



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2023 – 02:09 PM JST

PDB ID : 8I8L  
Title : Crystal structure of the ternary complex of Phosphopantetheine adenylyltransferase (PPAT) from *Enterobacter* sp. with Coenzyme-A and Phosphonoacetic acid at 2.23 Å resolution.  
Authors : Ahmad, N.; Sharma, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2023-02-04  
Resolution : 2.23 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.32.1  
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) : 2.32.1

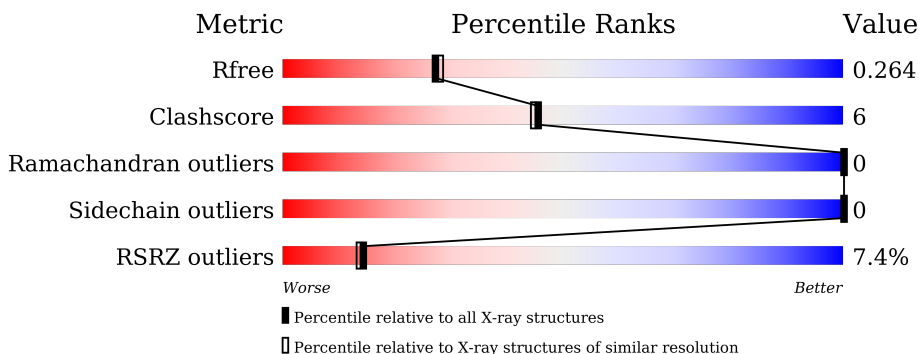
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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.



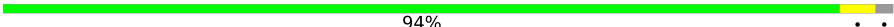
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	166	
1	B	166	
1	C	166	
1	D	166	
1	E	166	

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Mol	Chain	Length	Quality of chain
1	F	166	 94%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8142 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1246	796	216	224	10	0	0	0
1	B	166	1291	823	226	232	10	0	0	0
1	C	159	1246	796	216	224	10	0	0	0
1	D	159	1246	796	216	224	10	0	0	0
1	E	159	1246	796	216	224	10	0	0	0
1	F	163	1272	810	223	229	10	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

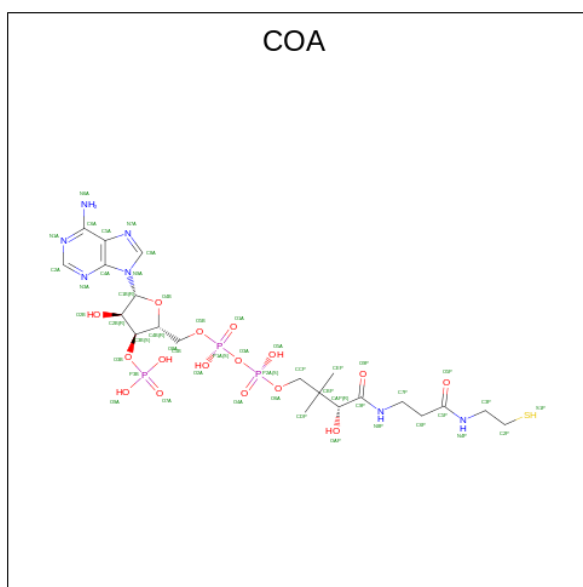
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A4W515
A	-5	LEU	-	expression tag	UNP A4W515
A	-4	VAL	-	expression tag	UNP A4W515
A	-3	ALA	-	expression tag	UNP A4W515
A	-2	ARG	-	expression tag	UNP A4W515
A	-1	GLY	-	expression tag	UNP A4W515
A	0	SER	-	expression tag	UNP A4W515
B	-6	GLY	-	expression tag	UNP A4W515
B	-5	LEU	-	expression tag	UNP A4W515
B	-4	VAL	-	expression tag	UNP A4W515
B	-3	ALA	-	expression tag	UNP A4W515
B	-2	ARG	-	expression tag	UNP A4W515
B	-1	GLY	-	expression tag	UNP A4W515
B	0	SER	-	expression tag	UNP A4W515
C	-6	GLY	-	expression tag	UNP A4W515
C	-5	LEU	-	expression tag	UNP A4W515
C	-4	VAL	-	expression tag	UNP A4W515

