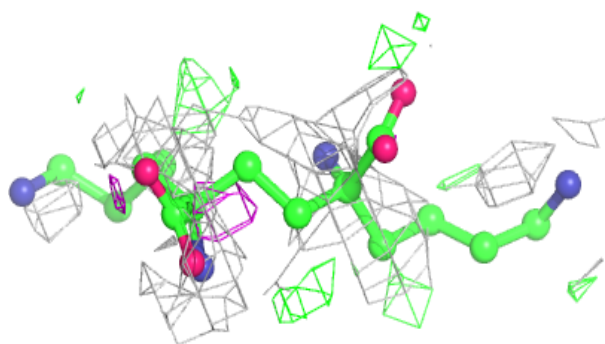
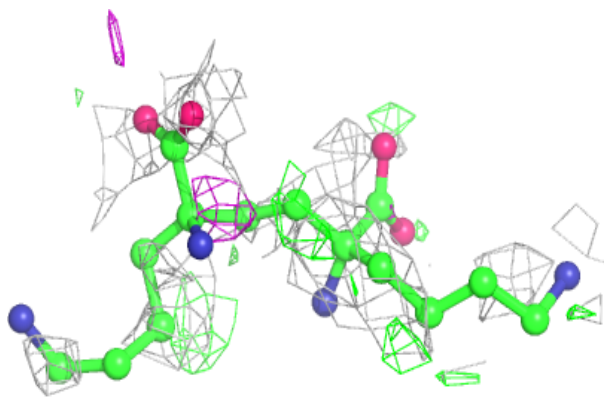
**Electron density around 3VN B 301:**

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

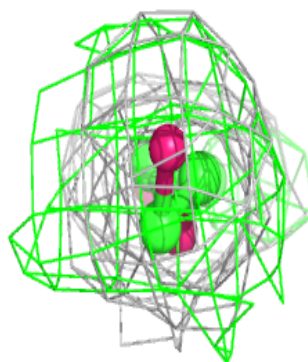
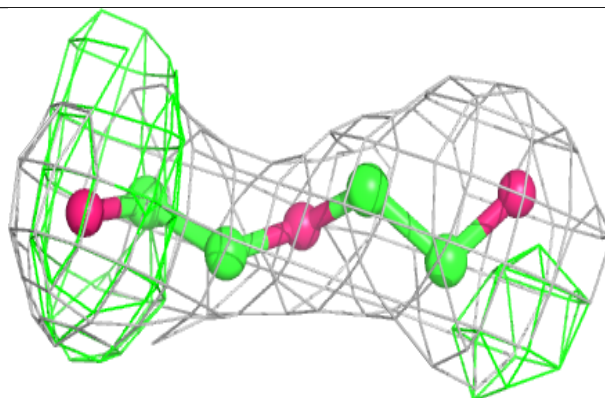
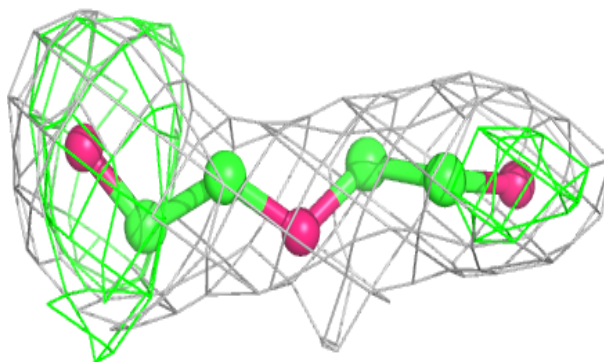


**Electron density around 3VN C 301:**

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

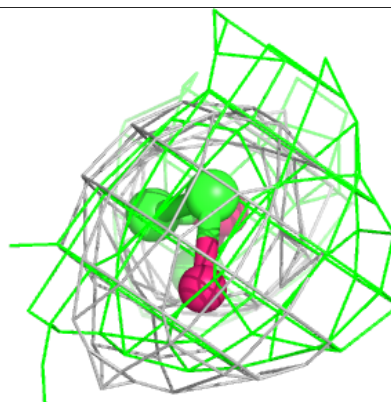
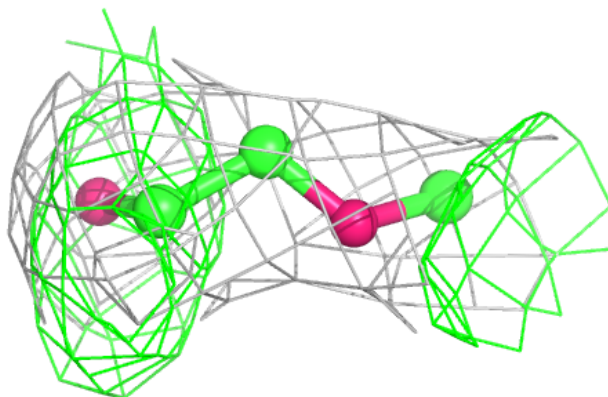
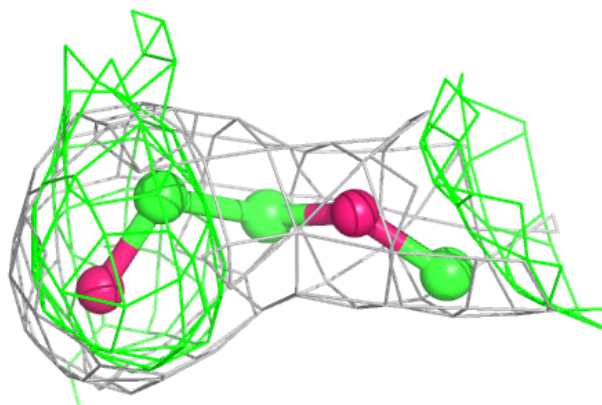
**Electron density around PEG D 304:**

