



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2021 – 10:08 AM EST

PDB ID : 7L4B
Title : Dihydrodipicolinate synthase (DHDPS) from *C.jejuni* with pyruvate bound in the active site in P1211 space group
Authors : Saran, S.; Sanders, D.A.R.
Deposited on : 2020-12-18
Resolution : 2.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	2.24
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)	:	2.24

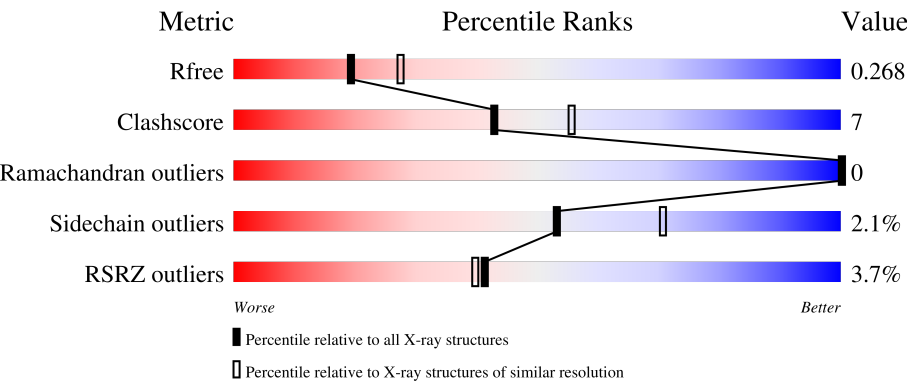
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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.



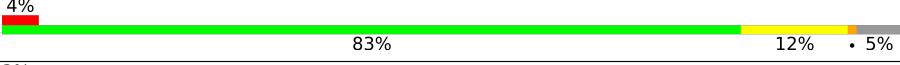



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	<div><div>2%</div><div><div></div><div>81%</div><div>14%</div><div>• 5%</div></div></div>
1	B	310	<div><div>%</div><div><div></div><div>83%</div><div>13%</div><div>5%</div></div></div>
1	C	310	<div><div>4%</div><div><div></div><div>78%</div><div>16%</div><div>• 5%</div></div></div>
1	D	310	<div><div>3%</div><div><div></div><div>81%</div><div>14%</div><div>5%</div></div></div>
1	E	310	<div><div>4%</div><div><div></div><div>81%</div><div>13%</div><div>• 5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	310	
1	G	310	
1	H	310	
1	I	310	
1	J	310	
1	K	310	
1	L	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	ACT	C	305	-	-	X	-
4	ACT	L	302	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27966 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
			2278	1449	379	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2275	1447	378	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2267	1442	375	437	13			
1	D	296	Total	C	N	O	S	0	0	0
			2257	1434	373	437	13			
1	E	294	Total	C	N	O	S	0	0	0
			2262	1440	375	434	13			
1	F	296	Total	C	N	O	S	0	0	0
			2271	1444	377	437	13			
1	G	296	Total	C	N	O	S	0	0	0
			2271	1444	377	437	13			
1	H	296	Total	C	N	O	S	0	0	0
			2279	1450	379	437	13			
1	I	296	Total	C	N	O	S	0	0	0
			2275	1447	378	437	13			
1	J	296	Total	C	N	O	S	0	0	0
			2279	1450	379	437	13			
1	K	296	Total	C	N	O	S	0	0	0
			2271	1444	378	436	13			
1	L	296	Total	C	N	O	S	0	0	0
			2271	1444	377	437	13			

There are 144 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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
G	-11	MET	-	expression tag	UNP Q9PPB4
G	-10	ARG	-	expression tag	UNP Q9PPB4
G	-9	GLY	-	expression tag	UNP Q9PPB4
G	-8	SER	-	expression tag	UNP Q9PPB4
G	-7	HIS	-	expression tag	UNP Q9PPB4
G	-6	HIS	-	expression tag	UNP Q9PPB4
G	-5	HIS	-	expression tag	UNP Q9PPB4
G	-4	HIS	-	expression tag	UNP Q9PPB4
G	-3	HIS	-	expression tag	UNP Q9PPB4
G	-2	HIS	-	expression tag	UNP Q9PPB4
G	-1	GLY	-	expression tag	UNP Q9PPB4
G	0	SER	-	expression tag	UNP Q9PPB4
H	-11	MET	-	expression tag	UNP Q9PPB4
H	-10	ARG	-	expression tag	UNP Q9PPB4
H	-9	GLY	-	expression tag	UNP Q9PPB4
H	-8	SER	-	expression tag	UNP Q9PPB4
H	-7	HIS	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

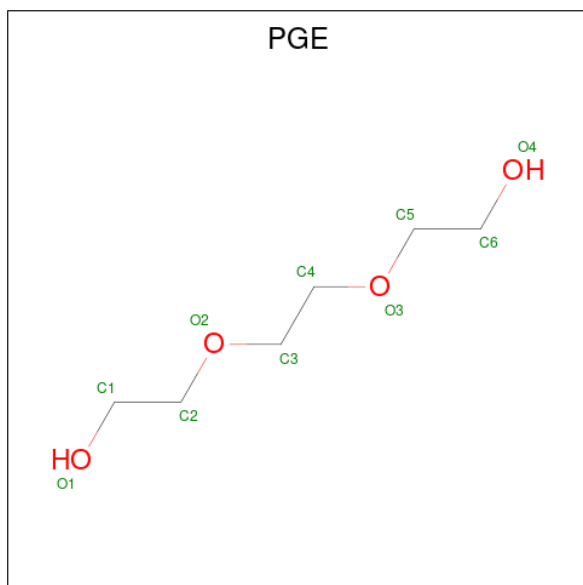
Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	HIS	-	expression tag	UNP Q9PPB4
H	-5	HIS	-	expression tag	UNP Q9PPB4
H	-4	HIS	-	expression tag	UNP Q9PPB4
H	-3	HIS	-	expression tag	UNP Q9PPB4
H	-2	HIS	-	expression tag	UNP Q9PPB4
H	-1	GLY	-	expression tag	UNP Q9PPB4
H	0	SER	-	expression tag	UNP Q9PPB4
I	-11	MET	-	expression tag	UNP Q9PPB4
I	-10	ARG	-	expression tag	UNP Q9PPB4
I	-9	GLY	-	expression tag	UNP Q9PPB4
I	-8	SER	-	expression tag	UNP Q9PPB4
I	-7	HIS	-	expression tag	UNP Q9PPB4
I	-6	HIS	-	expression tag	UNP Q9PPB4
I	-5	HIS	-	expression tag	UNP Q9PPB4
I	-4	HIS	-	expression tag	UNP Q9PPB4
I	-3	HIS	-	expression tag	UNP Q9PPB4
I	-2	HIS	-	expression tag	UNP Q9PPB4
I	-1	GLY	-	expression tag	UNP Q9PPB4
I	0	SER	-	expression tag	UNP Q9PPB4
J	-11	MET	-	expression tag	UNP Q9PPB4
J	-10	ARG	-	expression tag	UNP Q9PPB4
J	-9	GLY	-	expression tag	UNP Q9PPB4
J	-8	SER	-	expression tag	UNP Q9PPB4
J	-7	HIS	-	expression tag	UNP Q9PPB4
J	-6	HIS	-	expression tag	UNP Q9PPB4
J	-5	HIS	-	expression tag	UNP Q9PPB4
J	-4	HIS	-	expression tag	UNP Q9PPB4
J	-3	HIS	-	expression tag	UNP Q9PPB4
J	-2	HIS	-	expression tag	UNP Q9PPB4
J	-1	GLY	-	expression tag	UNP Q9PPB4
J	0	SER	-	expression tag	UNP Q9PPB4
K	-11	MET	-	expression tag	UNP Q9PPB4
K	-10	ARG	-	expression tag	UNP Q9PPB4
K	-9	GLY	-	expression tag	UNP Q9PPB4
K	-8	SER	-	expression tag	UNP Q9PPB4
K	-7	HIS	-	expression tag	UNP Q9PPB4
K	-6	HIS	-	expression tag	UNP Q9PPB4
K	-5	HIS	-	expression tag	UNP Q9PPB4
K	-4	HIS	-	expression tag	UNP Q9PPB4
K	-3	HIS	-	expression tag	UNP Q9PPB4
K	-2	HIS	-	expression tag	UNP Q9PPB4
K	-1	GLY	-	expression tag	UNP Q9PPB4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	SER	-	expression tag	UNP Q9PPB4
L	-11	MET	-	expression tag	UNP Q9PPB4
L	-10	ARG	-	expression tag	UNP Q9PPB4
L	-9	GLY	-	expression tag	UNP Q9PPB4
L	-8	SER	-	expression tag	UNP Q9PPB4
L	-7	HIS	-	expression tag	UNP Q9PPB4
L	-6	HIS	-	expression tag	UNP Q9PPB4
L	-5	HIS	-	expression tag	UNP Q9PPB4
L	-4	HIS	-	expression tag	UNP Q9PPB4
L	-3	HIS	-	expression tag	UNP Q9PPB4
L	-2	HIS	-	expression tag	UNP Q9PPB4
L	-1	GLY	-	expression tag	UNP Q9PPB4
L	0	SER	-	expression tag	UNP Q9PPB4

- Molecule 2 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
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

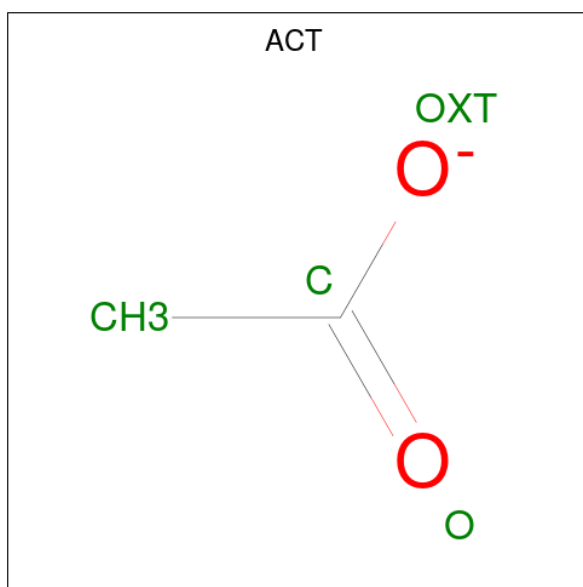
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 10 6 4	0	0
2	E	1	Total C O 10 6 4	0	0
2	E	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0
2	G	1	Total C O 10 6 4	0	0
2	H	1	Total C O 10 6 4	0	0
2	I	1	Total C O 10 6 4	0	0
2	J	1	Total C O 10 6 4	0	0
2	K	1	Total C O 10 6 4	0	0
2	L	1	Total C O 10 6 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

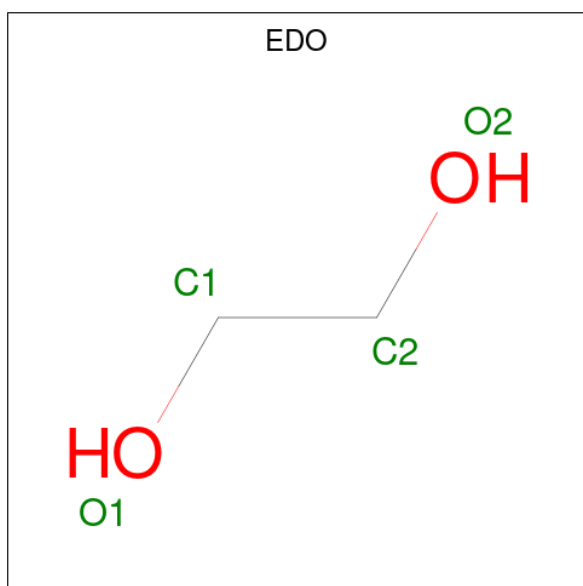
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

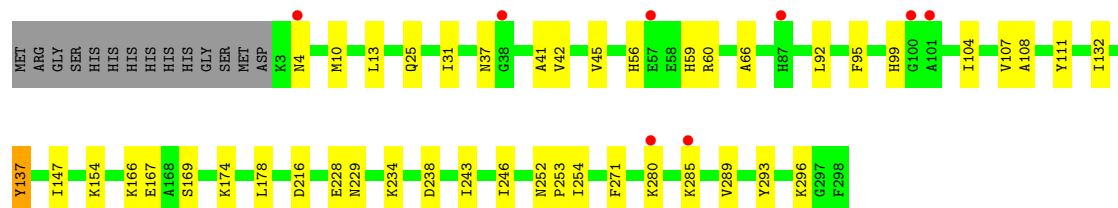
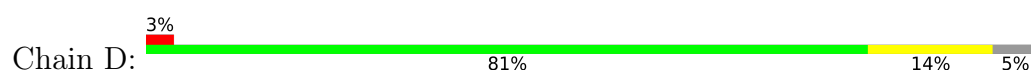
- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



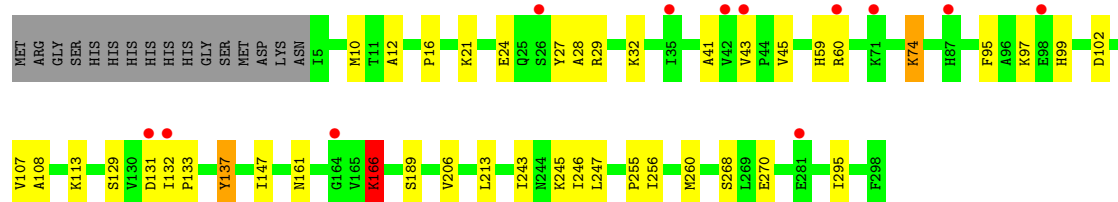
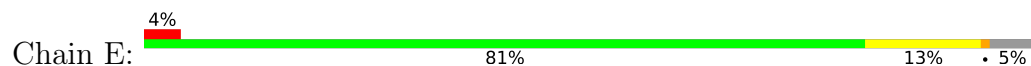
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

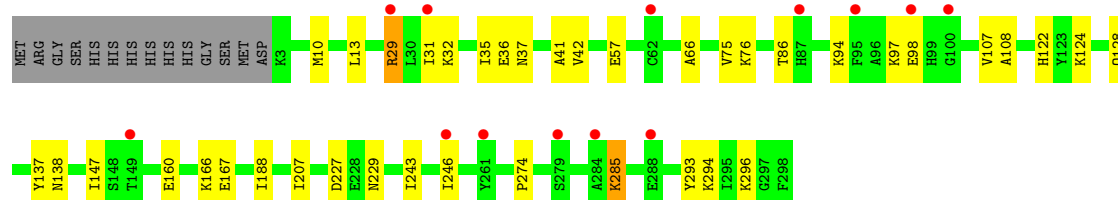
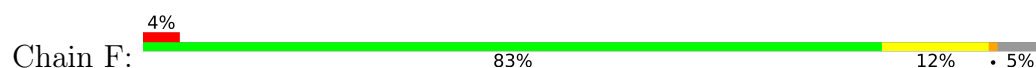
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	64	Total	O	0	0
			64	64		
6	C	43	Total	O	0	0
			43	43		
6	D	54	Total	O	0	0
			54	54		
6	E	38	Total	O	0	0
			38	38		
6	F	35	Total	O	0	0
			35	35		
6	G	53	Total	O	0	0
			53	53		
6	H	44	Total	O	0	0
			44	44		
6	I	47	Total	O	0	0
			47	47		
6	J	32	Total	O	0	0
			32	32		
6	K	46	Total	O	0	0
			46	46		
6	L	37	Total	O	0	0
			37	37		



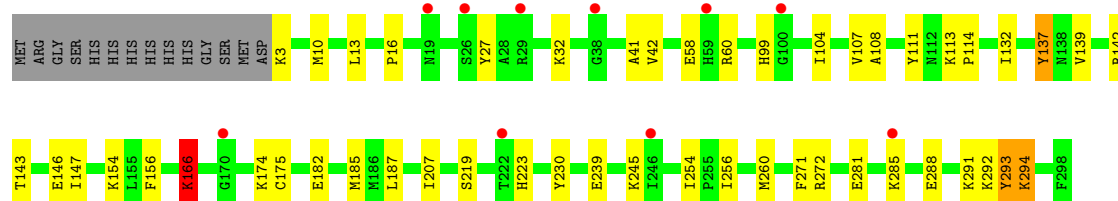
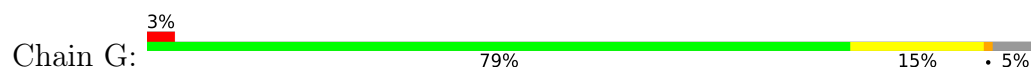
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



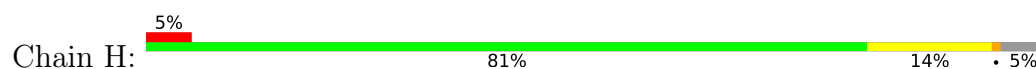
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

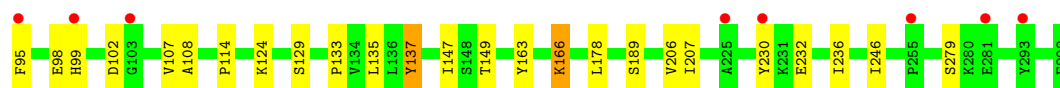


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



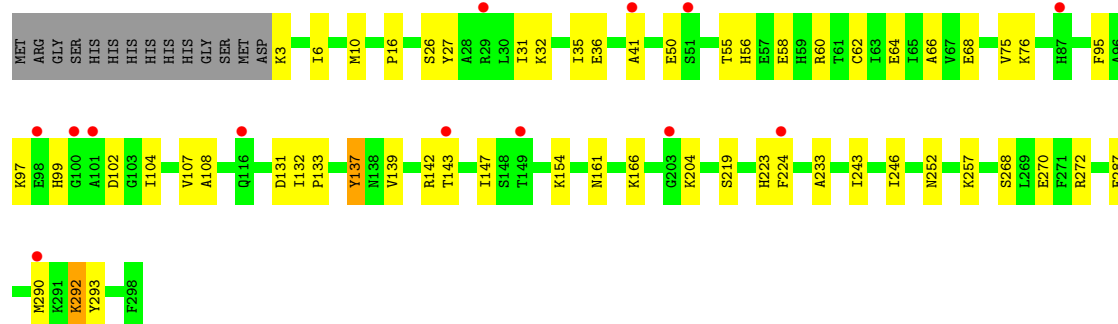
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase





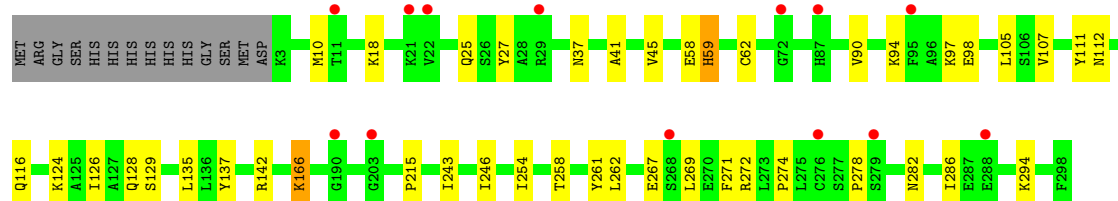
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain I: 4% 77% 17% 5%



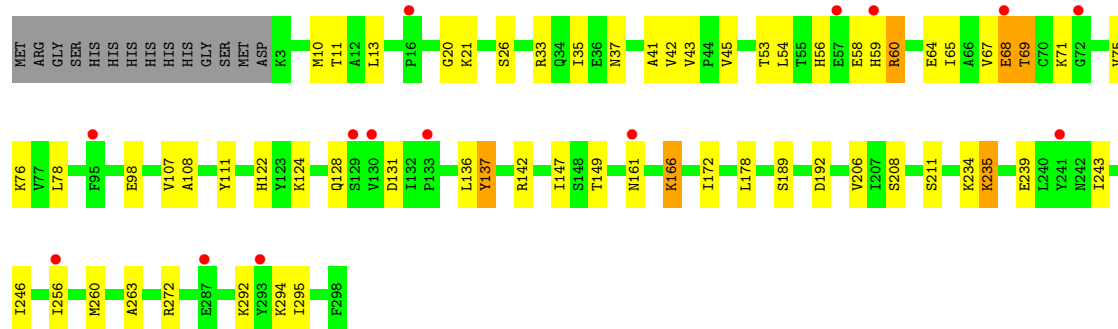
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain J: 4% 82% 13% 5%