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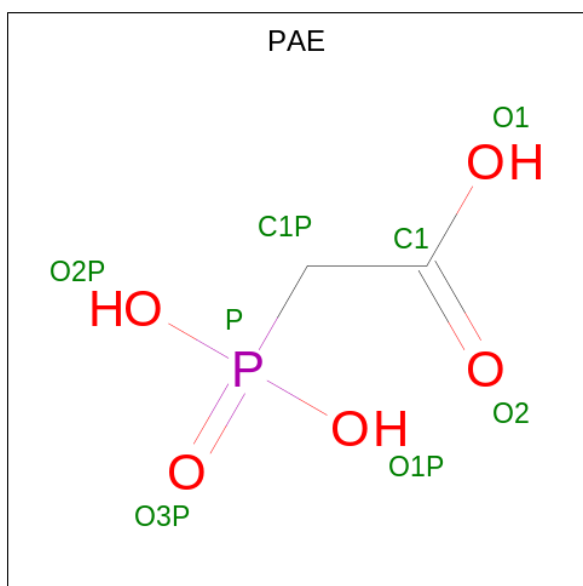
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ALA	-	expression tag	UNP A4W515
C	-2	ARG	-	expression tag	UNP A4W515
C	-1	GLY	-	expression tag	UNP A4W515
C	0	SER	-	expression tag	UNP A4W515
D	-6	GLY	-	expression tag	UNP A4W515
D	-5	LEU	-	expression tag	UNP A4W515
D	-4	VAL	-	expression tag	UNP A4W515
D	-3	ALA	-	expression tag	UNP A4W515
D	-2	ARG	-	expression tag	UNP A4W515
D	-1	GLY	-	expression tag	UNP A4W515
D	0	SER	-	expression tag	UNP A4W515
E	-6	GLY	-	expression tag	UNP A4W515
E	-5	LEU	-	expression tag	UNP A4W515
E	-4	VAL	-	expression tag	UNP A4W515
E	-3	ALA	-	expression tag	UNP A4W515
E	-2	ARG	-	expression tag	UNP A4W515
E	-1	GLY	-	expression tag	UNP A4W515
E	0	SER	-	expression tag	UNP A4W515
F	-6	GLY	-	expression tag	UNP A4W515
F	-5	LEU	-	expression tag	UNP A4W515
F	-4	VAL	-	expression tag	UNP A4W515
F	-3	ALA	-	expression tag	UNP A4W515
F	-2	ARG	-	expression tag	UNP A4W515
F	-1	GLY	-	expression tag	UNP A4W515
F	0	SER	-	expression tag	UNP A4W515

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	48	21	7	16	3	1	0	0
2	E	1	48	21	7	16	3	1	0	0

- Molecule 3 is PHOSPHONOACETIC ACID (three-letter code: PAE) (formula:  $C_2H_5O_5P$ ) (labeled as "Ligand of Interest" by depositor).



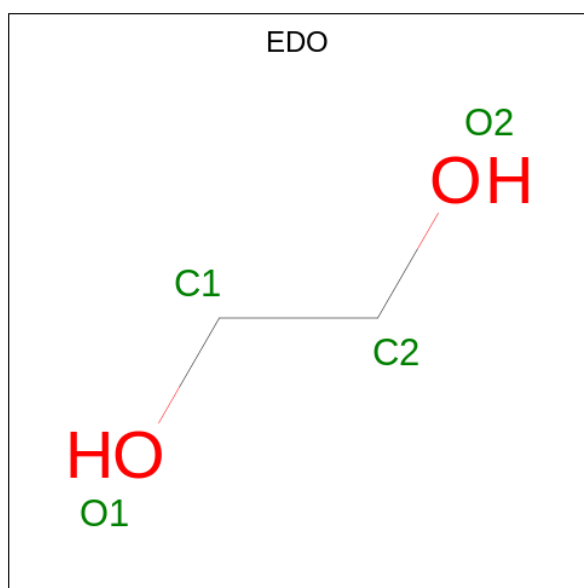
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
3	A	1	8	2	5	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	B	1	8	2	5	1	0	0
3	C	1	8	2	5	1	0	0
3	D	1	8	2	5	1	0	0
3	E	1	8	2	5	1	0	0
3	F	1	8	2	5	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