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

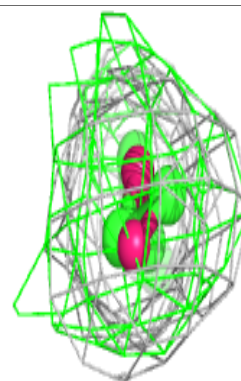
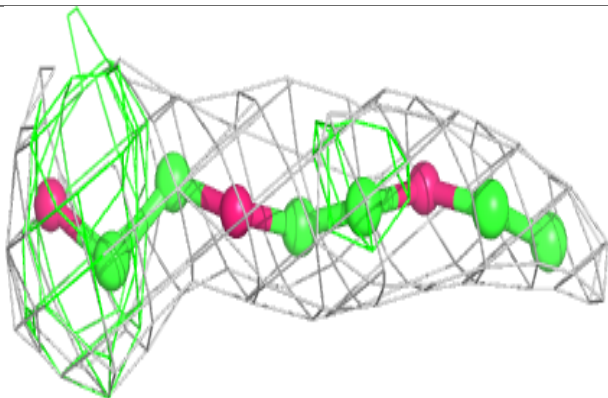
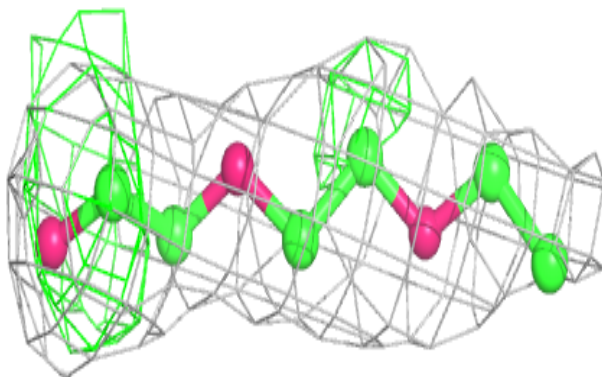


**Electron density around PEG B 304:**

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

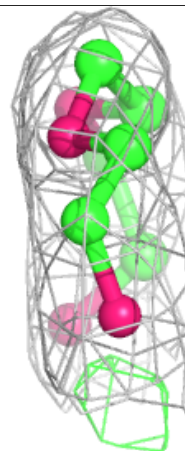
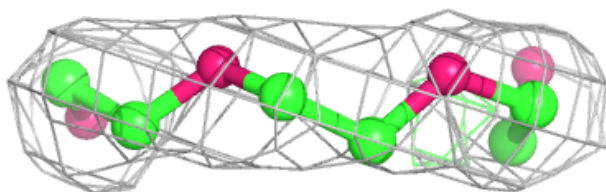
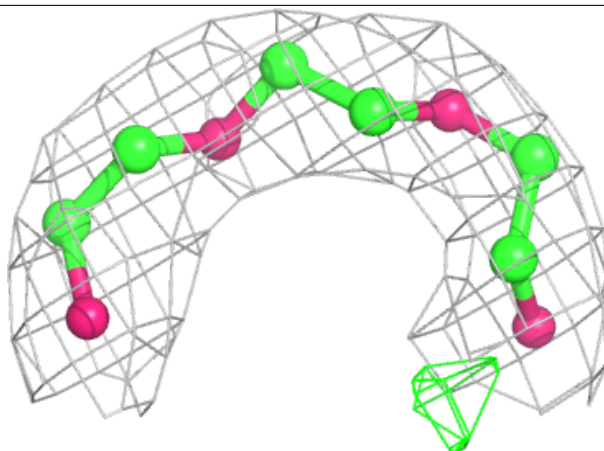
**Electron density around PGE A 303:**