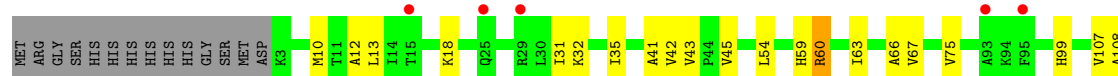
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

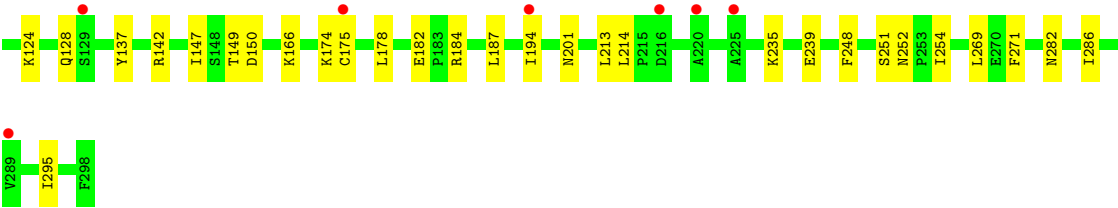
Chain K: 5% 75% 18% 5%



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain L: 4% 79% 16% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.51Å 200.36Å 122.24Å 90.00° 109.83° 90.00°	Depositor
Resolution (Å)	49.15 – 2.42 49.15 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.15-2.42) 88.0 (49.15-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.268 0.227 , 0.268	Depositor DCC
R_{free} test set	7072 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27966	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2300	0.57	0/3109
1	B	0.40	0/2297	0.55	0/3106
1	C	0.50	0/2291	0.58	0/3101
1	D	0.49	0/2281	0.55	0/3091
1	E	0.45	0/2286	0.57	0/3091
1	F	0.41	0/2295	0.56	0/3105
1	G	0.52	1/2295 (0.0%)	0.57	0/3105
1	H	0.40	0/2303	0.54	0/3113
1	I	0.46	0/2299	0.54	0/3109
1	J	0.44	0/2303	0.60	0/3113
1	K	0.47	0/2295	0.56	0/3103
1	L	0.50	0/2295	0.56	0/3105
All	All	0.45	1/27540 (0.0%)	0.56	0/37251

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	A	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	293	TYR	CE1-CZ	-5.38	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	KPI	Mainchain
1	E	166	KPI	Mainchain
1	G	166	KPI	Mainchain

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	2278	0	2316	35	0
1	B	2275	0	2307	25	0
1	C	2267	0	2282	40	0
1	D	2257	0	2254	30	0
1	E	2262	0	2299	33	0
1	F	2271	0	2297	23	0
1	G	2271	0	2296	33	0
1	H	2279	0	2318	33	0
1	I	2275	0	2307	34	0
1	J	2279	0	2319	32	0
1	K	2271	0	2296	43	0
1	L	2271	0	2296	32	0
2	A	10	0	14	3	0
2	B	10	0	14	1	0
2	C	20	0	28	0	0
2	D	10	0	14	1	0
2	E	20	0	28	1	0
2	F	10	0	14	0	0
2	G	10	0	14	1	0
2	H	10	0	14	0	0
2	I	10	0	14	1	0
2	J	10	0	14	1	0
2	K	10	0	14	0	0
2	L	10	0	14	0	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	J	1	0	0	0	0
4	C	4	0	3	5	0
4	F	4	0	3	0	0
4	L	4	0	3	4	0
5	J	4	0	6	0	0
6	A	54	0	0	1	0
6	B	64	0	0	2	0
6	C	43	0	0	0	0
6	D	54	0	0	1	0
6	E	38	0	0	0	0
6	F	35	0	0	2	0
6	G	53	0	0	1	0
6	H	44	0	0	2	0
6	I	47	0	0	3	0
6	J	32	0	0	0	0
6	K	46	0	0	1	0
6	L	37	0	0	0	0
All	All	27966	0	27798	376	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 7.