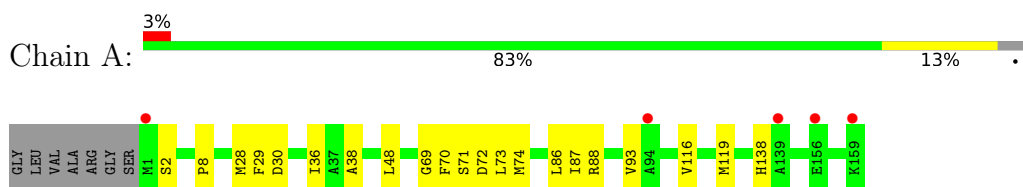
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	81	Total O 81 81	0	0
6	B	105	Total O 105 105	0	0
6	C	31	Total O 31 31	0	0
6	D	43	Total O 43 43	0	0
6	E	78	Total O 78 78	0	0
6	F	97	Total O 97 97	0	0



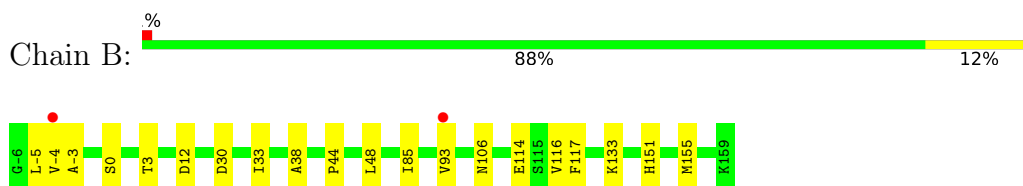
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

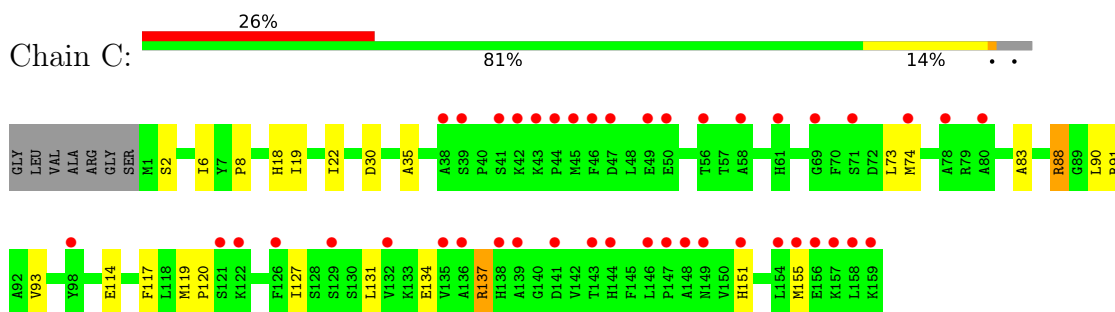
- Molecule 1: Phosphopantetheine adenylyltransferase



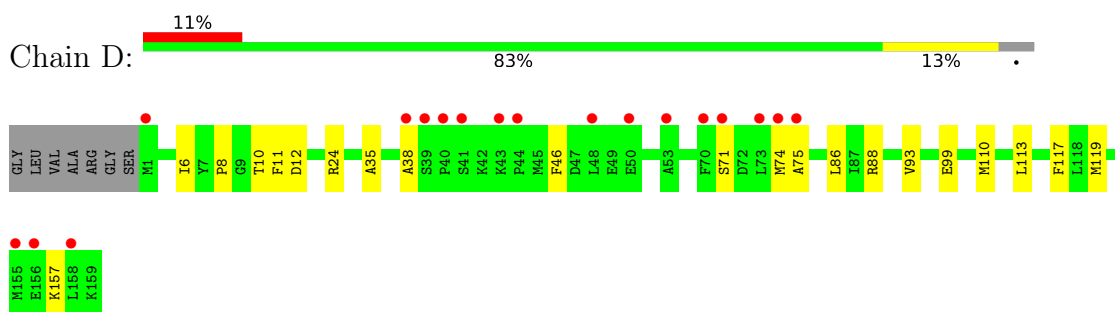
- Molecule 1: Phosphopantetheine adenylyltransferase



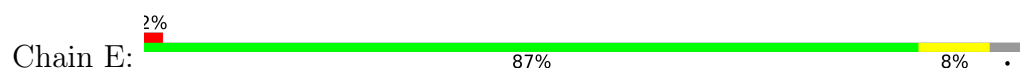
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