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



**Electron density around PGE B 303:**

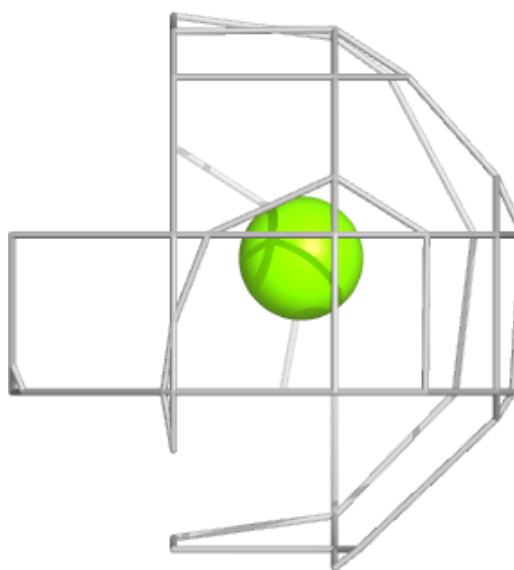
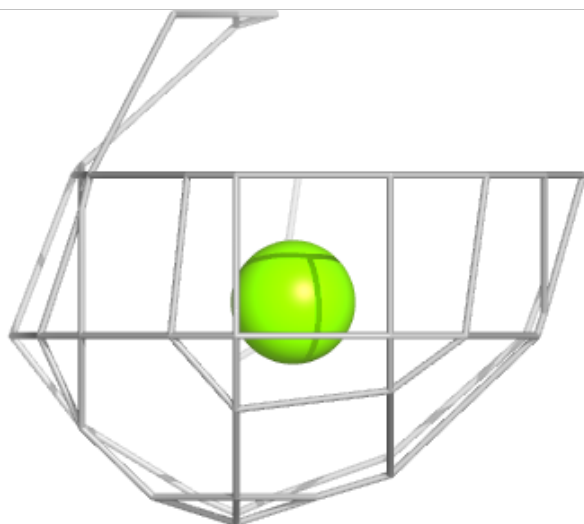
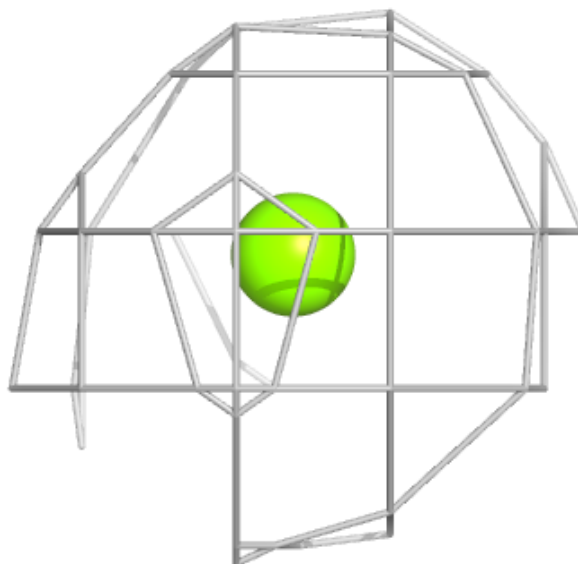
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





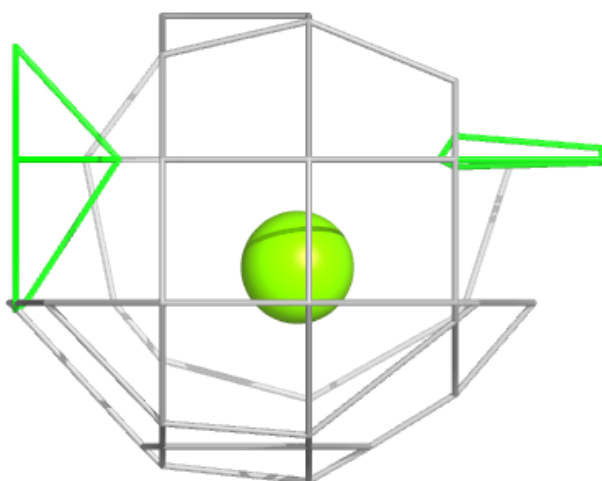
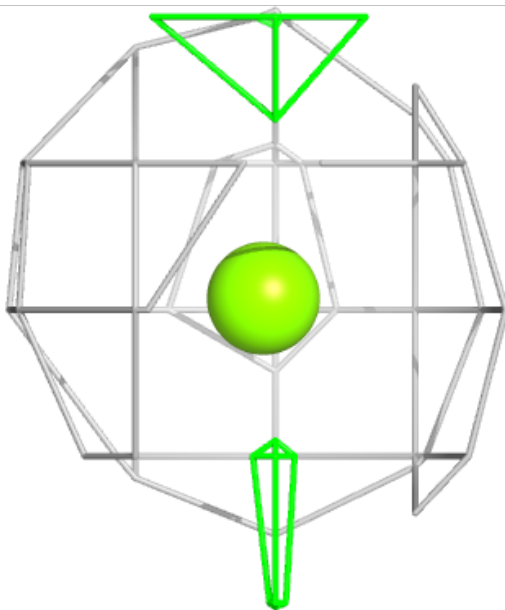
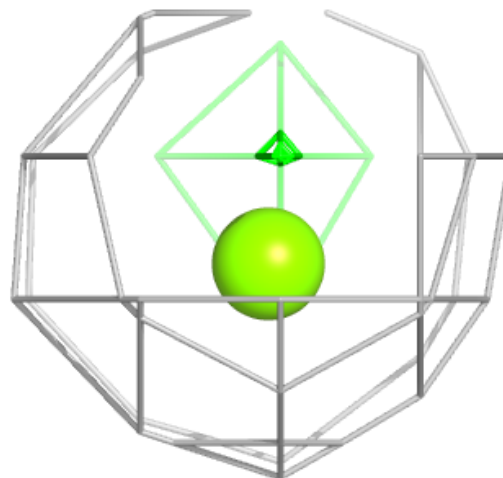
**Electron density around MG A 302:**