All (376) 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:E:60:ARG:HB2	1:E:95:PHE:CZ	1.86	1.10
1:E:60:ARG:HB2	1:E:95:PHE:HZ	1.16	1.06
1:J:45:VAL:HG11	1:J:59:HIS:CE1	2.07	0.90
1:K:65:ILE:O	1:K:69:THR:OG1	1.90	0.88
1:K:124:LYS:O	1:K:128:GLN:HG3	1.74	0.87
1:I:64:GLU:O	1:I:68:GLU:HG3	1.79	0.81
1:H:60:ARG:HB2	1:H:95:PHE:HZ	1.46	0.79
1:H:107:VAL:HA	1:H:137:TYR:HB3	1.68	0.76
1:L:60:ARG:HG2	1:L:99:HIS:CE1	2.19	0.76
1:I:107:VAL:HA	1:I:137:TYR:HB3	1.68	0.76
1:J:258:THR:HG22	1:J:269:LEU:HD11	1.68	0.75
1:K:56:HIS:O	1:K:60:ARG:HD3	1.86	0.75
1:E:60:ARG:CB	1:E:95:PHE:HZ	1.97	0.74
1:J:282:ASN:O	1:J:286:ILE:HD12	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.70	0.74
1:G:288:GLU:HA	1:G:291:LYS:HD2	1.69	0.74
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.69	0.73
1:L:251:SER:HA	4:L:302:ACT:H3	1.69	0.73
1:J:107:VAL:HA	1:J:137:TYR:HB3	1.70	0.73
1:K:67:VAL:O	1:K:71:LYS:HG3	1.88	0.72
1:K:208:SER:HB3	1:K:211:SER:HB2	1.72	0.72
1:L:235:LYS:O	1:L:239:GLU:HG3	1.89	0.72
1:D:60:ARG:HB2	1:D:95:PHE:CZ	2.24	0.72
1:C:67:VAL:HG22	1:C:77:VAL:HG21	1.73	0.71
1:K:107:VAL:HA	1:K:137:TYR:HB3	1.73	0.71
1:H:35:ILE:HG12	1:H:75:VAL:HG21	1.72	0.71
1:G:142:ARG:NH2	6:G:401:HOH:O	2.23	0.71
1:L:107:VAL:HA	1:L:137:TYR:HB3	1.73	0.70
1:L:60:ARG:CD	1:L:99:HIS:CE1	2.74	0.70
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.73	0.69
1:H:60:ARG:HB2	1:H:95:PHE:CZ	2.27	0.69
1:L:60:ARG:CG	1:L:99:HIS:CE1	2.75	0.69
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.75	0.69
1:B:288:GLU:O	1:B:291:LYS:HB2	1.92	0.69
1:I:35:ILE:HG12	1:I:75:VAL:HG21	1.74	0.69
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.74	0.68
1:C:252:ASN:H	4:C:305:ACT:H3	1.59	0.67
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.76	0.67
1:D:60:ARG:HB2	1:D:95:PHE:HZ	1.57	0.67
1:K:33:ARG:O	1:K:37:ASN:ND2	2.27	0.67
1:G:288:GLU:OE1	1:G:291:LYS:NZ	2.29	0.66
1:G:107:VAL:HA	1:G:137:TYR:HB3	1.76	0.66
1:I:287:GLU:HA	1:I:290:MET:HE2	1.77	0.65
1:A:108:ALA:HB2	1:A:147:ILE:HD11	1.79	0.65
1:A:67:VAL:HA	1:A:77:VAL:HG21	1.79	0.65
1:K:235:LYS:O	1:K:239:GLU:HG3	1.98	0.64
1:K:263:ALA:HB1	1:K:295:ILE:HG21	1.79	0.64
1:D:154:LYS:HD2	2:D:301:PGE:H4	1.80	0.64
1:K:35:ILE:HG12	1:K:75:VAL:HG21	1.79	0.64
1:I:55:THR:OG1	1:I:58:GLU:HG3	1.98	0.63
1:F:138:ASN:ND2	1:F:167:GLU:OE1	2.32	0.63
1:E:60:ARG:HB2	1:E:95:PHE:CE1	2.32	0.63
1:C:189:SER:HB3	1:C:206:VAL:HG12	1.81	0.62
1:A:60:ARG:HB2	1:A:95:PHE:CZ	2.33	0.62
1:B:142:ARG:NH2	6:B:405:HOH:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HG2	1:A:128:GLN:NE2	2.14	0.62
1:C:33:ARG:O	1:C:37:ASN:ND2	2.33	0.62
1:A:95:PHE:O	1:A:99:HIS:ND1	2.33	0.62
1:C:235:LYS:O	1:C:235:LYS:HD3	2.00	0.62
1:K:108:ALA:HB2	1:K:147:ILE:HD11	1.81	0.61
1:F:246:ILE:HD11	1:F:285:LYS:HG2	1.82	0.61
1:K:58:GLU:OE1	1:K:272:ARG:NH2	2.33	0.61
1:G:154:LYS:HD3	2:G:301:PGE:H62	1.83	0.61
1:D:108:ALA:HB2	1:D:147:ILE:HD11	1.82	0.61
1:D:296:LYS:NZ	6:D:401:HOH:O	2.33	0.61
1:J:45:VAL:CG1	1:J:59:HIS:CE1	2.83	0.61
1:B:47:THR:HG1	1:D:111:TYR:HH	1.46	0.60
1:F:31:ILE:O	1:F:35:ILE:HG12	2.01	0.60
1:E:21:LYS:NZ	1:E:24:GLU:OE2	2.33	0.60
1:K:45:VAL:HG11	1:K:59:HIS:CE1	2.36	0.60
1:B:13:LEU:HD11	1:B:42:VAL:HB	1.84	0.60
1:C:77:VAL:HG23	1:C:102:ASP:H	1.67	0.60
1:E:268:SER:OG	1:E:270:GLU:HG3	2.02	0.60
1:K:149:THR:HG23	1:K:178:LEU:HD23	1.82	0.59
1:K:294:LYS:NZ	6:K:404:HOH:O	2.34	0.59
1:A:13:LEU:HD11	1:A:42:VAL:HB	1.83	0.59
1:F:32:LYS:O	1:F:36:GLU:HG3	2.03	0.59
1:I:60:ARG:HB2	1:I:95:PHE:HZ	1.68	0.59
1:C:288:GLU:OE2	1:C:291:LYS:CE	2.50	0.58
1:J:254:ILE:O	1:J:258:THR:HG23	2.04	0.58
1:I:97:LYS:HE2	1:I:131:ASP:OD1	2.02	0.58
1:J:37:ASN:HD22	1:J:215:PRO:HG2	1.69	0.58
1:J:258:THR:HG21	1:J:278:PRO:HG3	1.85	0.57
1:L:282:ASN:O	1:L:286:ILE:HG13	2.05	0.57
1:L:182:GLU:OE2	1:L:184:ARG:NH1	2.38	0.57
1:C:248:PHE:HD2	4:C:305:ACT:H2	1.70	0.57
1:I:60:ARG:HB2	1:I:95:PHE:CZ	2.40	0.57
1:A:35:ILE:HG12	1:A:75:VAL:HG21	1.86	0.56
1:G:137:TYR:CZ	1:G:166:KPI:HEA	2.40	0.56
1:H:60:ARG:NE	1:H:99:HIS:CE1	2.73	0.56
1:I:10:MET:HG2	1:I:41:ALA:HB3	1.88	0.56
1:J:18:LYS:HE3	1:J:267:GLU:OE1	2.06	0.56
1:C:201:ASN:O	1:D:234:LYS:CE	2.53	0.56
1:H:166:KPI:HDA	1:H:207:ILE:HB	1.87	0.56
1:J:58:GLU:OE2	1:J:272:ARG:NH2	2.34	0.56
1:B:281:GLU:O	1:B:285:LYS:HG3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:VAL:HG13	1:K:54:LEU:HD12	1.88	0.56
1:F:76:LYS:NZ	6:F:401:HOH:O	2.36	0.55
1:G:230:TYR:CD2	1:H:230:TYR:HD2	2.24	0.55
1:J:126:ILE:O	1:J:129:SER:OG	2.24	0.55
1:C:90:VAL:HG13	1:C:129:SER:HB2	1.88	0.55
1:C:201:ASN:O	1:D:234:LYS:HE2	2.06	0.55
1:F:37:ASN:OD1	1:F:296:LYS:HD2	2.06	0.55
1:K:13:LEU:HD11	1:K:42:VAL:HB	1.87	0.55
1:B:231:LYS:H	1:B:231:LYS:HD2	1.70	0.55
1:E:108:ALA:HB2	1:E:147:ILE:HD11	1.88	0.55
1:J:112:ASN:HA	1:K:142:ARG:HH12	1.72	0.55
1:L:248:PHE:HD2	4:L:302:ACT:H2	1.72	0.55
1:H:74:LYS:NZ	6:H:401:HOH:O	2.26	0.55
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.90	0.54
1:C:27:TYR:CE2	1:C:62:CYS:HB3	2.43	0.54
1:G:10:MET:HG2	1:G:41:ALA:HB3	1.89	0.54
1:H:43:VAL:HG22	1:H:78:LEU:HB3	1.90	0.54
1:E:29:ARG:HA	1:E:32:LYS:HG3	1.89	0.54
1:K:10:MET:HG2	1:K:41:ALA:HB3	1.89	0.54
1:F:124:LYS:O	1:F:128:GLN:HG3	2.08	0.54
1:K:20:GLY:C	1:K:21:LYS:HD2	2.28	0.54
1:H:108:ALA:HB2	1:H:147:ILE:HD11	1.90	0.54
1:A:150:ASP:HB3	2:A:301:PGE:H3	1.89	0.53
1:E:60:ARG:HD3	1:E:99:HIS:CD2	2.43	0.53
1:I:243:ILE:HA	1:I:246:ILE:HG22	1.91	0.53
1:E:29:ARG:O	1:E:32:LYS:HB2	2.08	0.53
1:E:10:MET:HG2	1:E:41:ALA:HB3	1.91	0.53
1:J:10:MET:HG2	1:J:41:ALA:HB3	1.90	0.52
1:K:53:THR:HB	1:K:272:ARG:HG2	1.91	0.52
1:B:108:ALA:HB2	1:B:147:ILE:HD11	1.91	0.52
1:L:35:ILE:HG12	1:L:75:VAL:HG21	1.92	0.52
1:K:234:LYS:HE2	1:L:201:ASN:O	2.09	0.52
1:C:248:PHE:CD2	4:C:305:ACT:H2	2.44	0.52
1:L:175:CYS:HB3	1:L:187:LEU:HD21	1.90	0.52
1:H:10:MET:HG2	1:H:41:ALA:HB3	1.91	0.52
1:D:174:LYS:HD3	1:D:178:LEU:HD11	1.91	0.52
1:L:149:THR:HG23	1:L:178:LEU:HD23	1.92	0.52
1:E:161:ASN:OD1	1:E:161:ASN:N	2.33	0.52
1:L:13:LEU:HD11	1:L:42:VAL:HB	1.92	0.52
1:H:31:ILE:HD13	1:H:66:ALA:HA	1.91	0.51
1:J:105:LEU:HD13	1:J:135:LEU:HD23	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:O	1:A:235:LYS:HD3	2.10	0.51
1:D:167:GLU:OE1	1:D:169:SER:OG	2.23	0.51
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.75	0.51
1:G:58:GLU:OE1	1:G:272:ARG:NH1	2.36	0.51
1:A:60:ARG:NE	1:A:99:HIS:NE2	2.58	0.51
1:L:252:ASN:H	4:L:302:ACT:CH3	2.24	0.51
1:J:90:VAL:HG13	1:J:129:SER:HB3	1.93	0.51
1:G:256:ILE:O	1:G:260:MET:HG2	2.11	0.51
1:E:60:ARG:HD3	1:E:99:HIS:NE2	2.26	0.50
1:F:108:ALA:HB2	1:F:147:ILE:HD11	1.93	0.50
1:G:60:ARG:HG3	1:G:99:HIS:CE1	2.46	0.50
1:L:10:MET:HG2	1:L:41:ALA:HB3	1.94	0.50
1:I:108:ALA:HB2	1:I:147:ILE:HD11	1.93	0.50
1:L:213:LEU:HG	1:L:214:LEU:HG	1.92	0.50
1:A:10:MET:HG2	1:A:41:ALA:HB3	1.93	0.50
1:G:137:TYR:CE1	1:G:166:KPI:HEA	2.47	0.50
1:K:11:THR:OG1	1:K:211:SER:OG	2.28	0.50
1:B:35:ILE:HG12	1:B:75:VAL:HG21	1.94	0.50
1:B:10:MET:HG2	1:B:41:ALA:HB3	1.94	0.50
1:H:124:LYS:NZ	6:H:406:HOH:O	2.45	0.50
1:H:137:TYR:CE1	1:H:166:KPI:HEA	2.47	0.50
1:A:243:ILE:HA	1:A:246:ILE:HG22	1.92	0.49
1:E:243:ILE:HA	1:E:246:ILE:HG22	1.93	0.49
1:G:281:GLU:O	1:G:285:LYS:HB2	2.12	0.49
1:I:58:GLU:OE1	1:I:272:ARG:NH1	2.23	0.49
1:I:50:GLU:OE2	1:I:257:LYS:NZ	2.29	0.49
1:C:254:ILE:HA	1:C:271:PHE:CE2	2.47	0.49
1:K:208:SER:HB3	1:K:211:SER:CB	2.41	0.49
1:G:175:CYS:HB3	1:G:187:LEU:HD21	1.95	0.49
1:E:213:LEU:HD11	1:E:295:ILE:HD13	1.94	0.49
1:L:108:ALA:HB2	1:L:147:ILE:HD11	1.93	0.49
1:C:161:ASN:OD1	1:C:161:ASN:N	2.34	0.49
1:C:77:VAL:HG23	1:C:101:ALA:HA	1.95	0.49
1:A:18:LYS:HD3	1:A:267:GLU:OE2	2.13	0.48
1:I:31:ILE:HD13	1:I:66:ALA:HA	1.94	0.48
1:C:13:LEU:HD11	1:C:42:VAL:HB	1.94	0.48
1:I:99:HIS:ND1	6:I:405:HOH:O	2.34	0.48
1:G:288:GLU:CD	1:G:291:LYS:NZ	2.66	0.48
1:B:268:SER:HB3	1:B:270:GLU:HG3	1.96	0.48
1:I:104:ILE:HG23	1:I:132:ILE:HD11	1.95	0.48
1:K:21:LYS:HD2	1:K:21:LYS:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HD2	2:A:301:PGE:H22	1.96	0.48
1:A:21:LYS:HD3	1:A:272:ARG:NH2	2.29	0.48
1:H:60:ARG:NH1	1:H:99:HIS:HE1	2.11	0.48
1:L:60:ARG:HD2	1:L:99:HIS:CE1	2.47	0.48
1:B:88:GLU:HG2	1:B:92:LEU:HD11	1.96	0.48
1:G:146:GLU:OE2	1:G:174:LYS:NZ	2.34	0.48
1:A:231:LYS:HE2	1:A:231:LYS:HB2	1.62	0.48
1:C:229:ASN:HB3	1:C:232:GLU:OE1	2.14	0.48
1:K:208:SER:CB	1:K:211:SER:HB2	2.42	0.48
1:D:10:MET:HG2	1:D:41:ALA:HB3	1.95	0.47
1:D:45:VAL:HG11	1:D:59:HIS:CE1	2.48	0.47
1:A:60:ARG:HB2	1:A:95:PHE:CE2	2.49	0.47
1:B:94:LYS:NZ	6:B:408:HOH:O	2.37	0.47
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.97	0.47
1:K:64:GLU:O	1:K:68:GLU:CG	2.63	0.47
1:A:216:ASP:OD1	1:A:216:ASP:N	2.47	0.47
1:D:254:ILE:HA	1:D:271:PHE:CE2	2.49	0.47
1:E:245:LYS:HA	1:E:245:LYS:HD2	1.77	0.47
1:F:35:ILE:HG23	1:F:75:VAL:HG21	1.95	0.47
1:J:137:TYR:CE1	1:J:166:KPI:HEA	2.49	0.47
1:D:56:HIS:CE1	1:D:92:LEU:HD21	2.49	0.47
1:E:28:ALA:O	1:E:32:LYS:HG2	2.14	0.47
1:E:189:SER:HB3	1:E:206:VAL:HG12	1.96	0.47
1:J:94:LYS:HG3	1:J:129:SER:HB2	1.96	0.47
1:K:243:ILE:HA	1:K:246:ILE:HG22	1.97	0.47
1:D:285:LYS:O	1:D:289:VAL:HG23	2.14	0.47
1:K:192:ASP:OD1	1:K:208:SER:OG	2.24	0.47
1:L:45:VAL:HG13	1:L:54:LEU:HD12	1.97	0.47
1:K:56:HIS:O	1:K:60:ARG:CD	2.59	0.47
1:L:12:ALA:HA	1:L:43:VAL:HB	1.96	0.47
1:E:74:LYS:H	1:E:74:LYS:HG3	1.55	0.47
1:A:90:VAL:HG13	1:A:129:SER:HB3	1.97	0.47
1:L:147:ILE:O	1:L:174:LYS:NZ	2.39	0.47
1:B:67:VAL:HA	1:B:77:VAL:HG21	1.96	0.46
1:B:102:ASP:O	1:B:133:PRO:HD2	2.14	0.46
1:F:243:ILE:HA	1:F:246:ILE:HG22	1.97	0.46
1:A:60:ARG:CZ	1:A:99:HIS:NE2	2.78	0.46
1:B:235:LYS:O	1:B:239:GLU:HB2	2.15	0.46
1:H:4:ASN:HB3	1:H:133:PRO:HG3	1.96	0.46
1:D:95:PHE:O	1:D:99:HIS:CD2	2.68	0.46
1:K:136:LEU:O	1:K:166:KPI:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:TYR:CZ	1:H:166:KPI:HEA	2.51	0.46
1:L:60:ARG:CG	1:L:99:HIS:HE1	2.27	0.46
1:C:90:VAL:O	1:C:94:LYS:HG3	2.15	0.46
1:H:60:ARG:CZ	1:H:99:HIS:CE1	2.98	0.46
1:E:113:LYS:CE	1:L:142:ARG:HG2	2.46	0.46
1:J:27:TYR:CZ	1:J:62:CYS:HB3	2.51	0.46
1:C:27:TYR:CZ	1:C:62:CYS:HB3	2.50	0.46
1:E:45:VAL:HG11	1:E:59:HIS:CE1	2.51	0.46
1:F:188:ILE:HG21	1:F:207:ILE:HG13	1.98	0.46
1:G:288:GLU:CD	1:G:291:LYS:HZ3	2.18	0.46
1:H:59:HIS:O	1:H:63:ILE:HG13	2.16	0.46
1:B:84:ASN:HA	1:B:109:PRO:HB3	1.98	0.46
1:G:16:PRO:HD2	1:G:27:TYR:HD1	1.80	0.46
1:H:27:TYR:CZ	1:H:62:CYS:HB3	2.51	0.46
1:H:27:TYR:CE2	1:H:62:CYS:HB3	2.51	0.46
1:F:86:THR:HA	1:F:122:HIS:CE1	2.51	0.45
1:I:6:ILE:HG23	1:I:76:LYS:HE2	1.98	0.45
1:I:268:SER:OG	1:I:270:GLU:HG3	2.17	0.45
1:J:294:LYS:HA	1:J:294:LYS:HD3	1.75	0.45
1:E:95:PHE:O	1:E:95:PHE:CD1	2.69	0.45
1:H:60:ARG:CZ	1:H:99:HIS:HE1	2.30	0.45
1:J:111:TYR:O	1:K:142:ARG:NH1	2.49	0.45
1:A:124:LYS:HG2	1:A:128:GLN:HE21	1.82	0.45
1:E:247:LEU:HA	1:E:255:PRO:HB2	1.99	0.45
1:F:13:LEU:HD11	1:F:42:VAL:HB	1.98	0.45
1:C:102:ASP:O	1:C:133:PRO:HD2	2.17	0.45
1:H:10:MET:HA	1:H:41:ALA:O	2.16	0.45
1:H:189:SER:HB3	1:H:206:VAL:HG12	1.98	0.45
1:A:294:LYS:HA	1:A:294:LYS:HD3	1.74	0.45
1:L:248:PHE:CD2	4:L:302:ACT:H2	2.52	0.45
1:C:235:LYS:HD3	1:C:235:LYS:C	2.37	0.45
1:H:57:GLU:H	1:H:57:GLU:HG2	1.53	0.45
1:E:12:ALA:HA	1:E:43:VAL:HB	1.98	0.44
1:K:189:SER:HB3	1:K:206:VAL:HG12	1.98	0.44
1:J:10:MET:HA	1:J:41:ALA:O	2.17	0.44
1:A:86:THR:O	1:A:90:VAL:HG23	2.16	0.44
1:A:246:ILE:HD11	1:A:285:LYS:HB3	1.99	0.44
1:D:92:LEU:HA	1:D:95:PHE:HB3	1.99	0.44
1:G:245:LYS:HA	1:G:245:LYS:HD2	1.87	0.44
1:K:58:GLU:CD	1:K:272:ARG:HH22	2.21	0.44
1:A:280:LYS:HD2	1:A:280:LYS:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:MET:HG2	1:C:41:ALA:HB3	1.99	0.44
1:F:243:ILE:HB	1:F:293:TYR:CE2	2.53	0.44
1:G:292:LYS:HE2	1:G:293:TYR:CZ	2.52	0.44
1:J:269:LEU:HD21	1:J:271:PHE:HE1	1.81	0.44
1:C:91:GLY:HA2	1:C:94:LYS:HE3	1.99	0.44
1:C:252:ASN:H	4:C:305:ACT:CH3	2.29	0.44
1:D:243:ILE:HB	1:D:293:TYR:CE2	2.53	0.44
1:F:229:ASN:HB2	6:F:434:HOH:O	2.17	0.44
1:G:13:LEU:HD11	1:G:42:VAL:HB	1.99	0.44
1:D:104:ILE:HG23	1:D:132:ILE:HD11	1.98	0.44
1:I:16:PRO:HD2	1:I:27:TYR:HD1	1.81	0.44
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.33	0.44
1:G:254:ILE:HA	1:G:271:PHE:CE2	2.52	0.44
1:L:63:ILE:O	1:L:67:VAL:HG23	2.18	0.44
1:A:154:LYS:NZ	2:A:301:PGE:H62	2.32	0.44
1:C:108:ALA:HB2	1:C:147:ILE:HD11	1.98	0.44
1:C:231:LYS:HE3	1:D:228:GLU:OE1	2.17	0.44
1:I:219:SER:O	1:I:223:HIS:ND1	2.51	0.44
1:K:64:GLU:O	1:K:68:GLU:HG2	2.18	0.43
1:C:142:ARG:HH21	4:C:305:ACT:H3	1.83	0.43
1:E:29:ARG:HA	1:E:32:LYS:CG	2.48	0.43
1:G:294:LYS:HA	1:G:294:LYS:HD3	1.72	0.43
1:H:149:THR:HG23	1:H:178:LEU:HD23	1.99	0.43
1:J:243:ILE:HA	1:J:246:ILE:HG22	2.00	0.43
1:K:256:ILE:O	1:K:260:MET:HG2	2.18	0.43
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.87	0.43
1:G:166:KPI:HDA	1:G:207:ILE:HB	1.99	0.43
1:I:139:VAL:HG13	1:I:143:THR:HG23	2.00	0.43
1:C:135:LEU:HD13	1:C:163:TYR:CZ	2.54	0.43
1:D:31:ILE:HD13	1:D:66:ALA:HA	2.00	0.43
1:I:292:LYS:O	1:I:292:LYS:HG3	2.18	0.43
1:J:261:TYR:O	1:J:261:TYR:CG	2.70	0.43
1:D:13:LEU:HD11	1:D:42:VAL:HB	2.01	0.43
1:D:252:ASN:OD1	1:D:253:PRO:HA	2.18	0.43
1:F:293:TYR:C	1:F:294:LYS:HD2	2.38	0.43
1:G:108:ALA:HB2	1:G:147:ILE:HD11	1.99	0.43
1:A:161:ASN:OD1	1:A:161:ASN:N	2.44	0.43
1:E:137:TYR:CZ	1:E:166:KPI:HE	2.53	0.43
1:I:204:LYS:HA	1:I:204:LYS:HD3	1.89	0.43
1:B:154:LYS:HD3	2:B:301:PGE:H32	2.01	0.43
1:E:16:PRO:HD2	1:E:27:TYR:HD1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:NZ	6:A:402:HOH:O	2.27	0.42
1:B:245:LYS:HA	1:B:245:LYS:HD2	1.84	0.42
1:C:231:LYS:CE	1:D:228:GLU:OE1	2.67	0.42
1:E:102:ASP:O	1:E:133:PRO:HD2	2.19	0.42
1:F:94:LYS:O	1:F:98:GLU:HG3	2.20	0.42
1:H:246:ILE:HD12	1:H:246:ILE:HA	1.87	0.42
1:K:161:ASN:OD1	1:K:161:ASN:N	2.45	0.42
1:G:139:VAL:HG13	1:G:143:THR:HG23	2.02	0.42
1:I:154:LYS:HZ2	2:I:301:PGE:H5	1.84	0.42
1:I:243:ILE:HB	1:I:293:TYR:CE2	2.54	0.42
1:E:97:LYS:HG3	1:E:132:ILE:HG21	2.01	0.42
1:F:31:ILE:HD13	1:F:66:ALA:HA	2.00	0.42
1:J:269:LEU:HD23	1:J:269:LEU:O	2.19	0.42
1:J:274:PRO:HB3	1:K:122:HIS:HB2	2.02	0.42
1:A:47:THR:HG1	1:G:111:TYR:HH	1.67	0.42
1:B:43:VAL:HA	1:B:78:LEU:O	2.19	0.42
1:D:37:ASN:OD1	1:D:296:LYS:HD3	2.19	0.42
1:H:64:GLU:OE1	1:H:99:HIS:CE1	2.72	0.42
1:H:232:GLU:O	1:H:236:ILE:HG12	2.20	0.42
1:I:224:PHE:HB3	1:I:233:ALA:HB2	2.01	0.42
1:J:27:TYR:CE2	1:J:62:CYS:HB3	2.54	0.42
1:A:288:GLU:O	1:A:288:GLU:HG3	2.20	0.42
1:D:246:ILE:HD12	1:D:246:ILE:HA	1.90	0.42
1:I:58:GLU:OE2	6:I:401:HOH:O	2.21	0.42
1:L:124:LYS:O	1:L:128:GLN:HG3	2.20	0.42
1:A:249:CYS:SG	1:A:282:ASN:HB3	2.59	0.42
1:C:74:LYS:HB2	1:C:74:LYS:HE2	1.63	0.42
1:I:246:ILE:HD12	1:I:246:ILE:HA	1.79	0.42
1:J:112:ASN:HA	1:K:142:ARG:NH1	2.33	0.42
1:C:216:ASP:OD1	1:C:217:MET:N	2.52	0.42
1:I:3:LYS:N	6:I:413:HOH:O	2.52	0.42
1:B:231:LYS:H	1:B:231:LYS:CD	2.33	0.41
1:E:131:ASP:OD1	1:E:131:ASP:O	2.38	0.41
1:K:246:ILE:HD12	1:K:246:ILE:HA	1.91	0.41
1:F:29:ARG:HE	1:F:29:ARG:HB2	1.58	0.41
1:G:219:SER:O	1:G:223:HIS:ND1	2.53	0.41
1:L:31:ILE:HD13	1:L:66:ALA:HA	2.02	0.41
1:F:274:PRO:HB2	1:H:114:PRO:HB3	2.01	0.41
1:I:27:TYR:CE2	1:I:62:CYS:HB3	2.55	0.41
1:J:124:LYS:O	1:J:128:GLN:HG3	2.20	0.41
1:C:35:ILE:HD11	1:C:70:CYS:SG	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:LYS:HZ1	2:E:302:PGE:C5	2.33	0.41
1:G:113:LYS:HB2	1:G:113:LYS:HE3	1.90	0.41
1:G:104:ILE:HG23	1:G:132:ILE:HD11	2.01	0.41
1:J:45:VAL:HG12	1:J:45:VAL:O	2.20	0.41
1:L:254:ILE:HA	1:L:271:PHE:CE2	2.56	0.41
1:C:166:KPI:HE	1:C:207:ILE:HB	2.03	0.41
1:G:3:LYS:NZ	1:G:156:PHE:O	2.50	0.41
1:K:172:ILE:HG23	1:L:194:ILE:HG21	2.01	0.41
1:C:67:VAL:O	1:C:71:LYS:HG2	2.21	0.41
1:C:136:LEU:O	1:C:166:KPI:N	2.53	0.41
1:H:23:ASP:OD1	1:H:25:GLN:HG3	2.21	0.41
1:I:32:LYS:O	1:I:36:GLU:HB2	2.20	0.41
1:J:142:ARG:O	1:K:111:TYR:HA	2.21	0.41
1:L:45:VAL:HG11	1:L:59:HIS:CE1	2.55	0.41
1:L:213:LEU:HD11	1:L:295:ILE:HD13	2.01	0.41
1:E:256:ILE:O	1:E:260:MET:HG2	2.19	0.41
1:F:35:ILE:HG12	1:F:35:ILE:H	1.71	0.41
1:I:102:ASP:O	1:I:133:PRO:HD2	2.21	0.41
1:I:142:ARG:NH2	1:I:252:ASN:O	2.53	0.41
1:D:234:LYS:NZ	1:D:238:ASP:OD2	2.47	0.41
1:H:102:ASP:O	1:H:133:PRO:HD2	2.20	0.41
1:H:135:LEU:HD13	1:H:163:TYR:CZ	2.56	0.41
1:I:287:GLU:HA	1:I:290:MET:CE	2.47	0.41
1:K:43:VAL:HA	1:K:78:LEU:O	2.21	0.41
1:D:216:ASP:OD1	1:D:216:ASP:N	2.54	0.41
1:J:116:GLN:HB3	2:J:301:PGE:H42	2.02	0.41
1:A:274:PRO:HB2	1:G:114:PRO:HB3	2.04	0.40
1:G:182:GLU:HB3	1:G:185:MET:HE3	2.03	0.40
1:B:10:MET:HA	1:B:41:ALA:O	2.20	0.40
1:C:23:ASP:CG	1:C:26:SER:HB3	2.42	0.40
1:A:21:LYS:HD3	1:A:21:LYS:HA	1.92	0.40
1:A:102:ASP:O	1:A:133:PRO:HD2	2.21	0.40
1:B:256:ILE:O	1:B:260:MET:HG2	2.21	0.40
1:D:280:LYS:HD3	1:D:280:LYS:HA	1.85	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	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	B	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	C	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	D	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	E	291/310 (94%)	283 (97%)	8 (3%)	0	100	100
1	F	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	G	293/310 (94%)	283 (97%)	10 (3%)	0	100	100
1	H	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	I	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	J	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	K	293/310 (94%)	283 (97%)	10 (3%)	0	100	100
1	L	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
All	All	3514/3720 (94%)	3409 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	247/260 (95%)	245 (99%)	2 (1%)	81	91
1	B	246/260 (95%)	243 (99%)	3 (1%)	71	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	244/260 (94%)	237 (97%)	7 (3%)	42	61
1	D	242/260 (93%)	238 (98%)	4 (2%)	60	77
1	E	246/260 (95%)	243 (99%)	3 (1%)	71	84
1	F	246/260 (95%)	240 (98%)	6 (2%)	49	67
1	G	246/260 (95%)	242 (98%)	4 (2%)	62	78
1	H	248/260 (95%)	241 (97%)	7 (3%)	43	62
1	I	247/260 (95%)	242 (98%)	5 (2%)	55	72
1	J	248/260 (95%)	243 (98%)	5 (2%)	55	72
1	K	245/260 (94%)	235 (96%)	10 (4%)	30	47
1	L	246/260 (95%)	241 (98%)	5 (2%)	55	72
All	All	2951/3120 (95%)	2890 (98%)	61 (2%)	53	71

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	137	TYR
1	B	97	LYS
1	B	231	LYS
1	B	292	LYS
1	C	4	ASN
1	C	26	SER
1	C	87	HIS
1	C	98	GLU
1	C	145	CYS
1	C	231	LYS
1	C	235	LYS
1	D	4	ASN
1	D	25	GLN
1	D	137	TYR
1	D	229	ASN
1	E	74	LYS
1	E	129	SER
1	E	137	TYR
1	F	29	ARG
1	F	57	GLU
1	F	97	LYS
1	F	160	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	227	ASP
1	F	285	LYS
1	G	32	LYS
1	G	137	TYR
1	G	239	GLU
1	G	294	LYS
1	H	29	ARG
1	H	57	GLU
1	H	71	LYS
1	H	98	GLU
1	H	129	SER
1	H	137	TYR
1	H	279	SER
1	I	26	SER
1	I	56	HIS
1	I	137	TYR
1	I	161	ASN
1	I	292	LYS
1	J	25	GLN
1	J	59	HIS
1	J	97	LYS
1	J	98	GLU
1	J	262	LEU
1	K	26	SER
1	K	60	ARG
1	K	68	GLU
1	K	69	THR
1	K	76	LYS
1	K	98	GLU
1	K	131	ASP
1	K	137	TYR
1	K	235	LYS
1	K	292	LYS
1	L	18	LYS
1	L	32	LYS
1	L	60	ARG
1	L	150	ASP
1	L	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	242	ASN
1	B	242	ASN
1	C	4	ASN
1	C	117	GLN
1	D	25	GLN
1	D	56	HIS
1	H	99	HIS
1	J	19	ASN
1	J	59	HIS
1	K	59	HIS
1	L	4	ASN
1	L	99	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	KPI	H	166	1	10,13,14	1.43	1 (10%)	6,15,17	3.84	3 (50%)
1	KPI	L	166	1	10,13,14	1.88	1 (10%)	6,15,17	0.99	0
1	KPI	F	166	1	10,13,14	1.43	1 (10%)	6,15,17	2.47	3 (50%)
1	KPI	G	166	1	10,13,14	1.41	1 (10%)	6,15,17	4.21	3 (50%)
1	KPI	B	166	1	10,13,14	2.23	3 (30%)	6,15,17	1.43	0
1	KPI	J	166	1	10,13,14	0.67	0	6,15,17	3.06	4 (66%)
1	KPI	A	166	1	10,13,14	2.07	1 (10%)	6,15,17	1.91	2 (33%)
1	KPI	D	166	1	10,13,14	1.38	1 (10%)	6,15,17	2.22	2 (33%)
1	KPI	I	166	1	10,13,14	1.80	1 (10%)	6,15,17	1.74	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KPI	C	166	1	10,13,14	2.24	1 (10%)	6,15,17	2.09	2 (33%)
1	KPI	E	166	1	10,13,14	1.87	1 (10%)	6,15,17	2.78	2 (33%)
1	KPI	K	166	1	10,13,14	1.56	1 (10%)	6,15,17	1.43	1 (16%)