• Molecule 1: Phosphopantetheine adenylyltransferase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.93Å 78.62Å 106.98Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	42.63 – 2.23 42.63 – 2.23	Depositor EDS
% Data completeness (in resolution range)	95.9 (42.63-2.23) 95.9 (42.63-2.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, $R_{free}$	0.217 , 0.261 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	2677 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.013 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.023 for 1/2*h+3/2*k,1/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAE, GOL, EDO, COA

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	0.38	0/1273	0.73	0/1722
1	B	0.41	0/1318	0.76	0/1782
1	C	0.30	0/1273	0.68	0/1722
1	D	0.32	0/1273	0.67	0/1722
1	E	0.39	0/1273	0.73	0/1722
1	F	0.41	0/1299	0.69	0/1756
All	All	0.37	0/7709	0.71	0/10426

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	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	137	ARG	Sidechain
1	C	88	ARG	Sidechain

## 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	1246	0	1260	24	0
1	B	1291	0	1309	17	0
1	C	1246	0	1260	24	0
1	D	1246	0	1260	18	0
1	E	1246	0	1260	11	0
1	F	1272	0	1286	6	0
2	A	48	0	32	12	0
2	E	48	0	32	7	0
3	A	8	0	2	0	0
3	B	8	0	2	2	0
3	C	8	0	2	0	0
3	D	8	0	2	0	0
3	E	8	0	2	0	0
3	F	8	0	2	1	0
4	B	4	0	6	0	0
5	B	6	0	8	1	0
5	F	6	0	8	0	0
6	A	81	0	0	2	0
6	B	105	0	0	5	0
6	C	31	0	0	1	0
6	D	43	0	0	0	0
6	E	78	0	0	3	0
6	F	97	0	0	3	0
All	All	8142	0	7733	98	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 6.