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



**Electron density around MG D 301:**

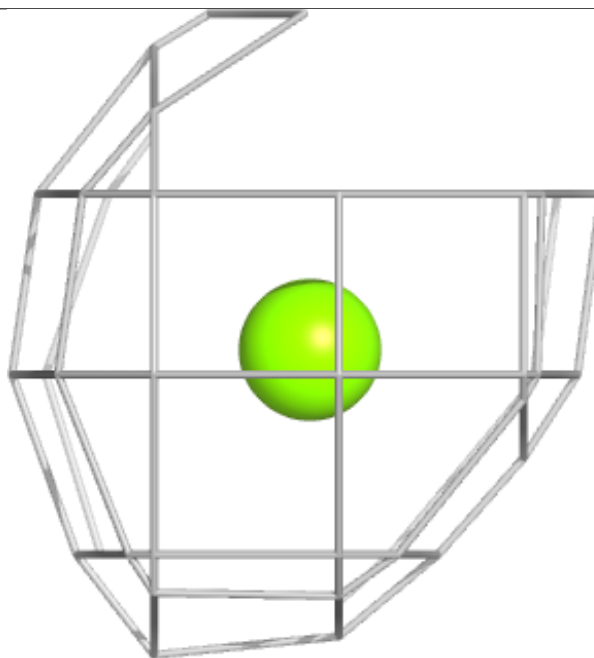
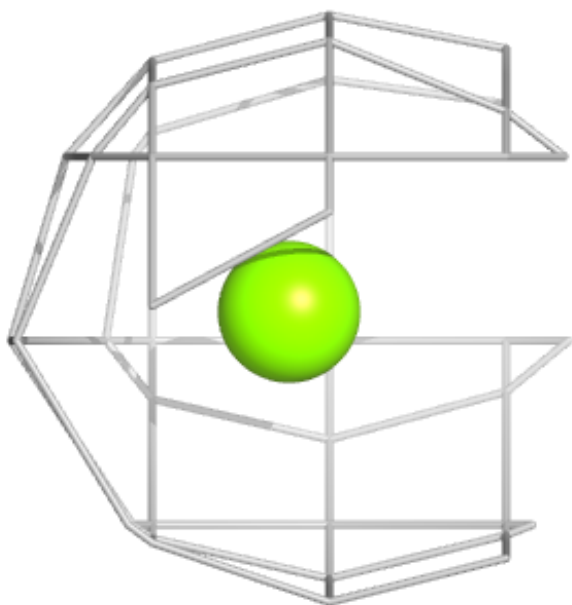
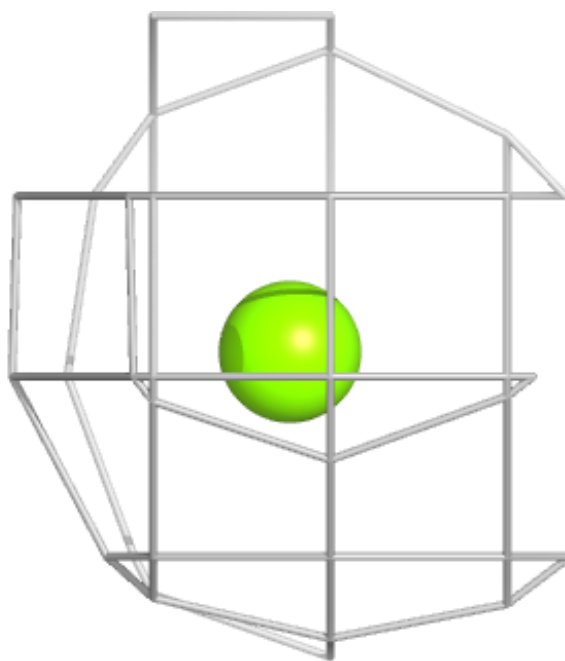
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





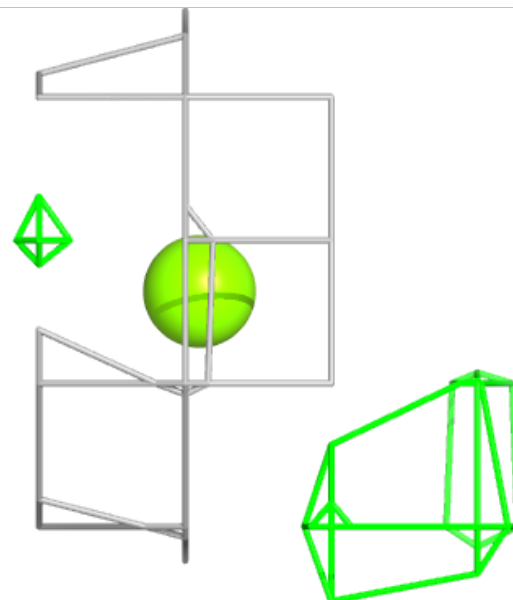
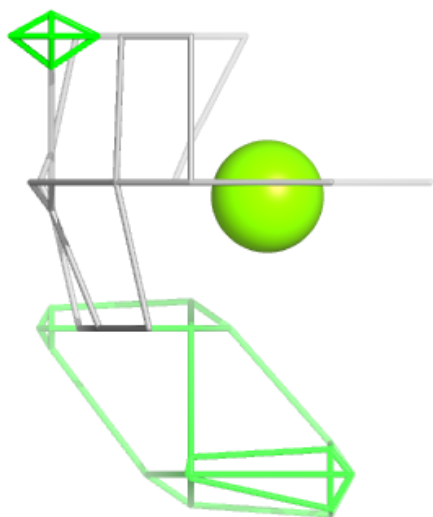
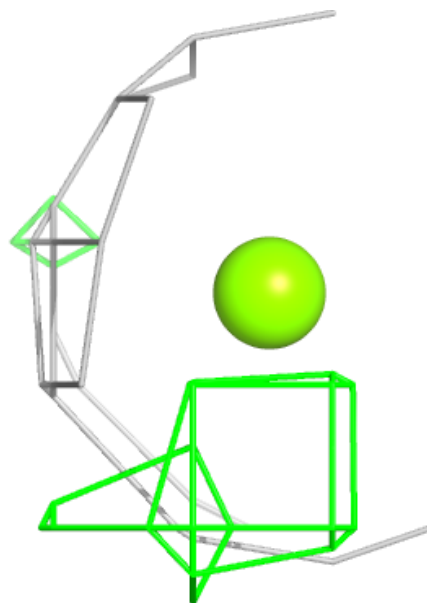
**Electron density around MG D 302:**