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
1	KPI	H	166	1	-	3/9/14/16	-
1	KPI	L	166	1	-	0/9/14/16	-
1	KPI	F	166	1	-	0/9/14/16	-
1	KPI	G	166	1	-	3/9/14/16	-
1	KPI	B	166	1	-	0/9/14/16	-
1	KPI	J	166	1	-	3/9/14/16	-
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	D	166	1	-	0/9/14/16	-
1	KPI	I	166	1	-	0/9/14/16	-
1	KPI	C	166	1	-	0/9/14/16	-
1	KPI	E	166	1	-	7/9/14/16	-
1	KPI	K	166	1	-	0/9/14/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	-6.43	1.42	1.52
1	A	166	KPI	CX2-CX1	-6.03	1.43	1.52
1	B	166	KPI	CX2-CX1	-5.76	1.43	1.52
1	L	166	KPI	CX2-CX1	-5.24	1.44	1.52
1	E	166	KPI	CX2-CX1	-5.17	1.44	1.52
1	I	166	KPI	CX2-CX1	-5.04	1.44	1.52
1	K	166	KPI	CX2-CX1	-4.36	1.45	1.52
1	H	166	KPI	O-C	4.18	1.36	1.19
1	G	166	KPI	O-C	4.11	1.36	1.19
1	D	166	KPI	CX2-CX1	-3.64	1.46	1.52
1	F	166	KPI	CX2-CX1	-3.51	1.46	1.52
1	B	166	KPI	CB-CA	-2.72	1.49	1.53
1	B	166	KPI	CA-N	-2.07	1.41	1.48

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	166	KPI	C1-CX1-CX2	-9.00	107.95	117.92
1	H	166	KPI	C1-CX1-CX2	-8.00	109.06	117.92
1	J	166	KPI	C1-CX1-CX2	-5.95	111.33	117.92
1	E	166	KPI	CE-NZ-CX1	5.48	136.49	121.77
1	G	166	KPI	CD-CE-NZ	4.38	118.63	110.66
1	F	166	KPI	C1-CX1-CX2	4.35	122.74	117.92
1	D	166	KPI	CE-NZ-CX1	4.27	133.26	121.77
1	H	166	KPI	CD-CE-NZ	3.88	117.73	110.66
1	C	166	KPI	CE-NZ-CX1	3.66	131.61	121.77
1	C	166	KPI	CD-CE-NZ	-3.53	104.23	110.66
1	A	166	KPI	CE-NZ-CX1	3.48	131.12	121.77
1	E	166	KPI	C1-CX1-NZ	-3.38	114.69	123.12
1	F	166	KPI	CE-NZ-CX1	3.12	130.15	121.77
1	K	166	KPI	CE-NZ-CX1	2.97	129.76	121.77
1	J	166	KPI	C1-CX1-NZ	2.89	130.34	123.12
1	I	166	KPI	C1-CX1-CX2	2.83	121.05	117.92
1	I	166	KPI	CE-NZ-CX1	2.67	128.95	121.77
1	H	166	KPI	C1-CX1-NZ	2.47	129.29	123.12
1	D	166	KPI	CD-CE-NZ	-2.46	106.18	110.66
1	A	166	KPI	CD-CE-NZ	-2.45	106.20	110.66
1	J	166	KPI	CD-CE-NZ	2.41	115.05	110.66
1	J	166	KPI	CD-CG-CB	-2.10	106.20	113.62
1	G	166	KPI	C1-CX1-NZ	2.09	128.34	123.12
1	F	166	KPI	CD-CE-NZ	-2.03	106.97	110.66

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	166	KPI	N-CA-CB-CG
1	E	166	KPI	CX2-CX1-NZ-CE
1	G	166	KPI	C1-CX1-NZ-CE
1	G	166	KPI	CX2-CX1-NZ-CE
1	H	166	KPI	C1-CX1-NZ-CE
1	H	166	KPI	CX2-CX1-NZ-CE
1	J	166	KPI	C1-CX1-NZ-CE
1	J	166	KPI	CX2-CX1-NZ-CE
1	E	166	KPI	CA-CB-CG-CD
1	E	166	KPI	C1-CX1-NZ-CE
1	E	166	KPI	C-CA-CB-CG
1	E	166	KPI	CE-CD-CG-CB
1	E	166	KPI	CG-CD-CE-NZ
1	J	166	KPI	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	H	166	KPI	CE-CD-CG-CB
1	G	166	KPI	CE-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	166	KPI	3	0
1	G	166	KPI	3	0
1	J	166	KPI	1	0
1	C	166	KPI	2	0
1	E	166	KPI	1	0
1	K	166	KPI	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 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	PGE	K	301	-	9,9,9	0.31	0	8,8,8	0.30	0
2	PGE	A	301	-	9,9,9	0.31	0	8,8,8	0.29	0
2	PGE	B	301	-	9,9,9	0.31	0	8,8,8	0.27	0
2	PGE	H	301	-	9,9,9	0.31	0	8,8,8	0.27	0
4	ACT	C	305	-	1,3,3	5.13	1 (100%)	0,3,3	-	-
2	PGE	C	301	-	9,9,9	0.32	0	8,8,8	0.24	0
4	ACT	F	303	-	1,3,3	6.69	1 (100%)	0,3,3	-	-
2	PGE	L	301	-	9,9,9	0.32	0	8,8,8	0.26	0
2	PGE	E	302	-	9,9,9	0.37	0	8,8,8	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PGE	F	301	-	9,9,9	0.31	0	8,8,8	0.25	0
2	PGE	G	301	-	9,9,9	0.32	0	8,8,8	0.26	0
2	PGE	J	301	-	9,9,9	0.31	0	8,8,8	0.34	0
5	EDO	J	303	-	3,3,3	0.48	0	2,2,2	0.24	0
2	PGE	C	302	-	9,9,9	0.31	0	8,8,8	0.29	0
4	ACT	L	302	-	1,3,3	3.78	1 (100%)	0,3,3	-	-
2	PGE	E	301	-	9,9,9	0.31	0	8,8,8	0.27	0
2	PGE	I	301	-	9,9,9	0.30	0	8,8,8	0.28	0
2	PGE	D	301	-	9,9,9	0.32	0	8,8,8	0.25	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	PGE	K	301	-	-	3/7/7/7	-
2	PGE	A	301	-	-	5/7/7/7	-
2	PGE	B	301	-	-	2/7/7/7	-
2	PGE	H	301	-	-	4/7/7/7	-
2	PGE	C	301	-	-	2/7/7/7	-
2	PGE	L	301	-	-	2/7/7/7	-
2	PGE	E	302	-	-	4/7/7/7	-
2	PGE	F	301	-	-	3/7/7/7	-
2	PGE	G	301	-	-	2/7/7/7	-
2	PGE	J	301	-	-	5/7/7/7	-
5	EDO	J	303	-	-	1/1/1/1	-
2	PGE	C	302	-	-	1/7/7/7	-
2	PGE	E	301	-	-	0/7/7/7	-
2	PGE	I	301	-	-	5/7/7/7	-
2	PGE	D	301	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	303	ACT	CH3-C	6.69	1.57	1.48
4	C	305	ACT	CH3-C	5.13	1.55	1.48
4	L	302	ACT	CH3-C	3.78	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PGE	O2-C3-C4-O3
2	I	301	PGE	O1-C1-C2-O2
2	J	301	PGE	O2-C3-C4-O3
2	K	301	PGE	O2-C3-C4-O3
2	D	301	PGE	O2-C3-C4-O3
2	E	302	PGE	O2-C3-C4-O3
2	A	301	PGE	O1-C1-C2-O2
2	K	301	PGE	C3-C4-O3-C5
2	H	301	PGE	O3-C5-C6-O4
2	I	301	PGE	O2-C3-C4-O3
2	E	302	PGE	O1-C1-C2-O2
2	E	302	PGE	O3-C5-C6-O4
2	H	301	PGE	O2-C3-C4-O3
2	A	301	PGE	O3-C5-C6-O4
2	B	301	PGE	O1-C1-C2-O2
5	J	303	EDO	O1-C1-C2-O2
2	F	301	PGE	O3-C5-C6-O4
2	G	301	PGE	C1-C2-O2-C3
2	F	301	PGE	C1-C2-O2-C3
2	H	301	PGE	C3-C4-O3-C5
2	G	301	PGE	C6-C5-O3-C4
2	J	301	PGE	C6-C5-O3-C4
2	F	301	PGE	C6-C5-O3-C4
2	A	301	PGE	C1-C2-O2-C3
2	J	301	PGE	O1-C1-C2-O2
2	I	301	PGE	C6-C5-O3-C4
2	K	301	PGE	C1-C2-O2-C3
2	L	301	PGE	O3-C5-C6-O4
2	C	302	PGE	O2-C3-C4-O3
2	B	301	PGE	C6-C5-O3-C4
2	J	301	PGE	C1-C2-O2-C3
2	D	301	PGE	C6-C5-O3-C4
2	I	301	PGE	C4-C3-O2-C2
2	A	301	PGE	C6-C5-O3-C4
2	E	302	PGE	C1-C2-O2-C3
2	I	301	PGE	O3-C5-C6-O4
2	H	301	PGE	C1-C2-O2-C3
2	J	301	PGE	O3-C5-C6-O4
2	C	301	PGE	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

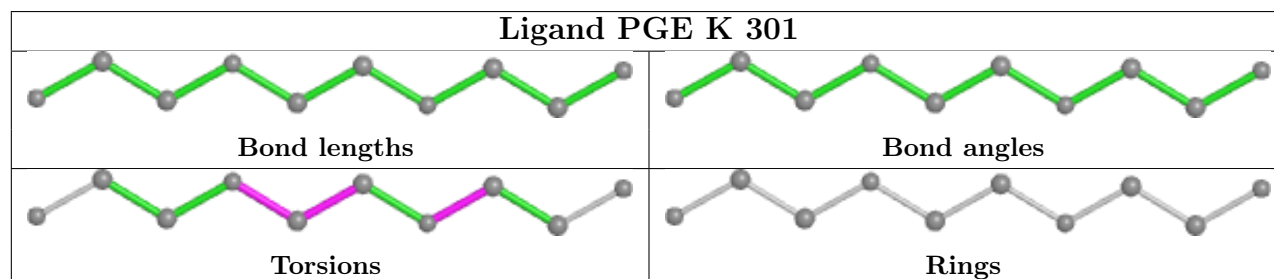
Mol	Chain	Res	Type	Atoms
2	C	301	PGE	C1-C2-O2-C3
2	L	301	PGE	O1-C1-C2-O2

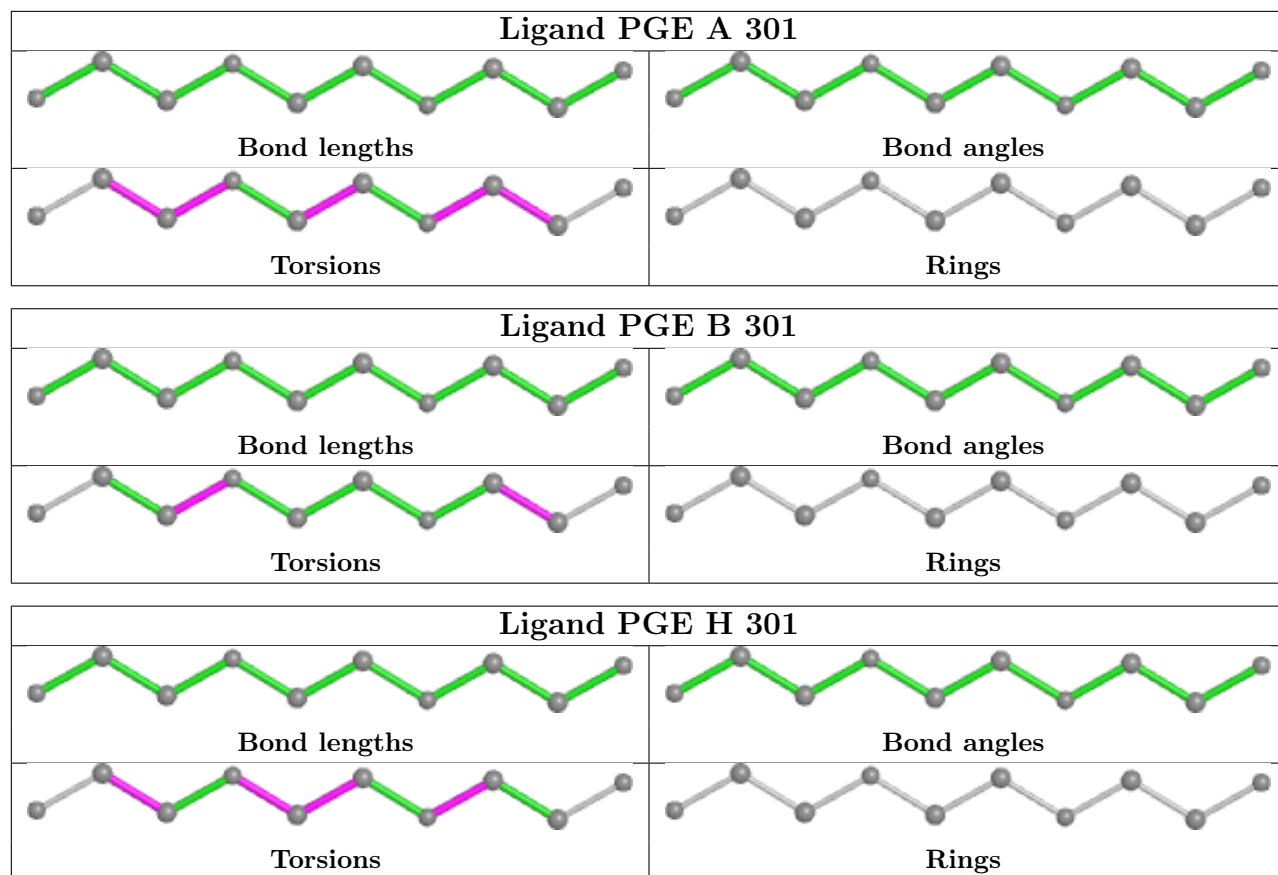
There are no ring outliers.

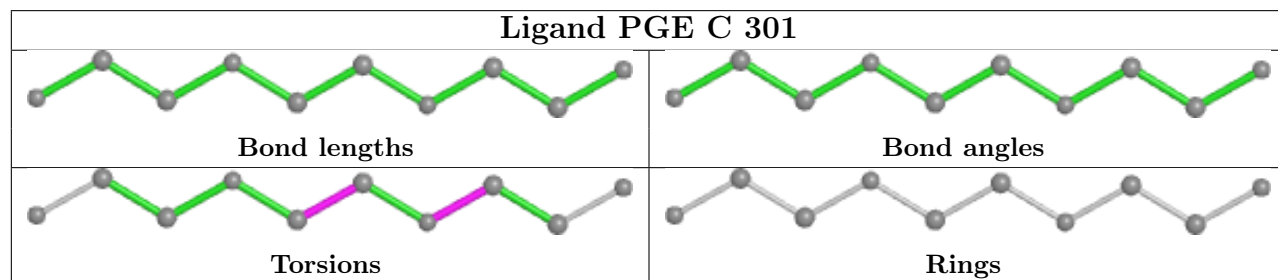
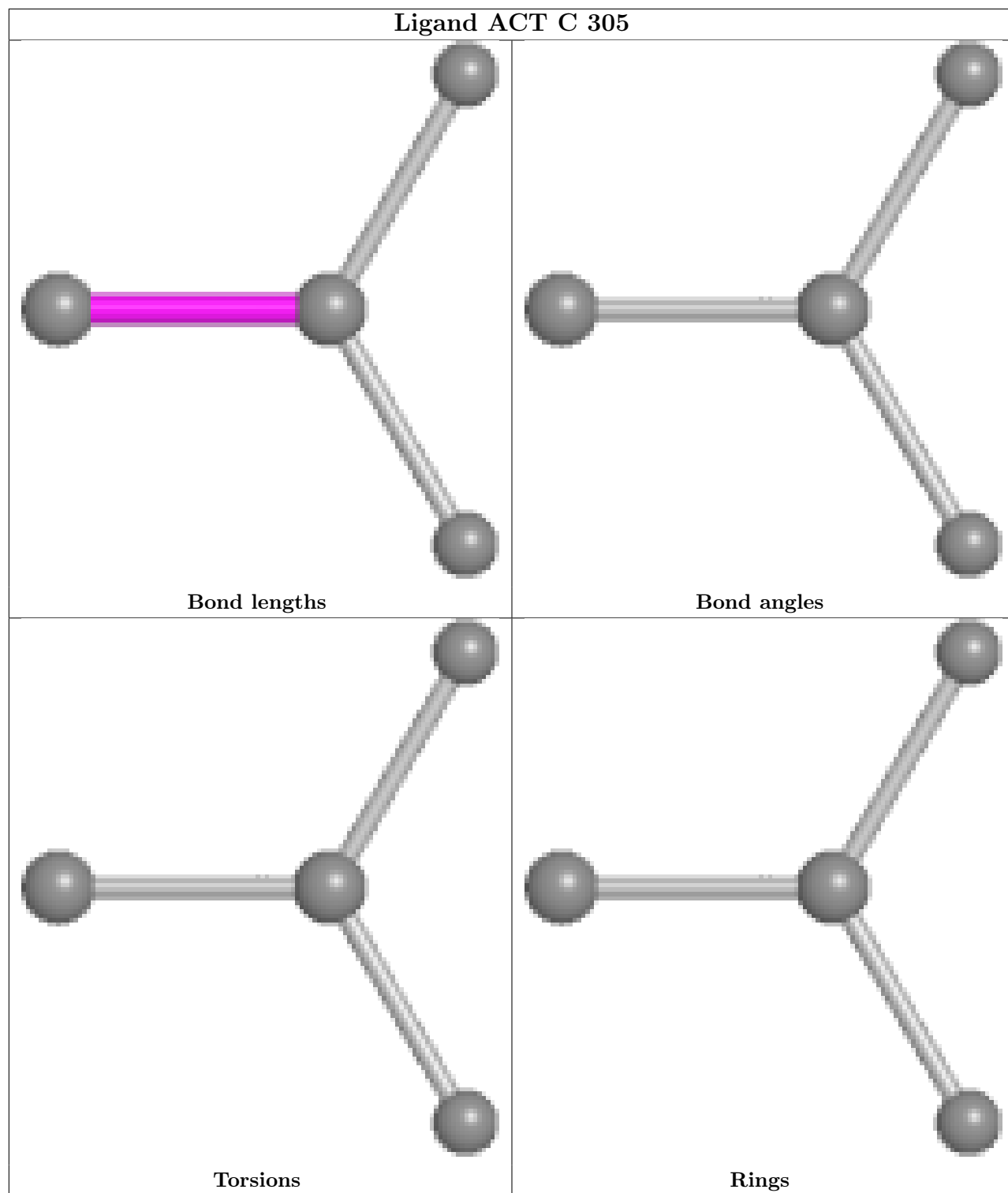
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PGE	3	0
2	B	301	PGE	1	0
4	C	305	ACT	5	0
2	E	302	PGE	1	0
2	G	301	PGE	1	0
2	J	301	PGE	1	0
4	L	302	ACT	4	0
2	I	301	PGE	1	0
2	D	301	PGE	1	0