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



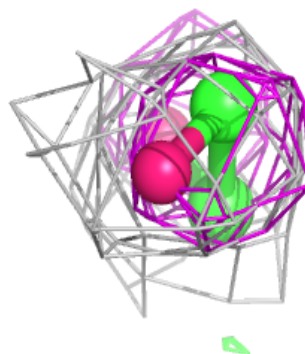
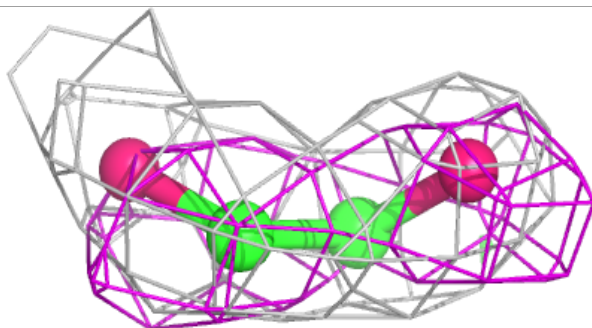
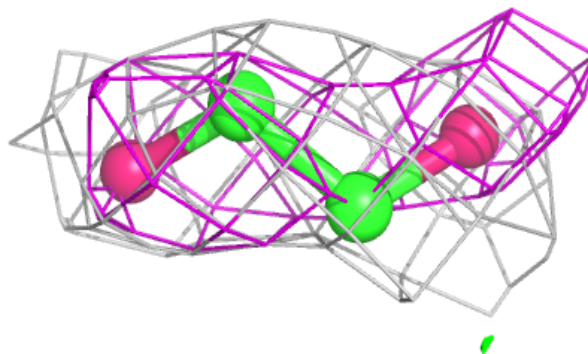
**Electron density around MG B 302:**

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

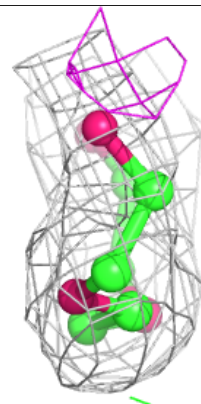
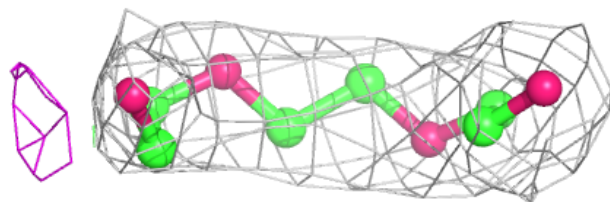
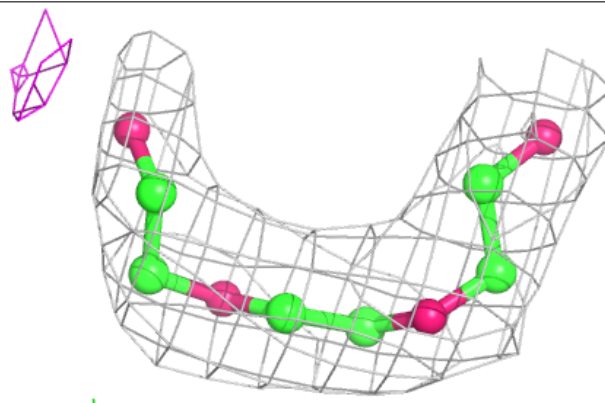


**Electron density around EDO D 305:**

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

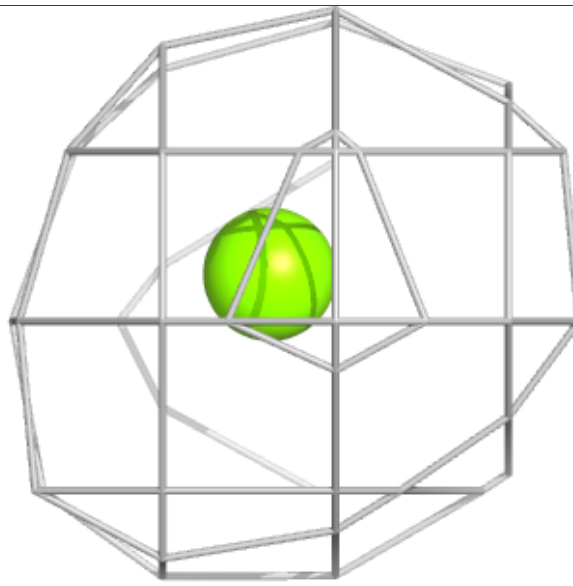
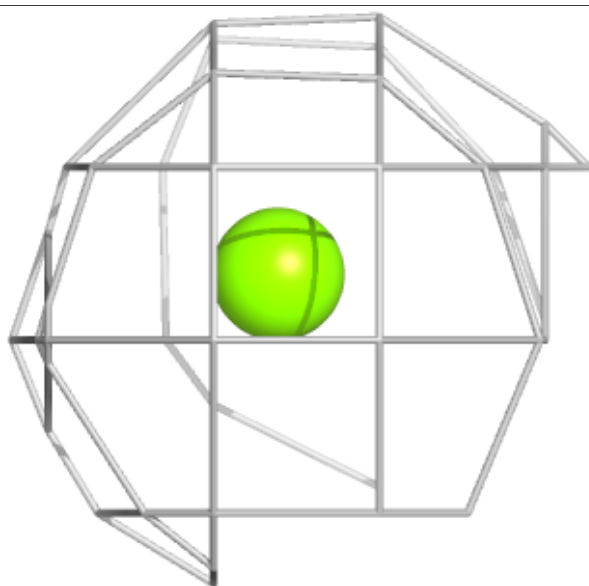
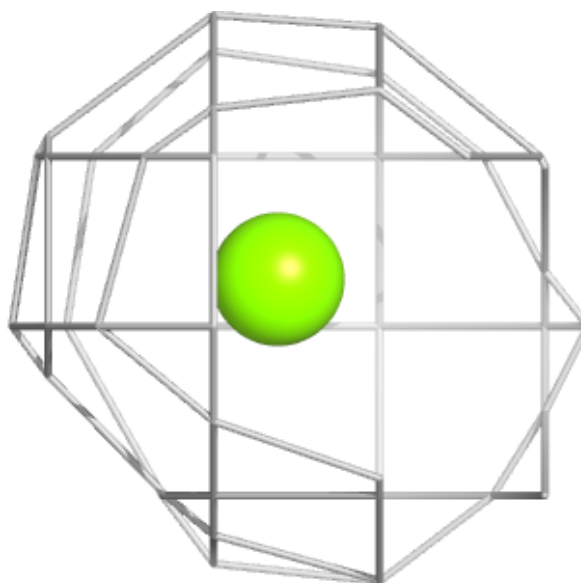
**Electron density around PGE D 303:**