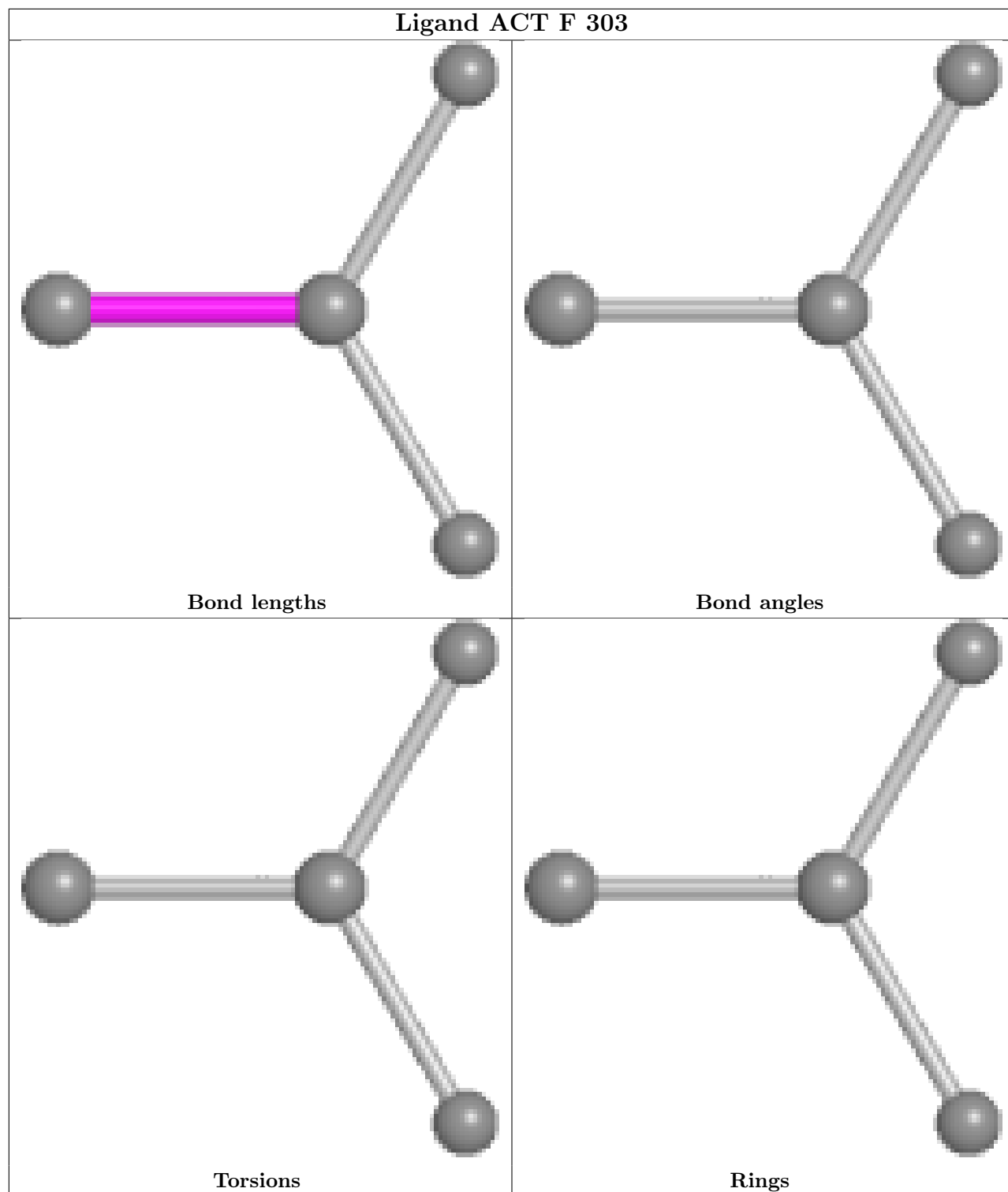
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



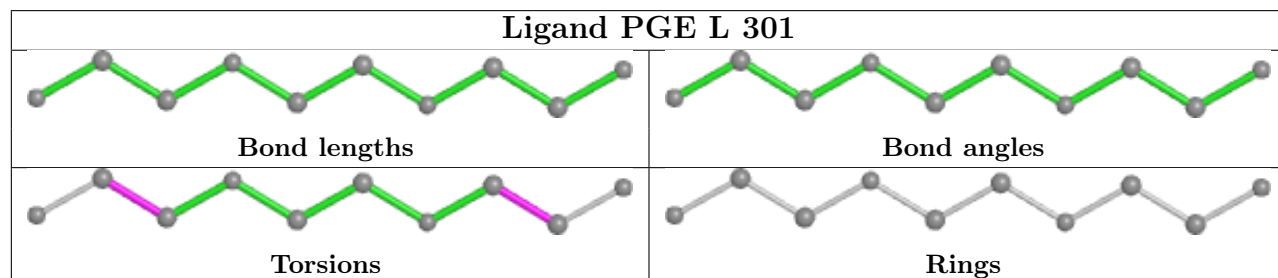


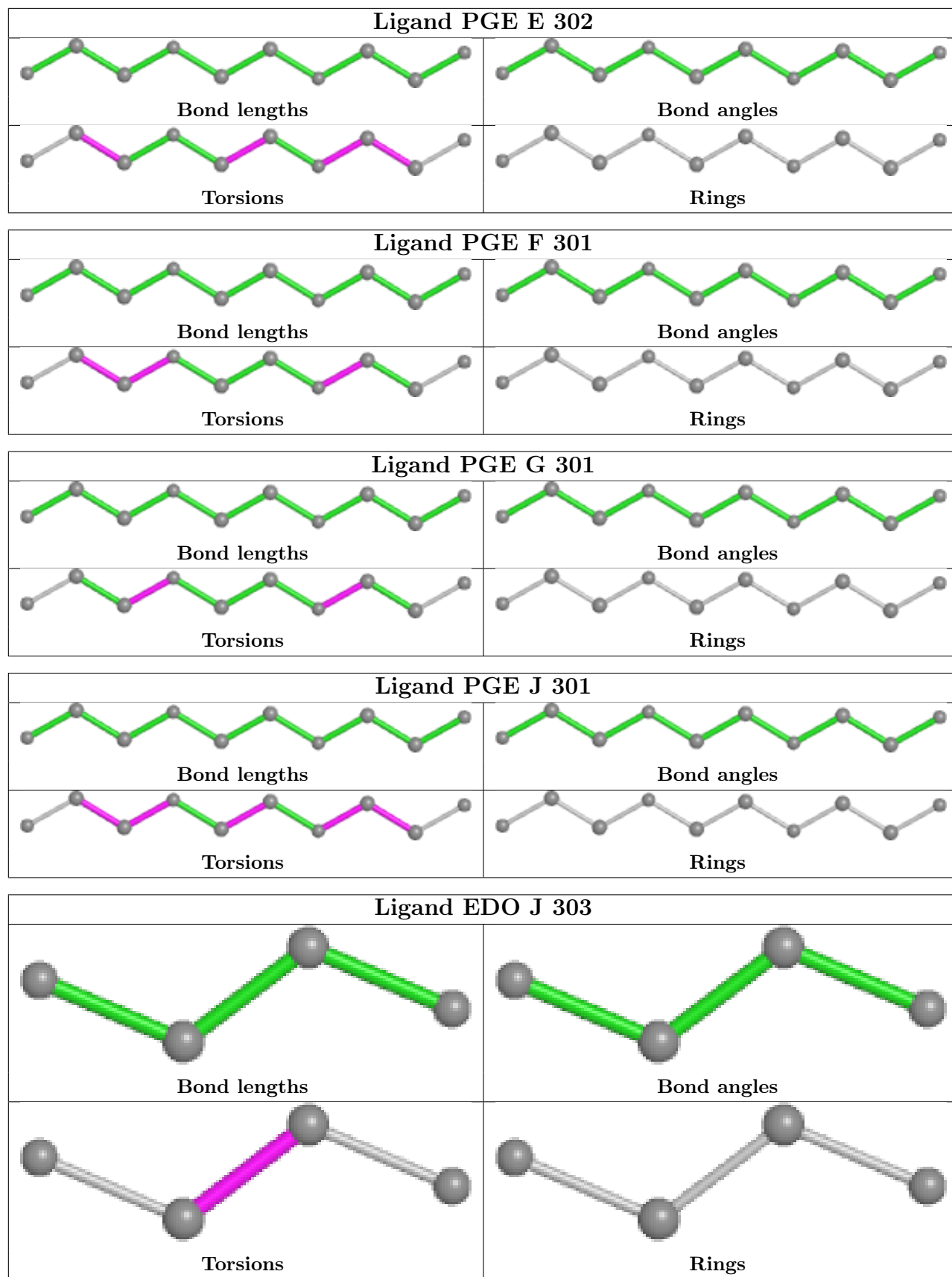


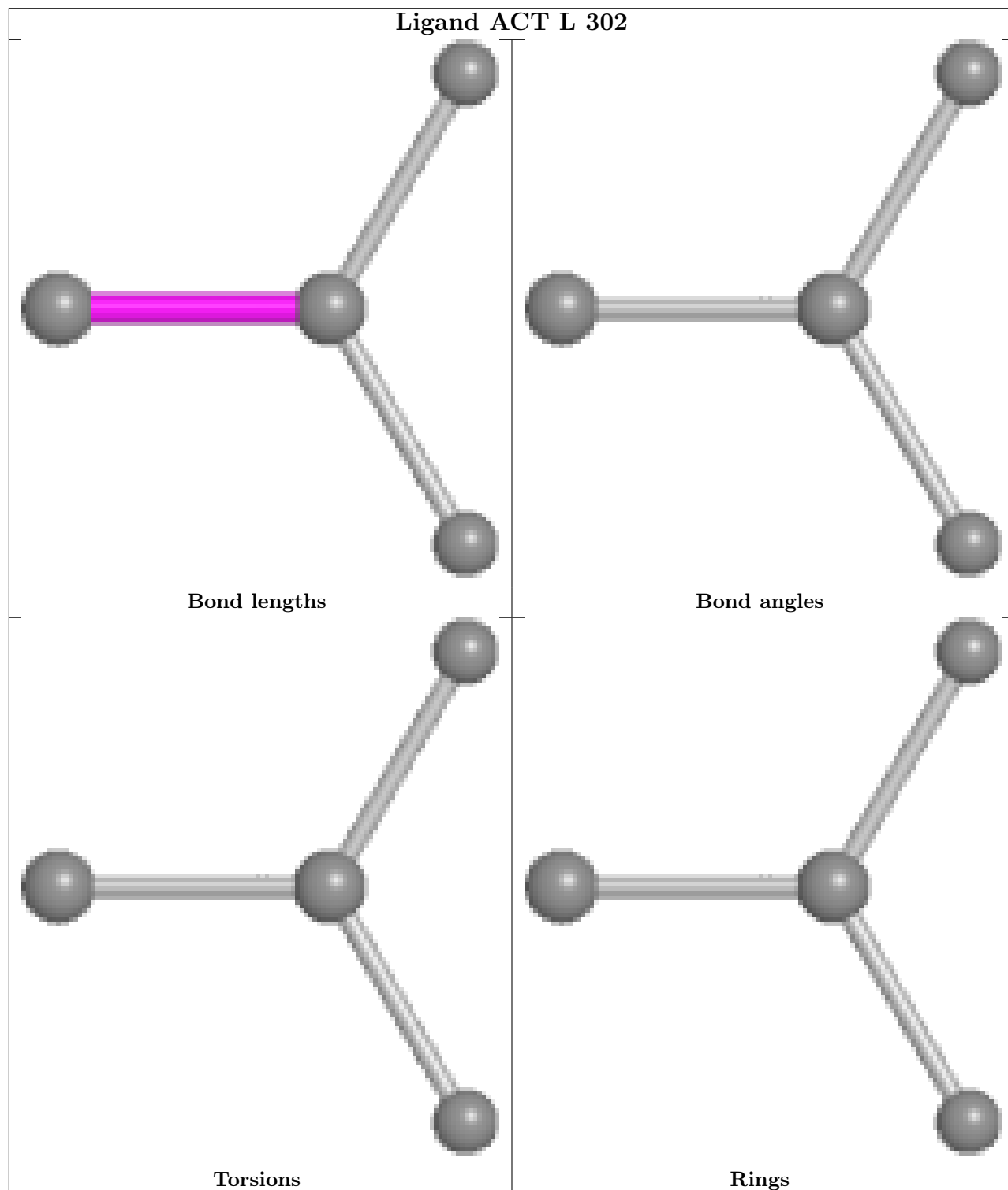
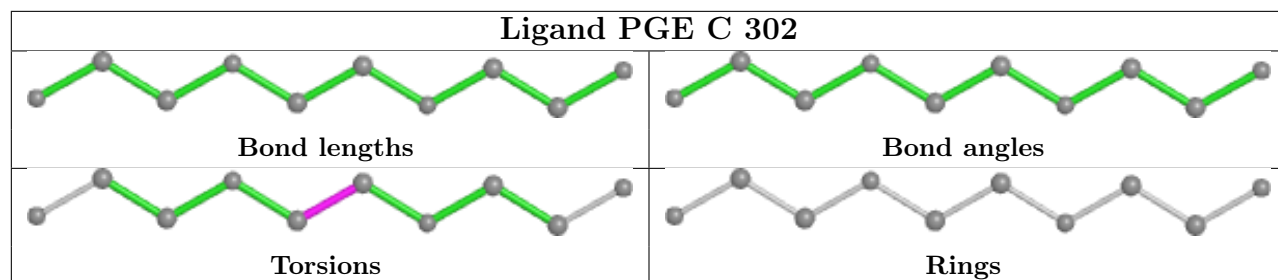
Ligand ACT F 303

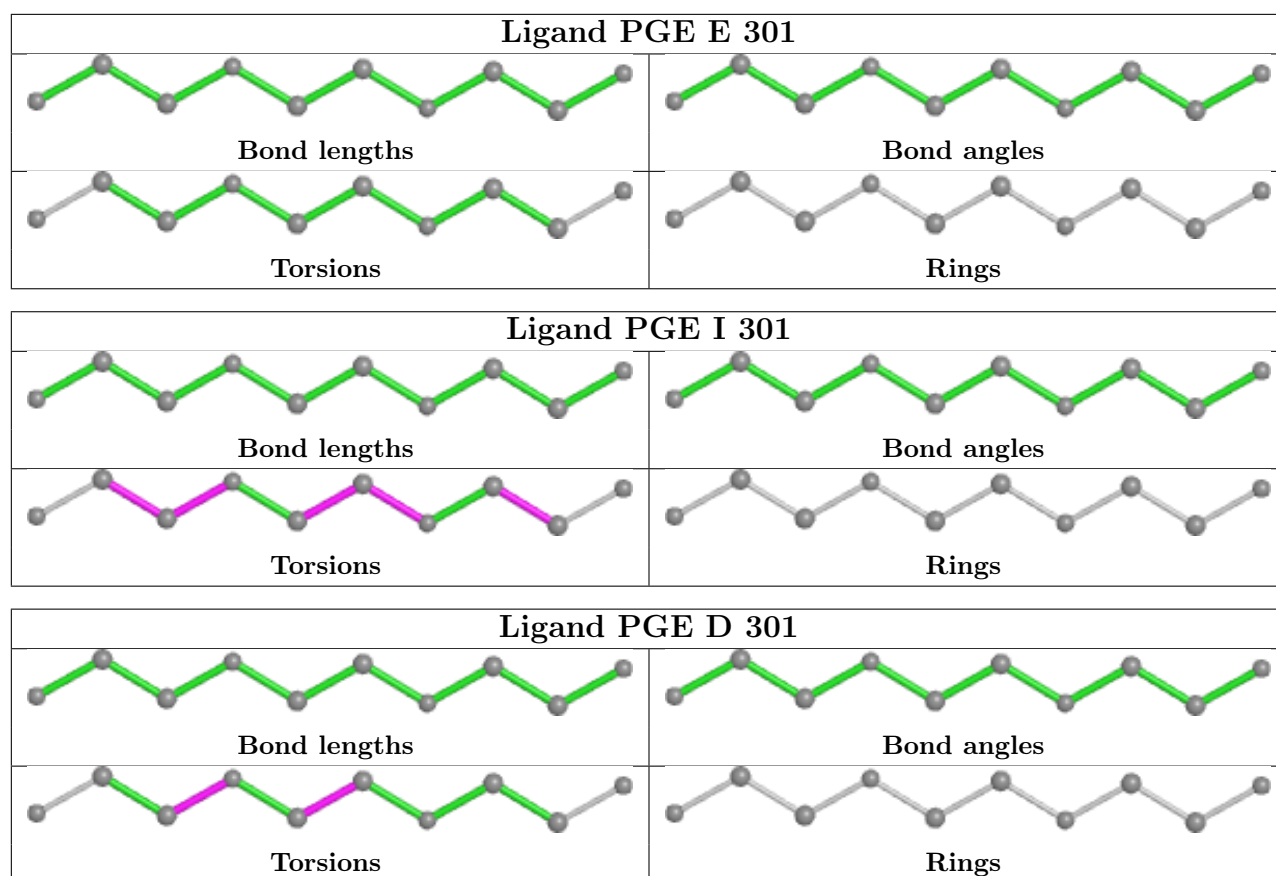


Ligand PGE L 301









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/310 (95%)	0.10	7 (2%) 59 56	34, 49, 72, 91	0
1	B	295/310 (95%)	0.07	4 (1%) 75 73	37, 50, 70, 98	0
1	C	295/310 (95%)	0.10	11 (3%) 41 40	34, 50, 71, 87	0
1	D	295/310 (95%)	0.09	8 (2%) 54 52	36, 49, 73, 89	0
1	E	293/310 (94%)	0.14	12 (4%) 37 35	30, 54, 75, 97	0
1	F	295/310 (95%)	0.14	13 (4%) 34 32	36, 51, 73, 105	0
1	G	295/310 (95%)	0.14	10 (3%) 45 43	36, 51, 70, 89	0
1	H	295/310 (95%)	0.23	15 (5%) 28 26	38, 53, 73, 103	0
1	I	295/310 (95%)	0.15	13 (4%) 34 32	37, 53, 73, 90	0
1	J	295/310 (95%)	0.23	13 (4%) 34 32	40, 56, 83, 96	0
1	K	295/310 (95%)	0.22	14 (4%) 31 29	41, 55, 77, 108	0
1	L	295/310 (95%)	0.15	12 (4%) 37 35	24, 57, 81, 97	0
All	All	3538/3720 (95%)	0.15	132 (3%) 41 40	24, 53, 75, 108	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	164	GLY	5.2
1	H	95	PHE	4.9
1	F	288	GLU	4.7
1	I	41	ALA	4.6
1	E	131	ASP	4.4
1	K	95	PHE	4.3
1	K	68	GLU	4.0
1	H	255	PRO	4.0
1	H	90	VAL	3.9
1	H	103	GLY	3.9
1	D	280	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	25	GLN	3.9
1	D	87	HIS	3.7
1	I	100	GLY	3.7
1	D	101	ALA	3.7
1	E	43	VAL	3.5
1	I	98	GLU	3.5
1	K	129	SER	3.4
1	E	60	ARG	3.4
1	E	98	GLU	3.3
1	H	293	TYR	3.3
1	L	220	ALA	3.3
1	C	129	SER	3.3
1	B	103	GLY	3.2
1	L	95	PHE	3.2
1	D	100	GLY	3.2
1	H	86	THR	3.2
1	G	100	GLY	3.2
1	L	15	THR	3.2
1	F	98	GLU	3.1
1	A	60	ARG	3.1
1	G	29	ARG	3.1
1	J	288	GLU	3.1
1	G	19	ASN	3.1
1	G	26	SER	3.1
1	C	4	ASN	3.1
1	H	91	GLY	3.1
1	I	51	SER	3.0
1	E	35	ILE	3.0
1	E	26	SER	3.0
1	F	261	TYR	3.0
1	H	99	HIS	2.9
1	F	87	HIS	2.9
1	F	246	ILE	2.9
1	C	262	LEU	2.9
1	I	87	HIS	2.9
1	K	133	PRO	2.9
1	G	38	GLY	2.8
1	L	289	VAL	2.8
1	E	87	HIS	2.8
1	J	276	CYS	2.8
1	C	86	THR	2.8
1	J	11	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	87	HIS	2.7
1	F	100	GLY	2.7
1	L	216	ASP	2.7
1	L	129	SER	2.7
1	D	285	LYS	2.7
1	J	29	ARG	2.6
1	J	203	GLY	2.6
1	C	98	GLU	2.6
1	A	128	GLN	2.6
1	K	16	PRO	2.6
1	A	230	TYR	2.6
1	F	95	PHE	2.5
1	K	287	GLU	2.5
1	H	59	HIS	2.5
1	K	293	TYR	2.5
1	F	279	SER	2.5
1	G	285	LYS	2.5
1	J	21	LYS	2.4
1	H	93	ALA	2.4
1	H	230	TYR	2.4
1	I	290	MET	2.4
1	F	62	CYS	2.4
1	K	72	GLY	2.4
1	A	27	TYR	2.4
1	K	57	GLU	2.4
1	G	59	HIS	2.3
1	E	132	ILE	2.3
1	L	225	ALA	2.3
1	E	42	VAL	2.3
1	J	22	VAL	2.3
1	A	152	ILE	2.3
1	I	116	GLN	2.3
1	C	16	PRO	2.3
1	K	256	ILE	2.3
1	J	95	PHE	2.3
1	I	143	THR	2.3
1	I	149	THR	2.3
1	K	241	TYR	2.3
1	L	93	ALA	2.3
1	C	103	GLY	2.3
1	H	225	ALA	2.3
1	K	130	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	161	ASN	2.3
1	E	281	GLU	2.3
1	G	170	GLY	2.3
1	G	246	ILE	2.3
1	I	101	ALA	2.3
1	J	279	SER	2.2
1	C	95	PHE	2.2
1	L	29	ARG	2.2
1	B	152	ILE	2.2
1	F	29	ARG	2.2
1	C	293	TYR	2.2
1	L	175	CYS	2.2
1	F	31	ILE	2.2
1	D	4	ASN	2.2
1	C	267	GLU	2.2
1	E	71	LYS	2.2
1	I	203	GLY	2.2
1	K	59	HIS	2.2
1	J	72	GLY	2.2
1	D	57	GLU	2.2
1	H	63	ILE	2.1
1	I	29	ARG	2.1
1	D	38	GLY	2.1
1	G	222	THR	2.1
1	F	284	ALA	2.0
1	A	77	VAL	2.0
1	I	224	PHE	2.0
1	L	25	GLN	2.0
1	L	194	ILE	2.0
1	A	168	ALA	2.0
1	B	75	VAL	2.0
1	J	268	SER	2.0
1	J	190	GLY	2.0
1	C	283	PHE	2.0
1	H	281	GLU	2.0
1	F	149	THR	2.0
1	B	230	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	D	166	14/15	0.84	0.27	45,49,57,57	0
1	KPI	K	166	14/15	0.86	0.18	45,52,59,61	0
1	KPI	I	166	14/15	0.87	0.16	55,58,61,64	0
1	KPI	L	166	14/15	0.87	0.21	45,50,51,52	0
1	KPI	J	166	14/15	0.88	0.16	44,51,62,64	0
1	KPI	B	166	14/15	0.90	0.15	36,42,59,61	0
1	KPI	G	166	14/15	0.90	0.29	46,51,57,59	0
1	KPI	E	166	14/15	0.91	0.15	42,48,59,64	0
1	KPI	A	166	14/15	0.91	0.17	33,43,52,54	0
1	KPI	F	166	14/15	0.93	0.13	52,54,64,66	0
1	KPI	H	166	14/15	0.94	0.14	33,41,50,50	0
1	KPI	C	166	14/15	0.96	0.12	40,46,54,58	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	L	302	4/4	0.55	0.24	73,79,80,82	0
2	PGE	E	302	10/10	0.68	0.20	57,68,70,70	0
2	PGE	L	301	10/10	0.70	0.18	65,66,70,72	0
5	EDO	J	303	4/4	0.72	0.23	63,64,65,67	0
4	ACT	C	305	4/4	0.75	0.25	62,68,70,71	0
3	MG	C	303	1/1	0.81	0.09	47,47,47,47	0
3	MG	F	302	1/1	0.83	0.23	54,54,54,54	0
2	PGE	E	301	10/10	0.83	0.23	72,72,74,76	0
2	PGE	D	301	10/10	0.84	0.20	59,61,65,67	0
2	PGE	A	301	10/10	0.85	0.18	59,62,68,68	0
2	PGE	C	301	10/10	0.86	0.16	52,58,61,63	0
3	MG	D	302	1/1	0.86	0.25	59,59,59,59	0
2	PGE	K	301	10/10	0.87	0.17	66,72,80,81	0
2	PGE	B	301	10/10	0.88	0.18	62,63,66,66	0