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



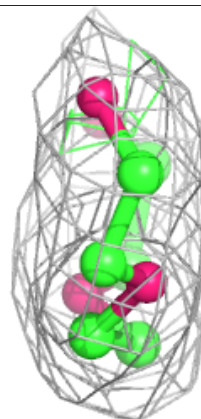
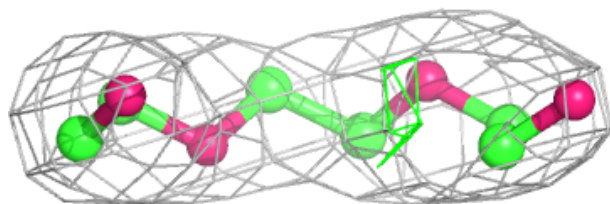
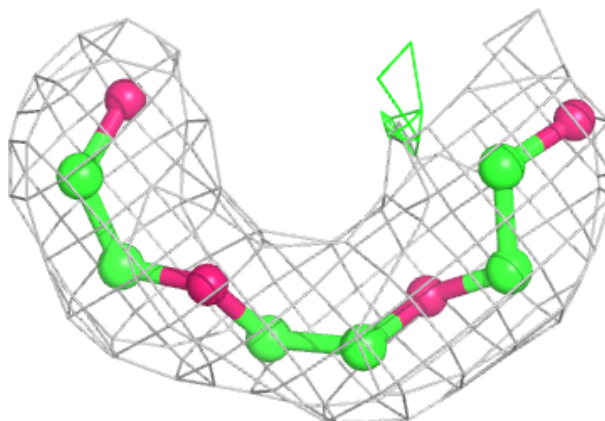
**Electron density around MG A 301:**

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



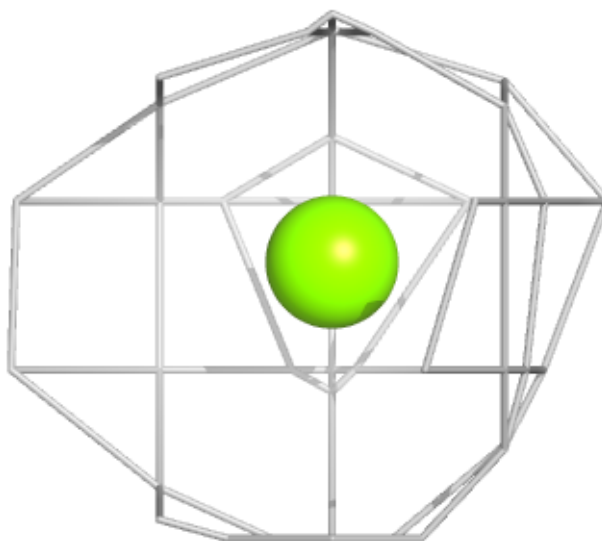
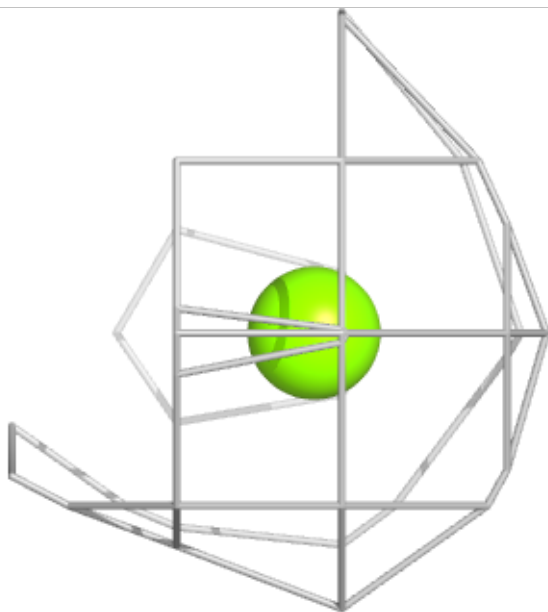
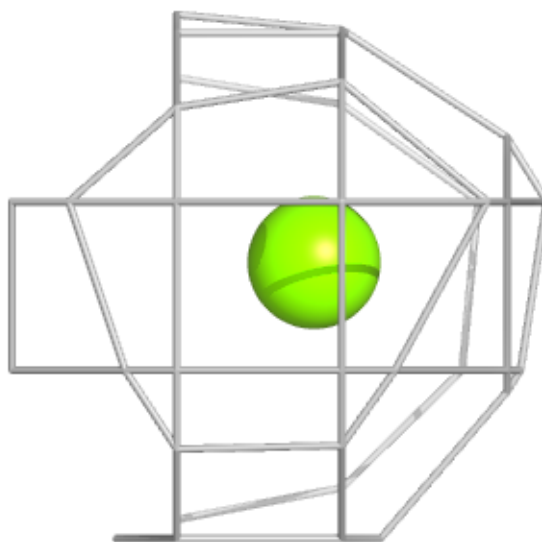
**Electron density around PGE C 306:**