Continued on next page...

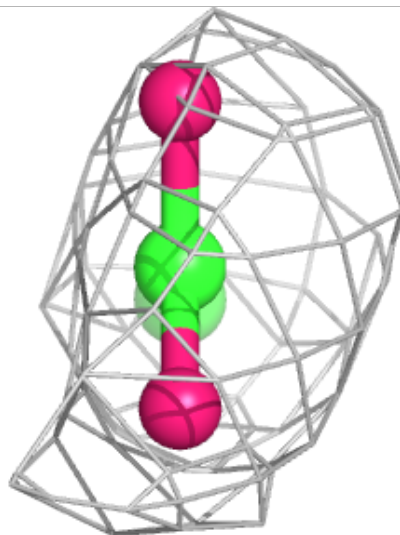
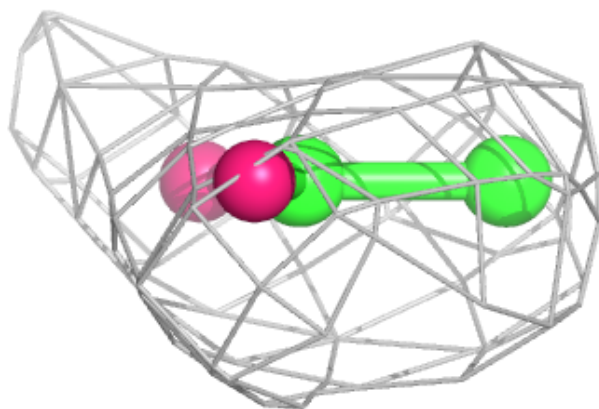
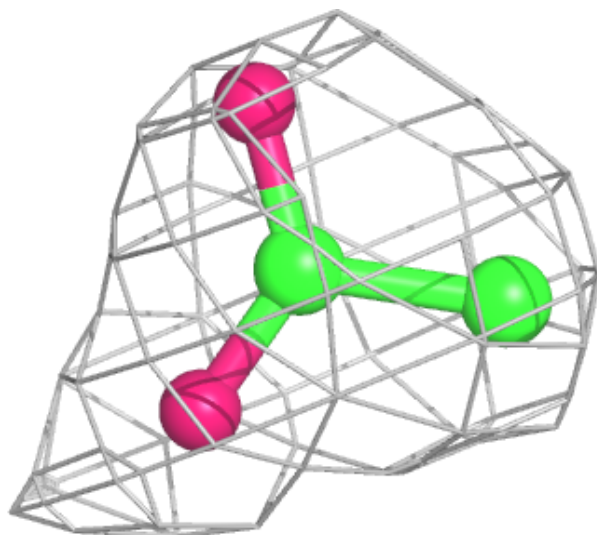
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	I	301	10/10	0.89	0.15	60,66,71,71	0
3	MG	C	304	1/1	0.89	0.20	53,53,53,53	0
3	MG	J	302	1/1	0.89	0.19	61,61,61,61	0
3	MG	A	302	1/1	0.90	0.23	55,55,55,55	0
2	PGE	H	301	10/10	0.90	0.14	60,61,65,67	0
2	PGE	J	301	10/10	0.90	0.18	56,61,64,66	0
2	PGE	C	302	10/10	0.91	0.12	63,66,69,70	0
2	PGE	F	301	10/10	0.91	0.17	52,59,62,62	0
3	MG	E	303	1/1	0.92	0.17	59,59,59,59	0
2	PGE	G	301	10/10	0.95	0.14	55,58,60,62	0
4	ACT	F	303	4/4	0.95	0.18	53,54,55,56	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.

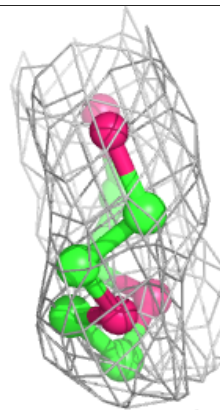
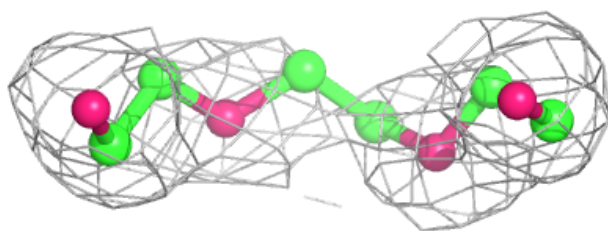
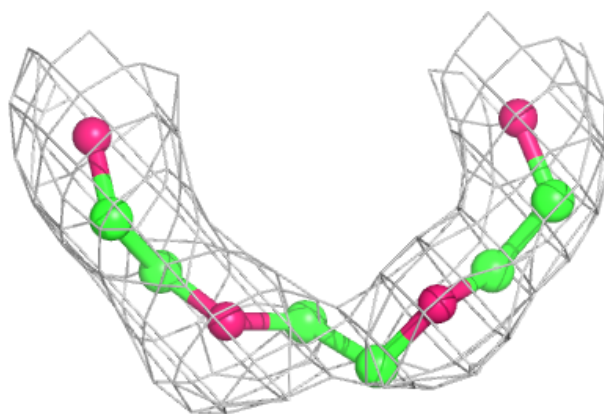
Electron density around ACT L 302:

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



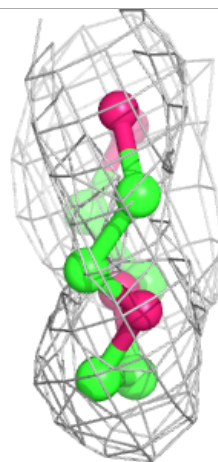
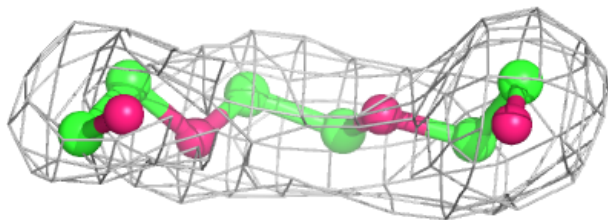
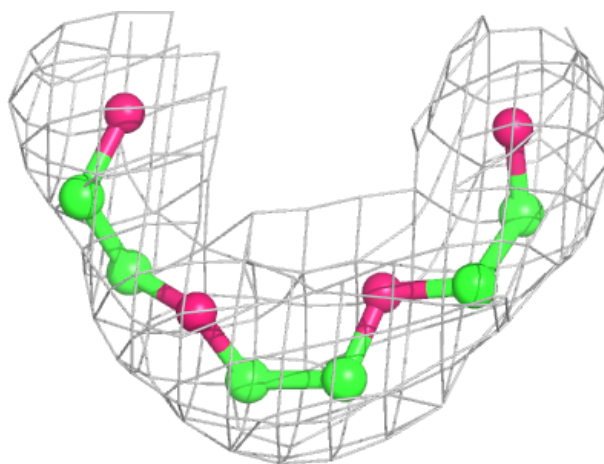
Electron density around PGE E 302:

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



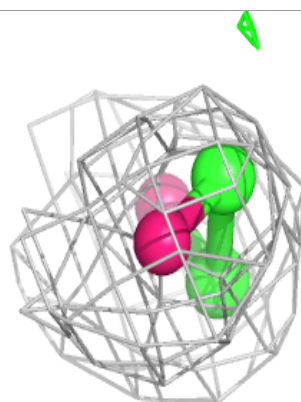
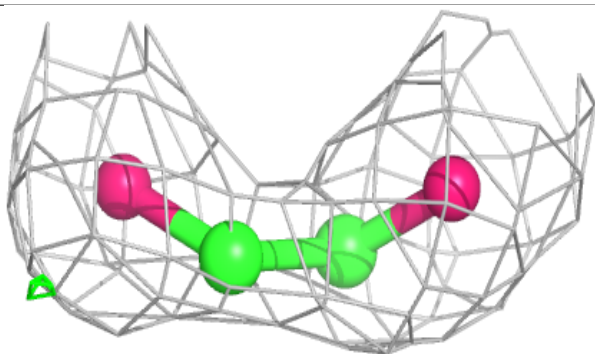
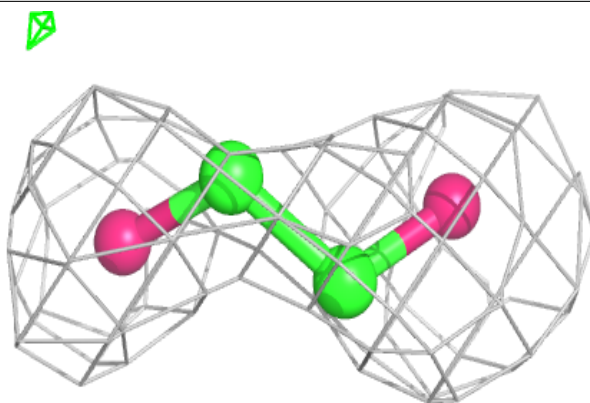
Electron density around PGE L 301:

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



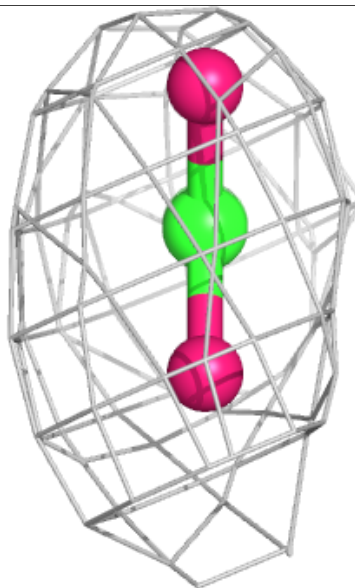
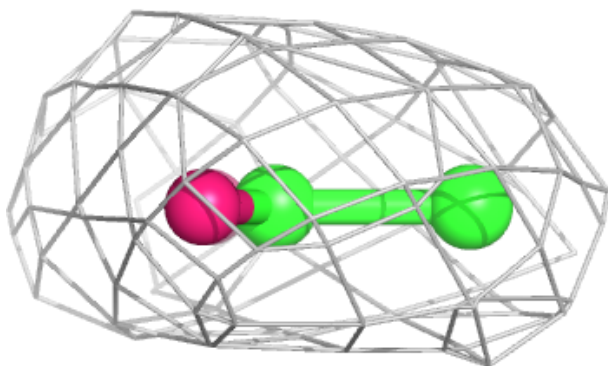
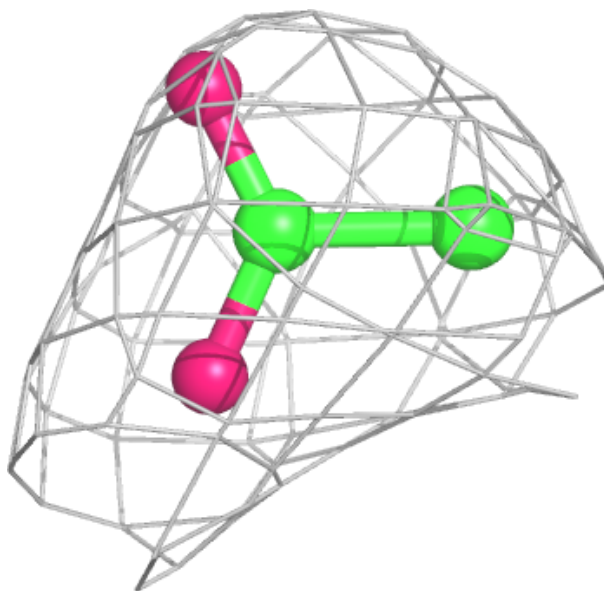
Electron density around EDO J 303:

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



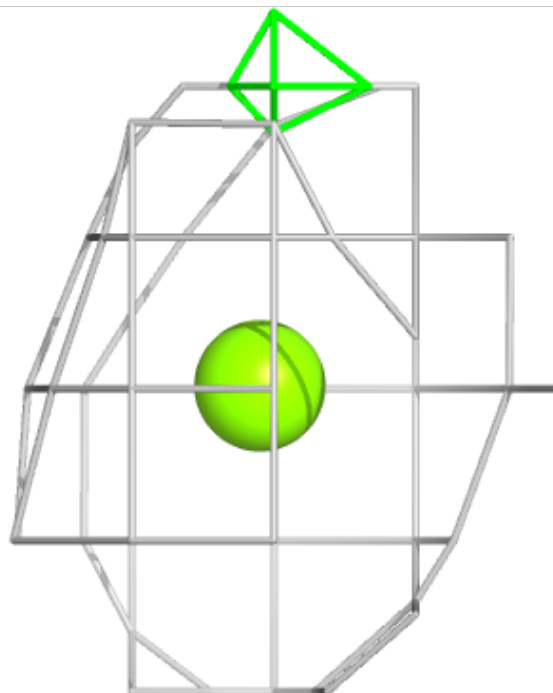
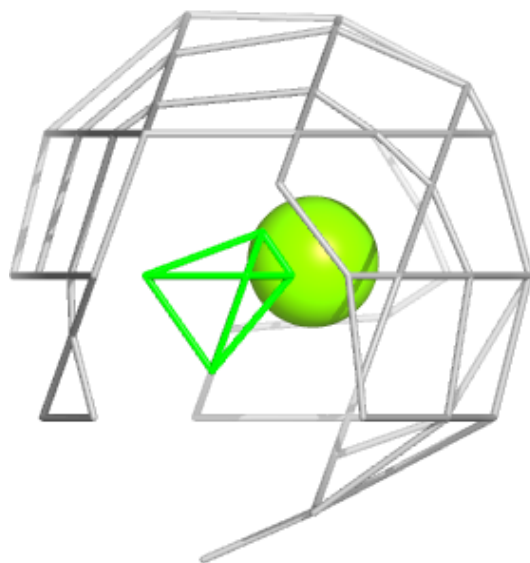
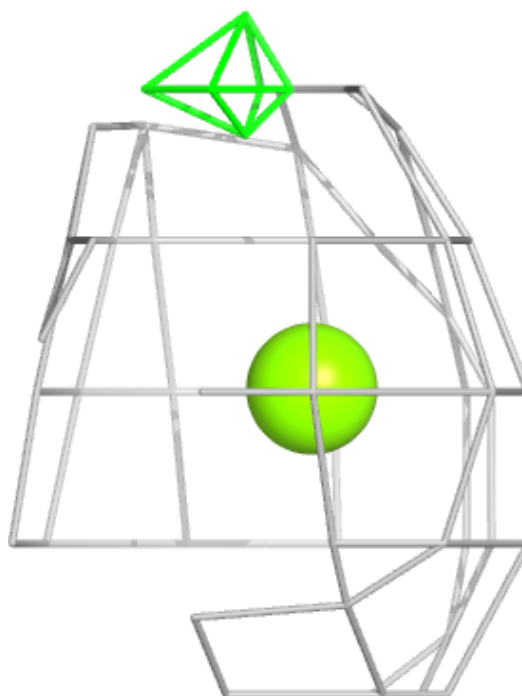
Electron density around ACT C 305:

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



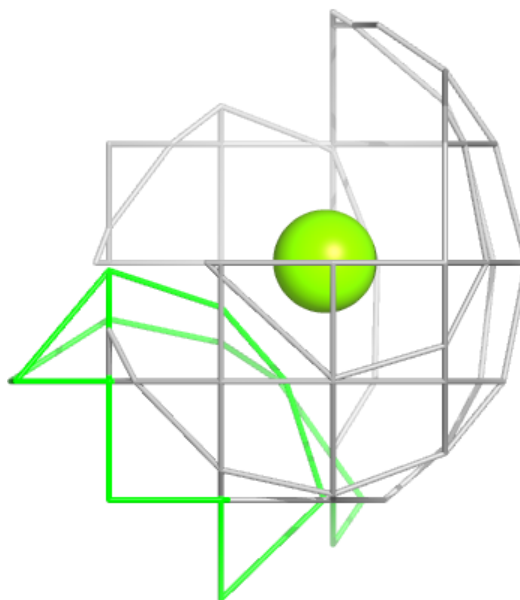
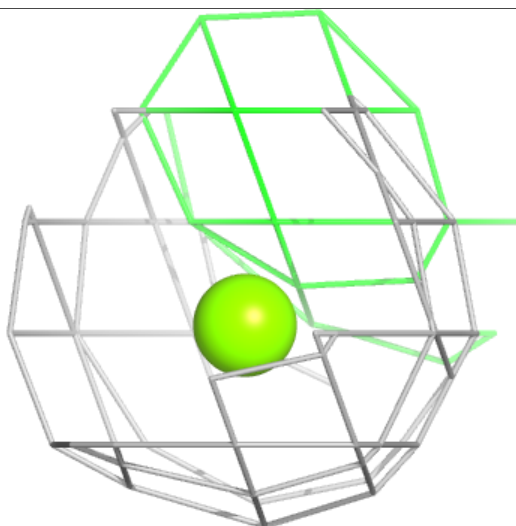
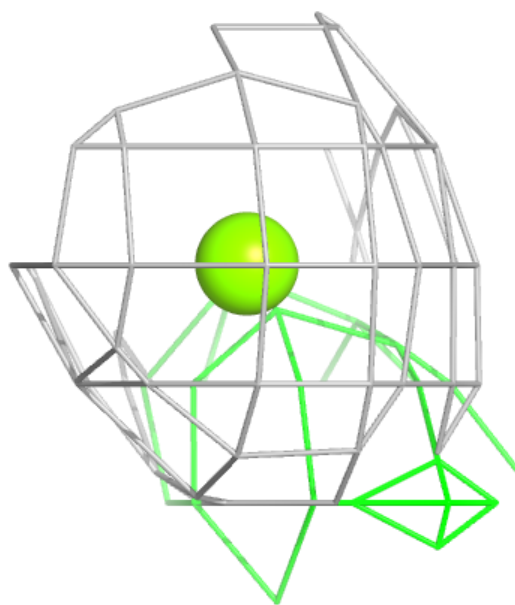
Electron density around MG C 303:

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



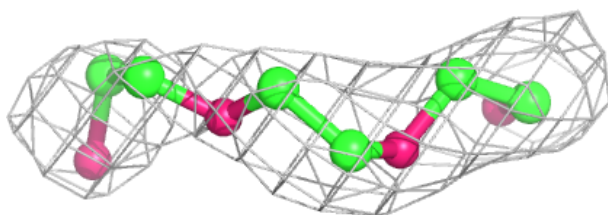
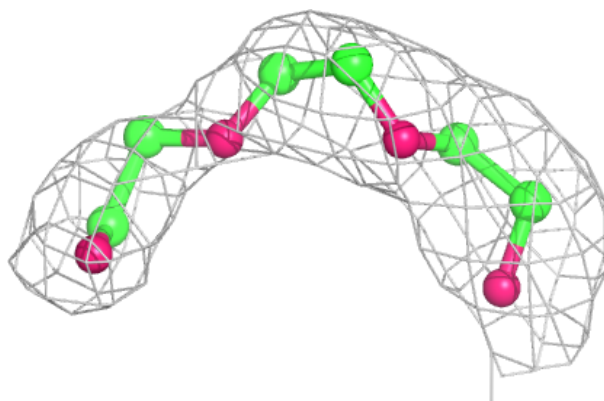
Electron density around MG F 302:

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

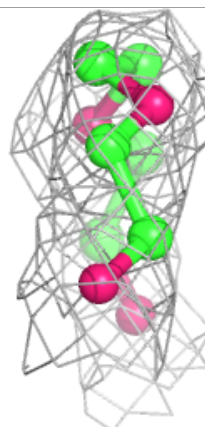
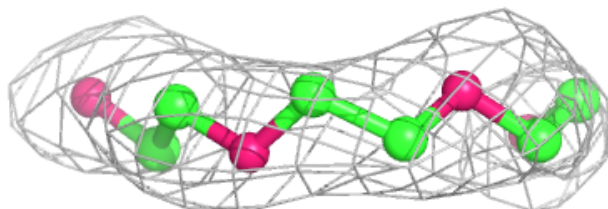
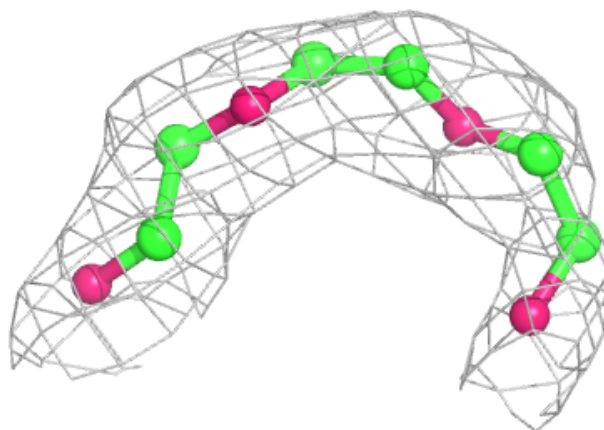


Electron density around PGE E 301:

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

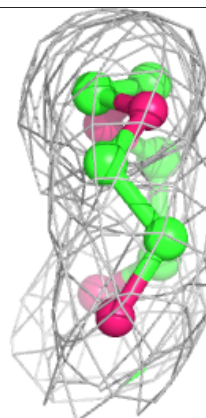
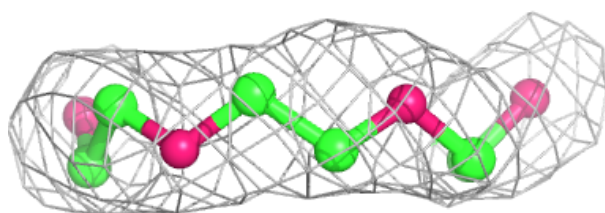
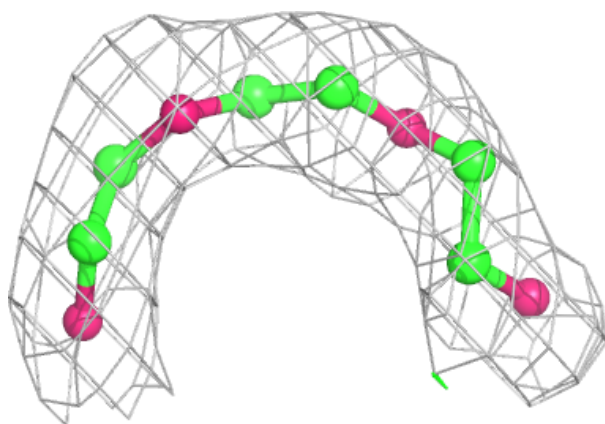
**Electron density around PGE D 301:**

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



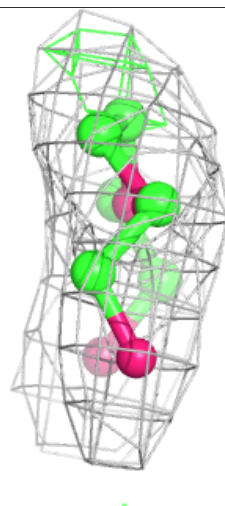
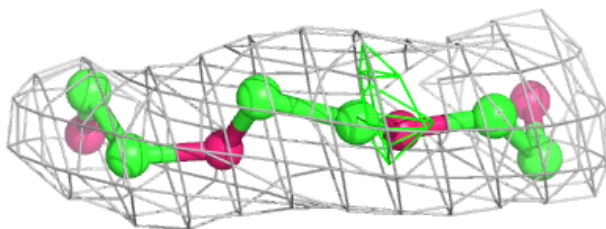
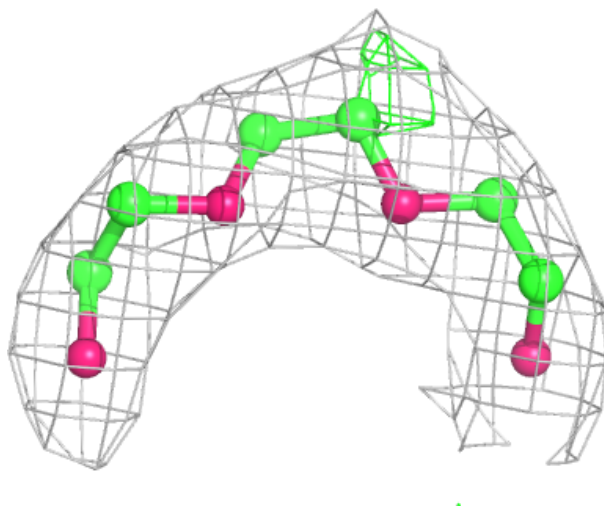
Electron density around PGE A 301:

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



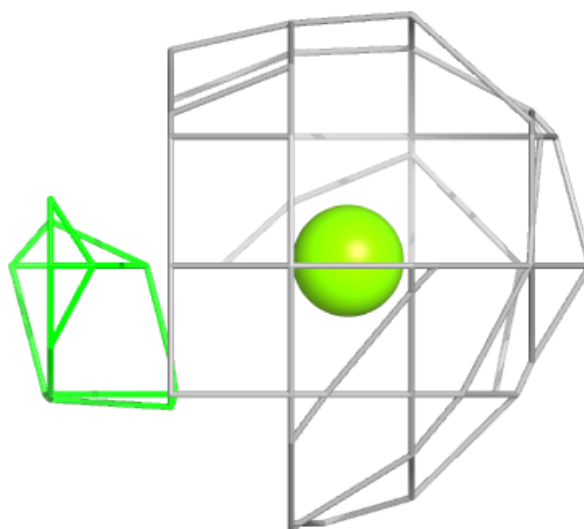
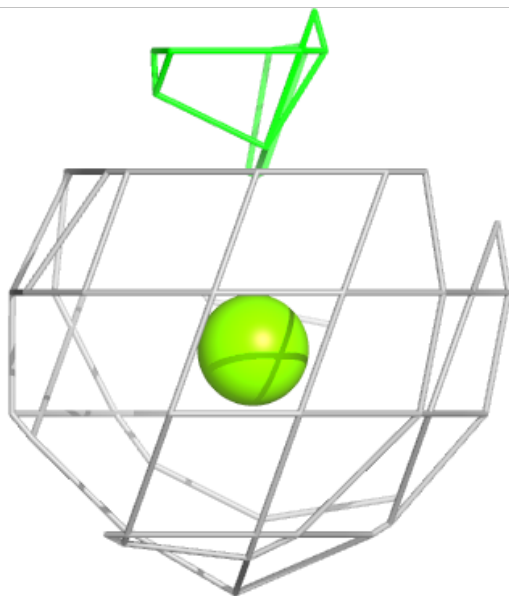
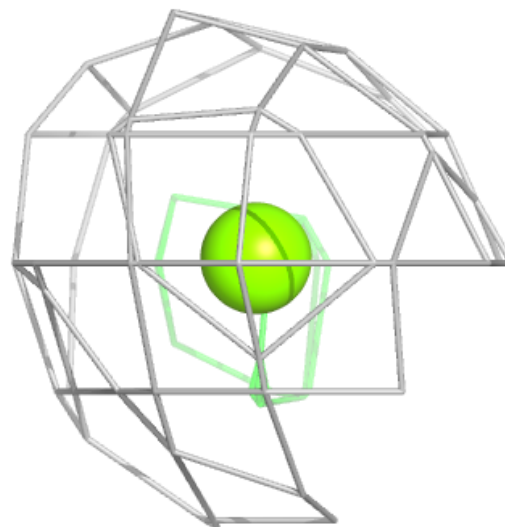
Electron density around PGE C 301:

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



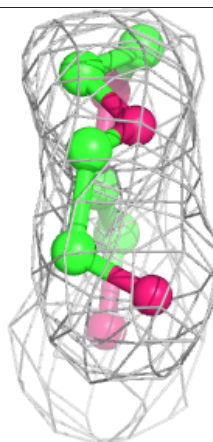
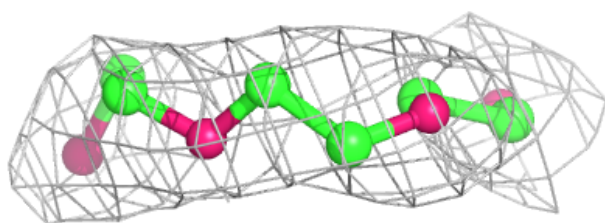
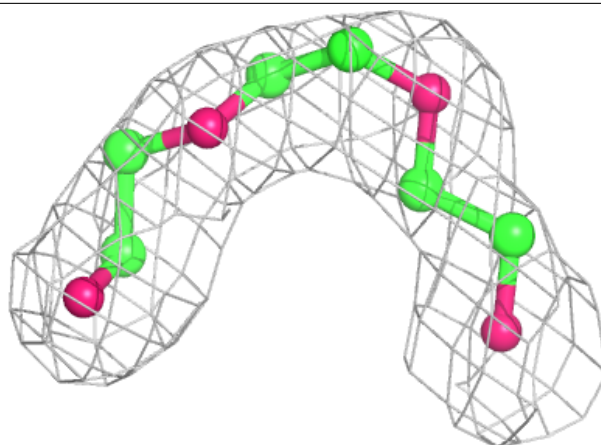
Electron density around MG D 302:

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

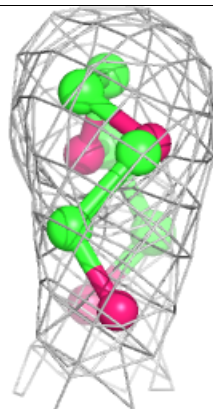
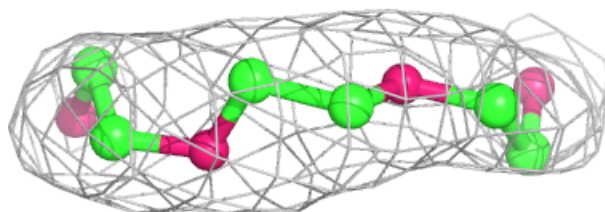
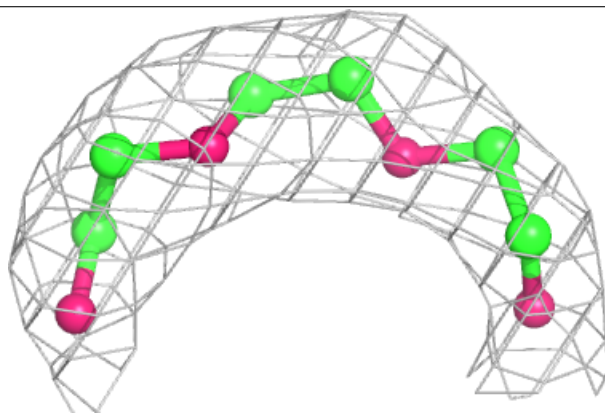


Electron density around PGE K 301:

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

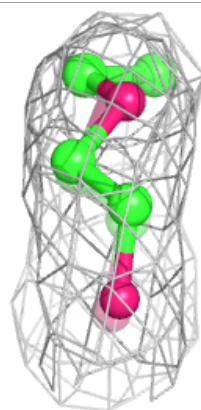
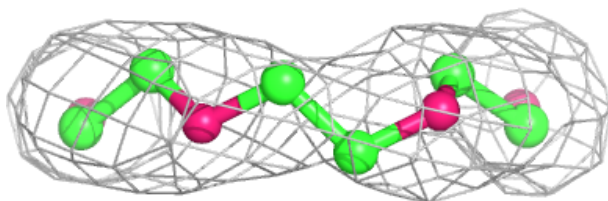
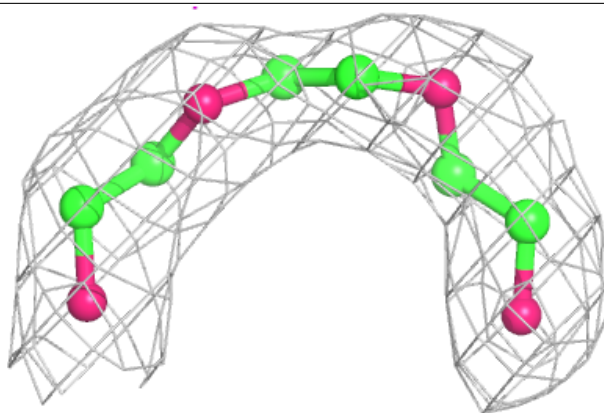
**Electron density around PGE B 301:**

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



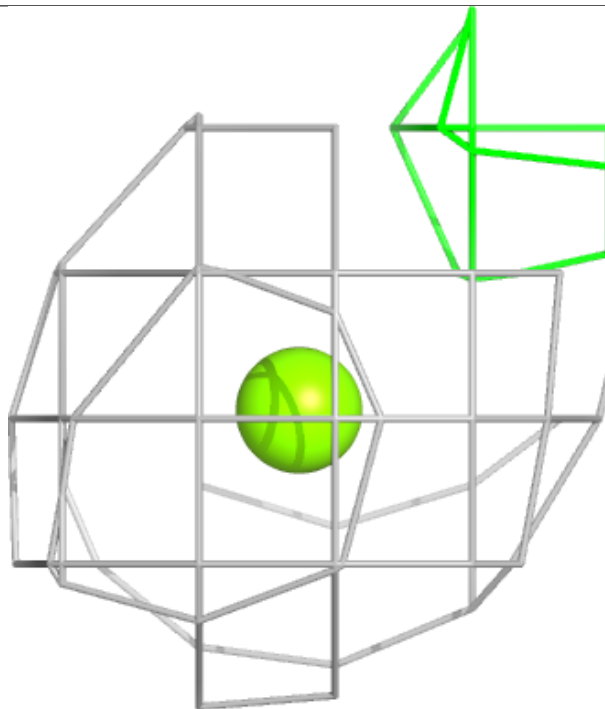
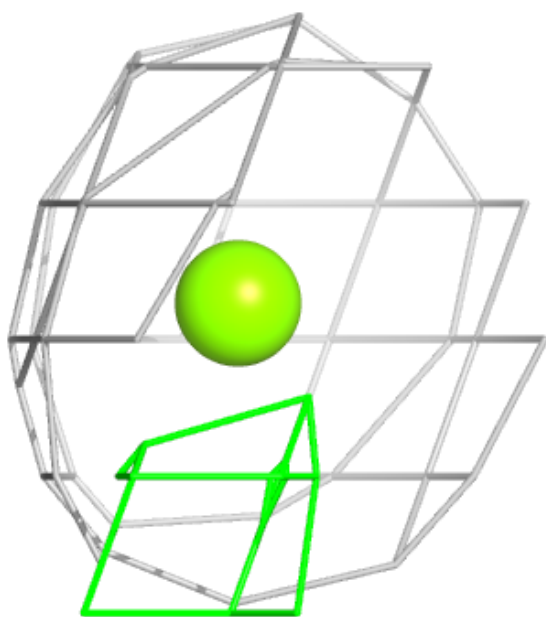
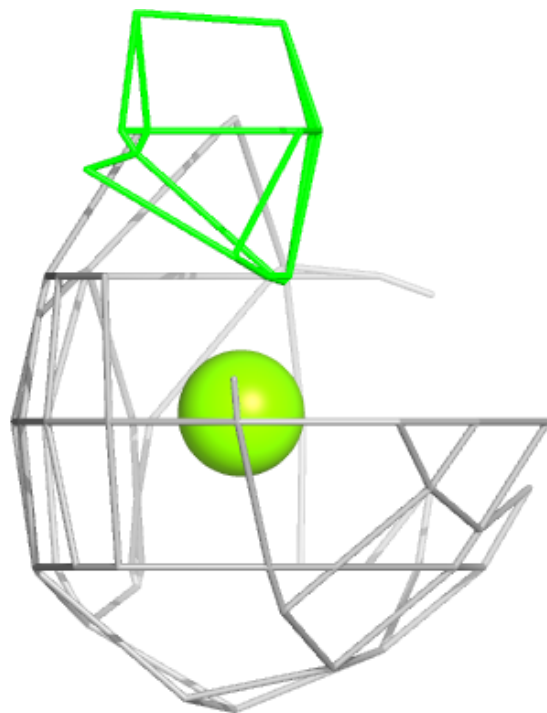
Electron density around PGE I 301:

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



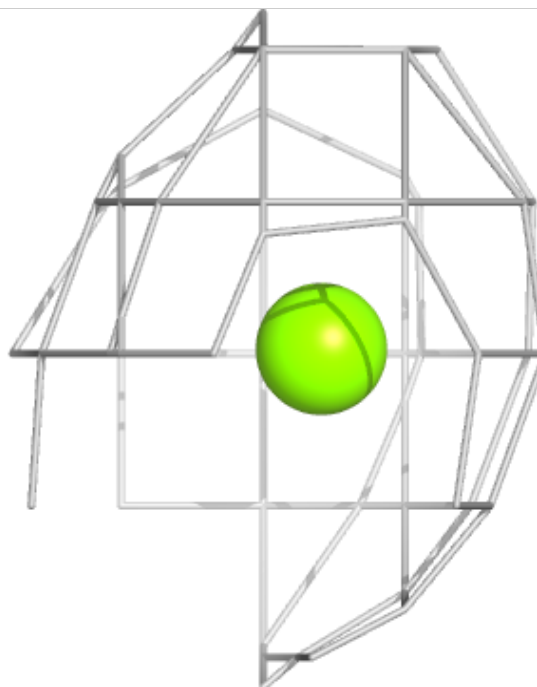
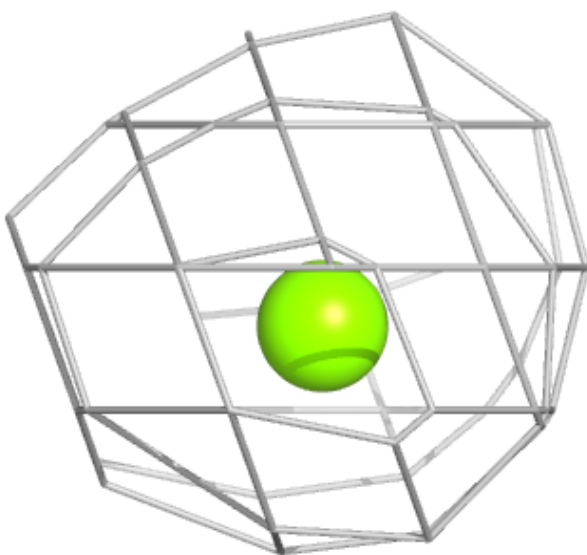
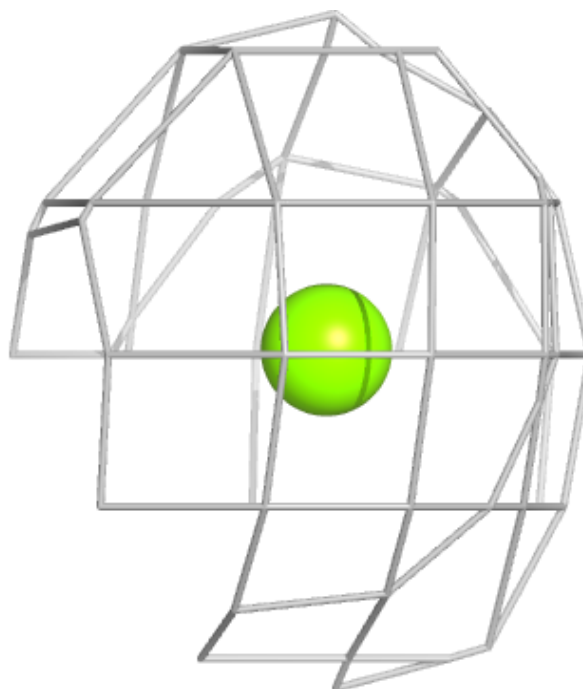
Electron density around MG C 304:

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



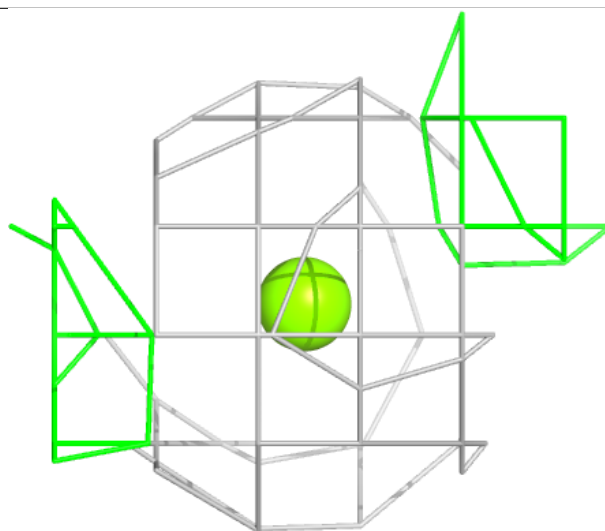
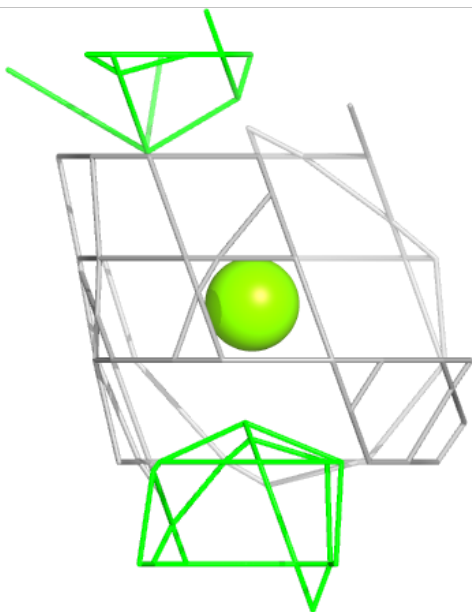
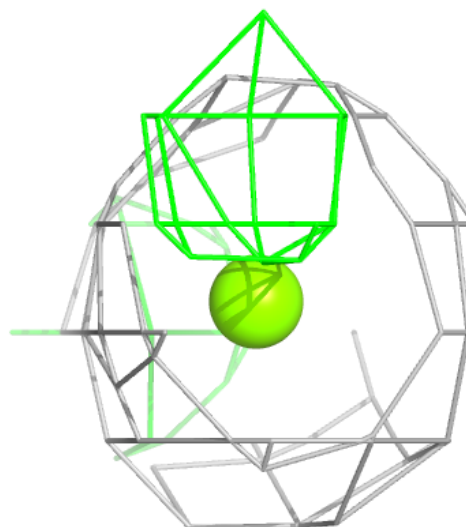
Electron density around MG J 302:

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



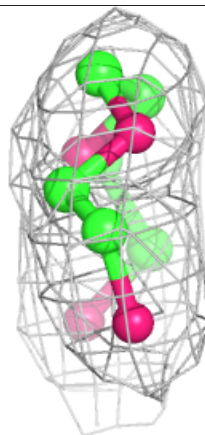
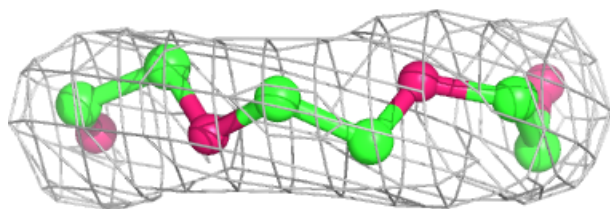
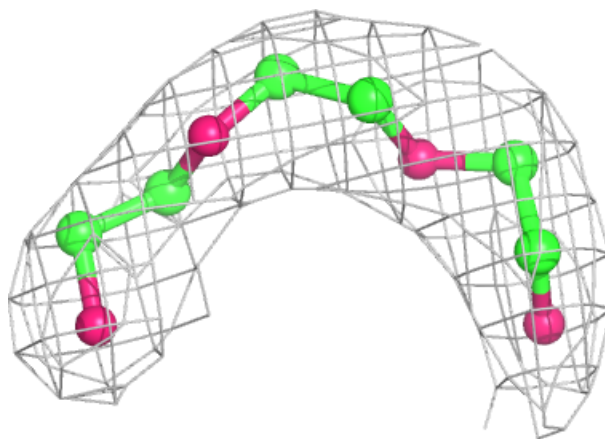
Electron density around MG A 302:

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



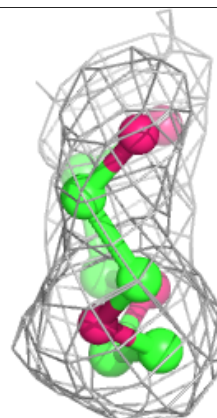
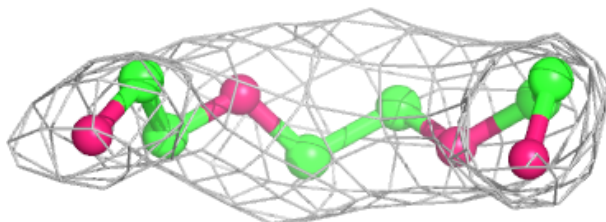
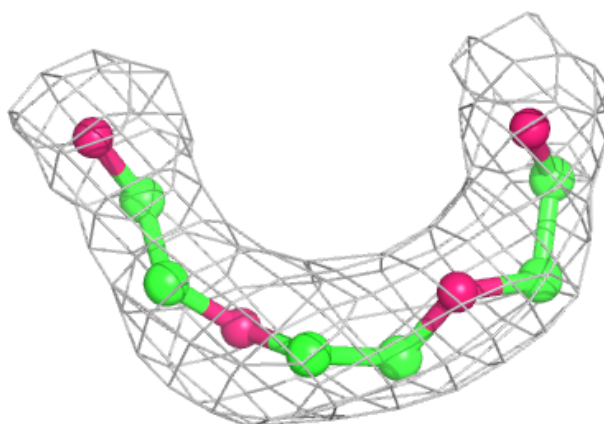
Electron density around PGE H 301:

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

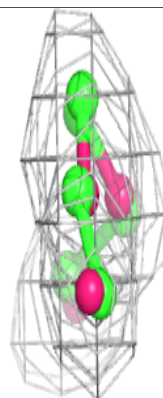
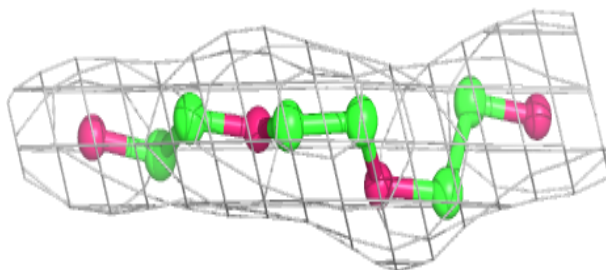
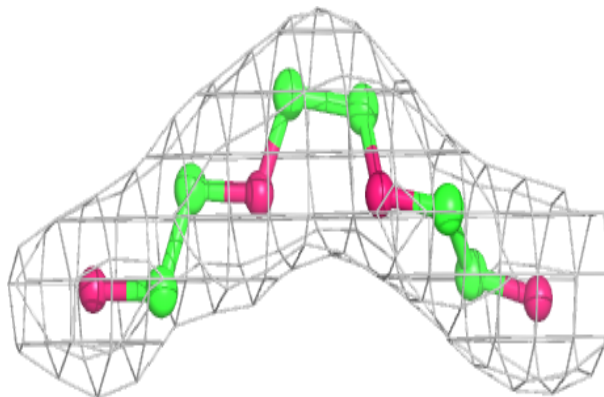


Electron density around PGE J 301:

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

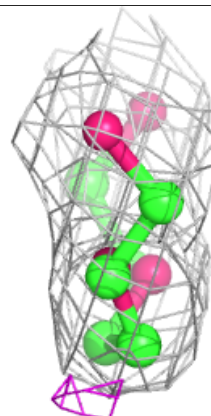
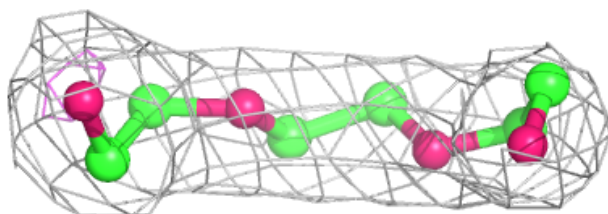
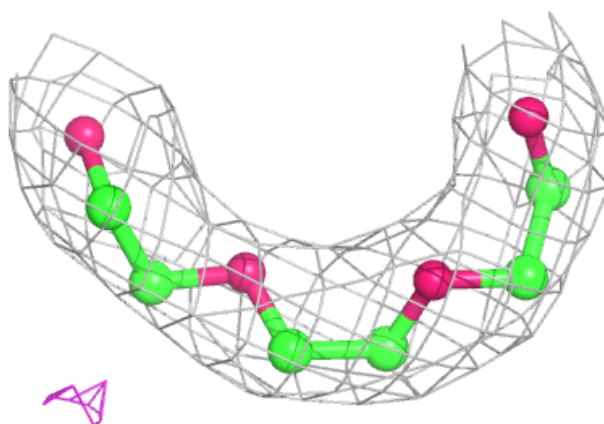
**Electron density around PGE C 302:**

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



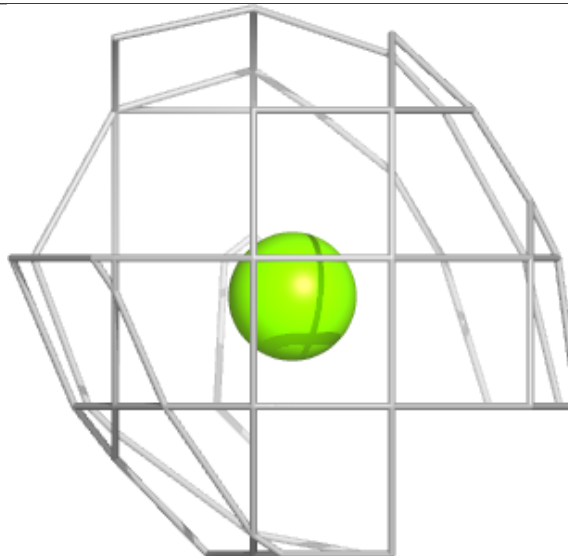
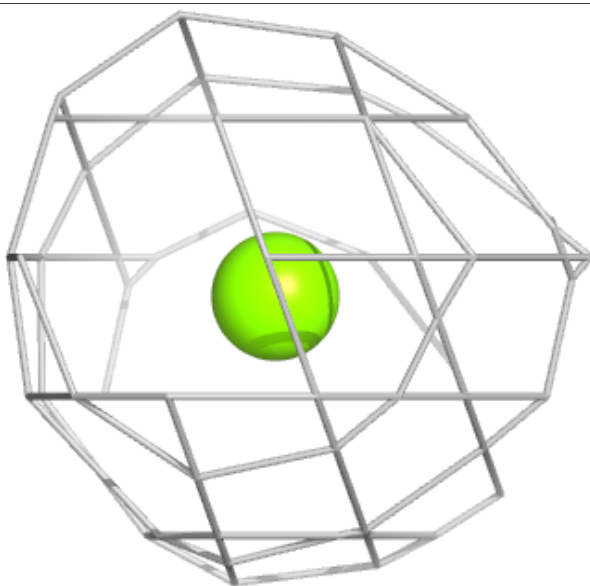
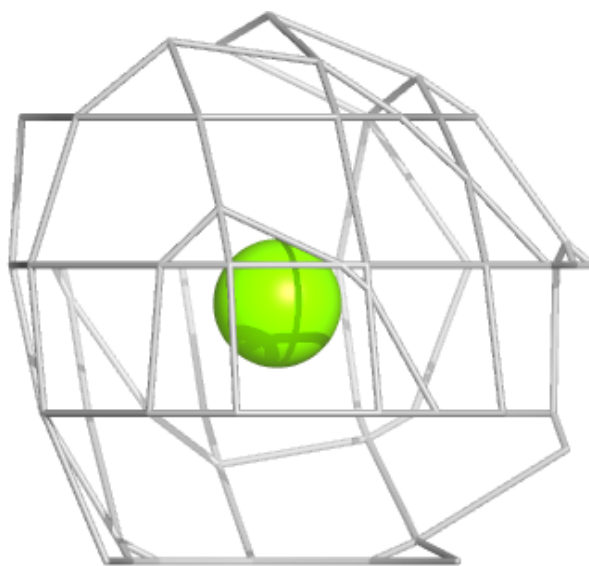
Electron density around PGE F 301:

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



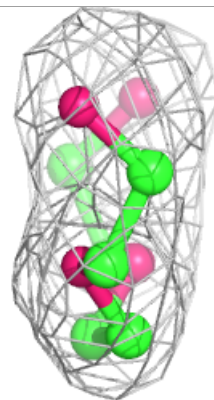
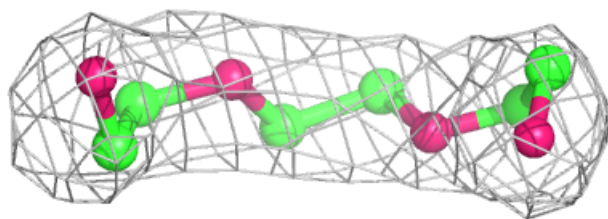
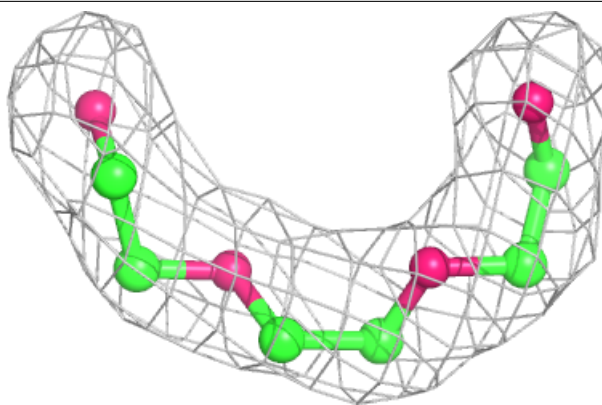
Electron density around MG E 303:

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



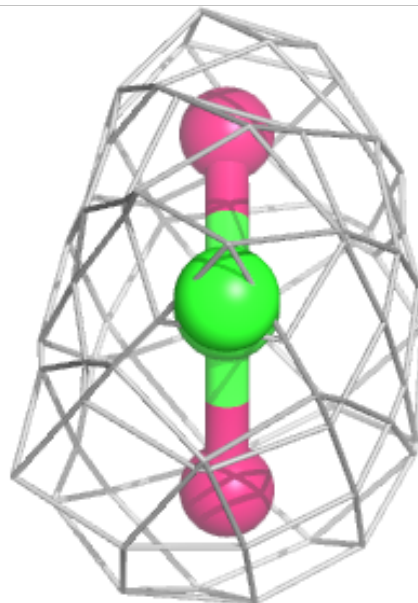
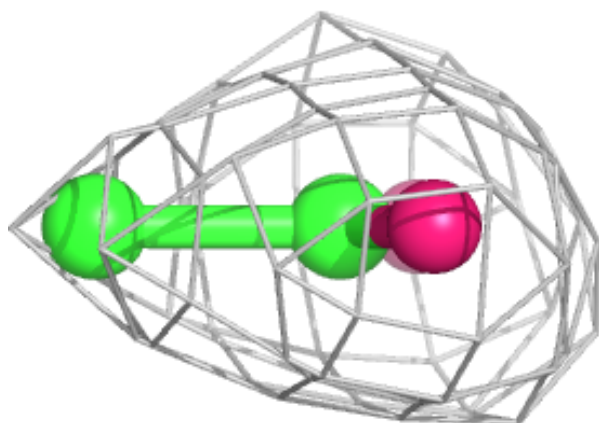
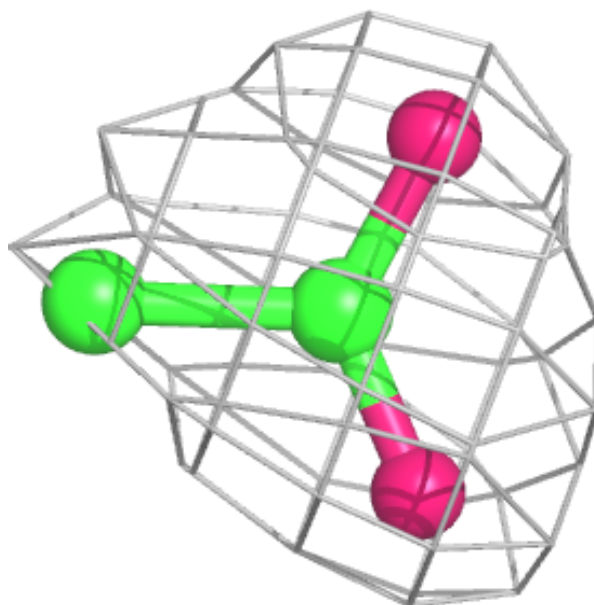
Electron density around PGE G 301:

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



Electron density around ACT F 303:

$2mF_o-DF_c$ (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.