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



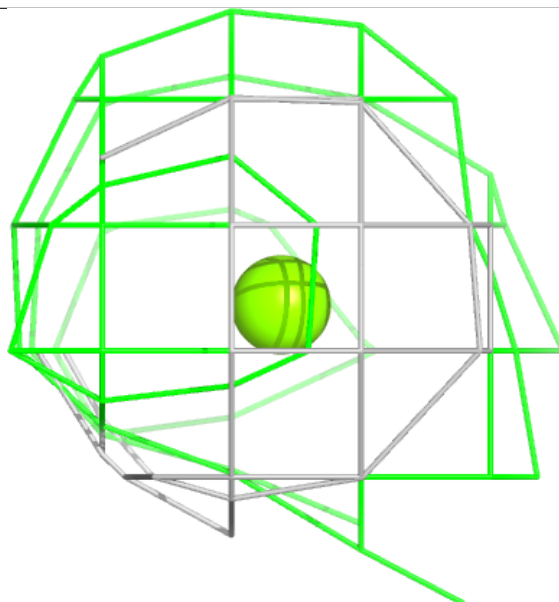
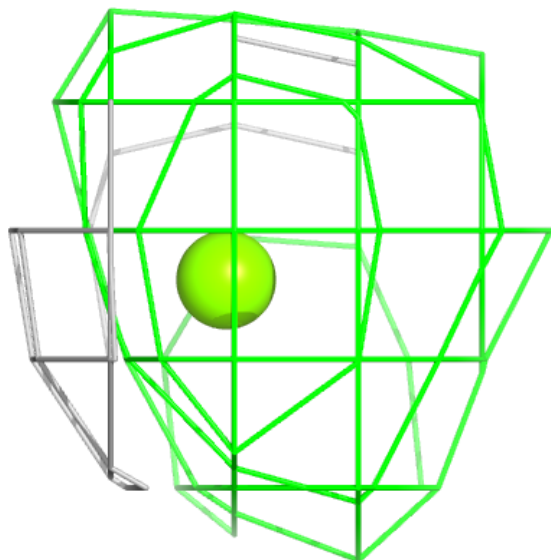
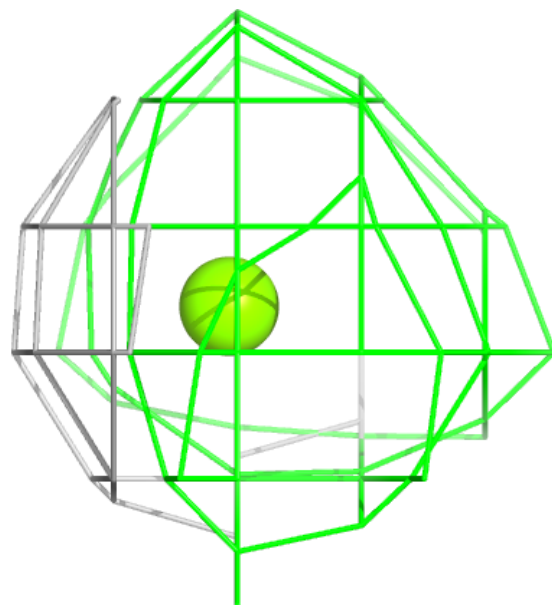
**Electron density around MG C 305:**

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



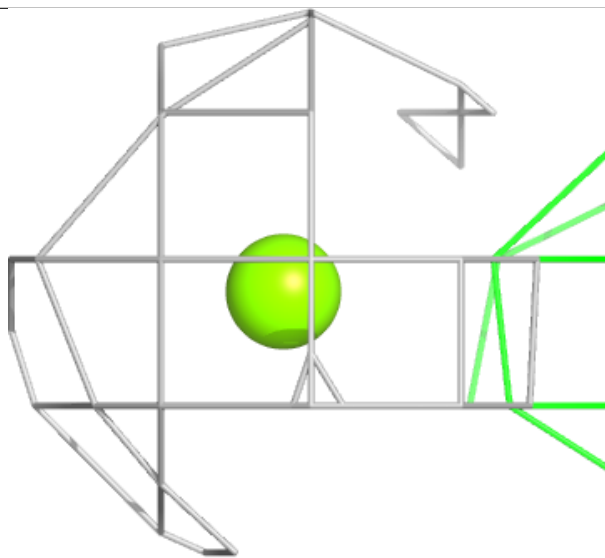
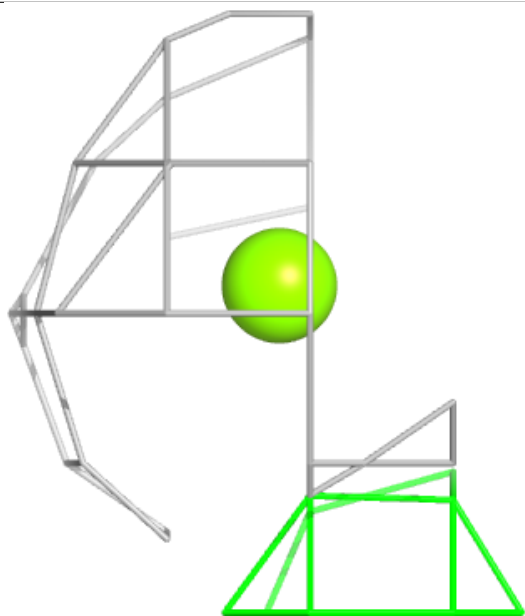
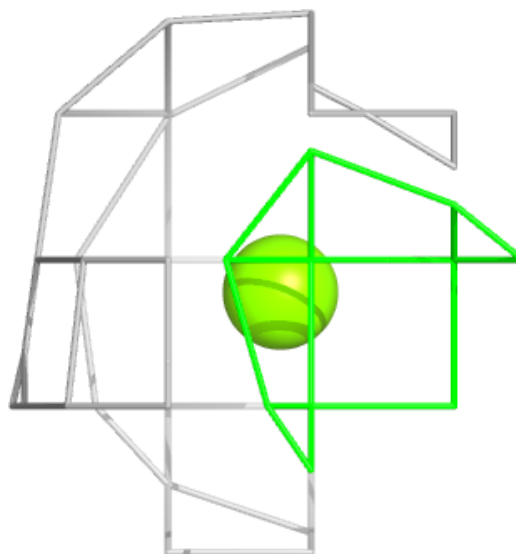
**Electron density around MG C 302:**

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



**Electron density around MG C 303:**

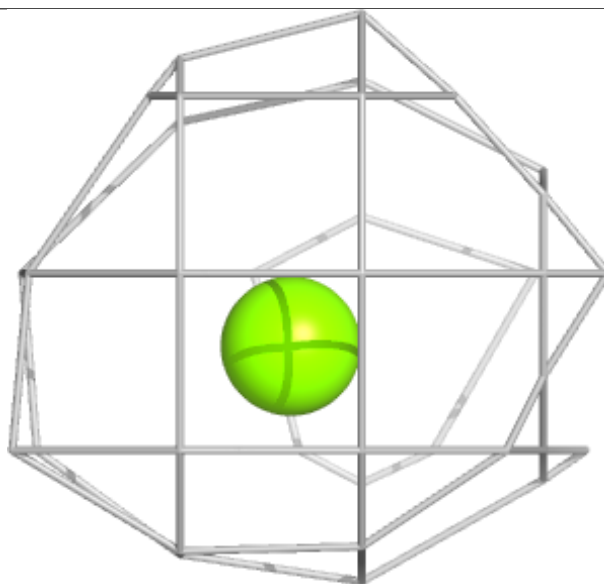
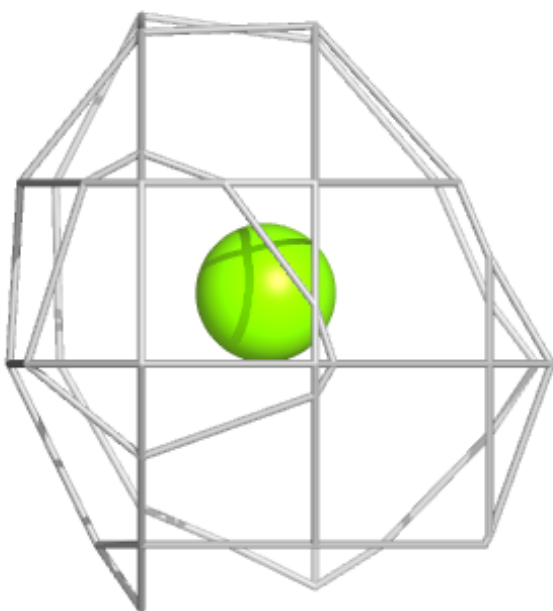
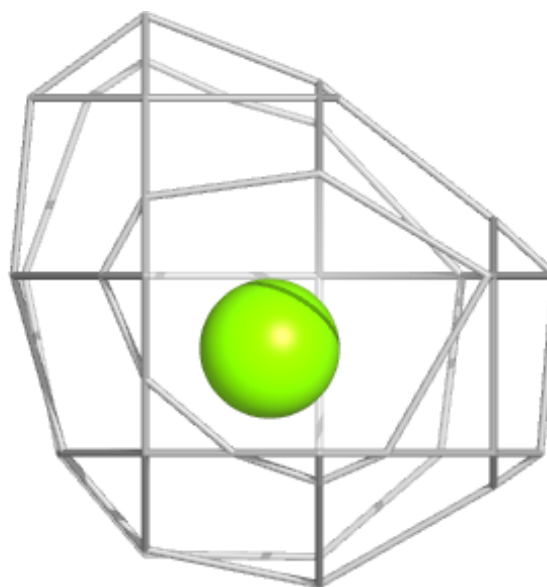
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG C 304:**

$2mF_o-DF_c$  (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.