All (98) 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:73:LEU:HA	2:A:201:COA:CDP	2.02	0.89
2:E:202:COA:O9A	2:E:202:COA:O2A	1.97	0.82
1:B:114:GLU:HG3	6:B:303:HOH:O	1.79	0.82
1:A:73:LEU:HA	2:A:201:COA:H131	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:PAE:O1P	6:B:301:HOH:O	2.00	0.78
1:A:70:PHE:O	2:A:201:COA:H62	1.88	0.73
1:B:-5:LEU:HD23	1:B:-5:LEU:O	1.89	0.73
1:B:-4:VAL:O	6:B:302:HOH:O	2.06	0.73
3:B:203:PAE:P	6:B:301:HOH:O	2.52	0.66
2:E:202:COA:H133	2:E:202:COA:H72	1.79	0.65
1:E:72:ASP:OD1	6:E:301:HOH:O	2.14	0.64
1:B:33:ILE:HD11	6:B:330:HOH:O	1.98	0.62
1:D:38:ALA:HB2	1:D:71:SER:HB3	1.82	0.62
1:E:15:THR:O	1:E:19:ILE:HG12	1.99	0.62
1:A:30:ASP:HA	1:B:0:SER:HB2	1.84	0.60
1:E:30:ASP:HA	1:F:0:SER:HB2	1.83	0.60
6:A:378:HOH:O	1:B:-3:ALA:HB2	2.01	0.59
1:D:88:ARG:HB2	1:D:117:PHE:CD1	2.38	0.59
1:B:106:ASN:OD1	5:B:202:GOL:C1	2.53	0.57
1:A:71:SER:HA	2:A:201:COA:C6P	2.35	0.57
1:C:127:ILE:O	1:C:127:ILE:HG13	2.04	0.56
1:A:71:SER:HA	2:A:201:COA:H62	1.88	0.56
1:A:74:MET:H	2:A:201:COA:H132	1.72	0.55
1:F:108:HIS:CE1	6:F:337:HOH:O	2.61	0.54
1:C:2:SER:HA	1:C:30:ASP:OD2	2.08	0.54
1:C:93:VAL:HG22	1:D:93:VAL:HG13	1.89	0.53
2:E:202:COA:O4A	2:E:202:COA:H4B	2.07	0.53
1:E:121:SER:HB3	6:E:322:HOH:O	2.10	0.51
1:C:151:HIS:O	1:C:155:MET:HG2	2.11	0.51
1:A:86:LEU:C	1:A:86:LEU:HD23	2.31	0.51
1:C:90:LEU:O	1:C:120:PRO:HD3	2.10	0.51
1:A:138:HIS:HB2	1:C:73:LEU:HG	1.93	0.51
1:E:73:LEU:HA	2:E:202:COA:O5A	2.11	0.50
1:D:10:THR:HG22	1:D:12:ASP:HB2	1.94	0.50
1:D:74:MET:O	1:D:75:ALA:HB3	2.12	0.50
1:F:158:LEU:O	1:F:159:LYS:C	2.50	0.50
1:B:3:THR:O	1:B:30:ASP:HB2	2.12	0.49
1:F:-3:ALA:N	6:F:306:HOH:O	2.40	0.49
1:C:114:GLU:OE2	1:D:24:ARG:NE	2.43	0.48
1:D:88:ARG:NH2	1:D:99:GLU:OE2	2.46	0.48
1:E:8:PRO:HA	1:E:35:ALA:O	2.14	0.48
1:D:46:PHE:CE1	1:D:157:LYS:HG3	2.49	0.48
1:C:8:PRO:HA	1:C:35:ALA:O	2.14	0.47
1:C:88:ARG:HB2	1:C:117:PHE:CD1	2.50	0.47
1:A:72:ASP:OD1	6:A:301:HOH:O	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HG2	1:B:117:PHE:CE2	2.50	0.46
1:C:93:VAL:HG22	1:D:93:VAL:CG1	2.46	0.46
1:D:8:PRO:HA	1:D:35:ALA:O	2.15	0.46
1:A:38:ALA:HA	1:A:48:LEU:HD13	1.97	0.46
1:A:36:ILE:O	1:A:69:GLY:HA2	2.16	0.46
1:A:28:MET:HE3	1:B:114:GLU:HG2	1.98	0.46
1:F:3:THR:O	1:F:30:ASP:HB2	2.16	0.46
1:B:12:ASP:OD2	1:B:133:LYS:NZ	2.49	0.45
1:C:19:ILE:HA	1:C:22:ILE:HD12	1.97	0.45
1:E:71:SER:HB2	2:E:202:COA:O5P	2.17	0.45
1:E:93:VAL:O	1:E:96:PHE:HB3	2.17	0.45
1:A:70:PHE:CE2	2:A:201:COA:H71	2.52	0.45
1:C:18:HIS:O	1:C:22:ILE:HG13	2.17	0.45
1:A:2:SER:HA	1:A:30:ASP:OD2	2.17	0.44
1:D:110:MET:HG2	1:D:113:LEU:HB2	1.99	0.44
1:C:90:LEU:O	1:C:120:PRO:CD	2.65	0.44
1:C:127:ILE:HA	1:C:131:LEU:HD22	2.00	0.44
1:D:10:THR:O	1:D:11:PHE:C	2.56	0.44
1:D:119:MET:HE3	1:D:119:MET:HB2	1.90	0.43
2:E:202:COA:H51A	2:E:202:COA:H8A	2.01	0.43
1:E:74:MET:N	2:E:202:COA:O5A	2.47	0.43
1:B:38:ALA:CB	1:B:48:LEU:HD22	2.48	0.43
1:C:134:GLU:HA	1:C:134:GLU:OE1	2.19	0.43
3:F:202:PAE:H11	6:F:345:HOH:O	2.18	0.42
1:A:88:ARG:NH2	2:A:201:COA:H51A	2.35	0.42
1:B:151:HIS:O	1:B:155:MET:HG2	2.19	0.42
1:D:88:ARG:HB2	1:D:117:PHE:CE1	2.54	0.42
1:E:38:ALA:HA	1:E:48:LEU:HD13	2.01	0.42
1:C:134:GLU:OE1	1:C:137:ARG:HD3	2.18	0.42
1:C:127:ILE:HA	1:C:131:LEU:CD2	2.50	0.42
1:B:3:THR:HB	1:B:85:ILE:CD1	2.50	0.42
1:C:91:ARG:HH21	1:C:91:ARG:HG2	1.85	0.41
1:C:114:GLU:HG3	6:C:302:HOH:O	2.19	0.41
1:A:73:LEU:HA	2:A:201:COA:H132	1.97	0.41
1:C:6:ILE:HG23	1:C:83:ALA:CB	2.50	0.41
1:C:127:ILE:O	1:C:127:ILE:CG1	2.67	0.41
1:D:74:MET:HA	1:D:74:MET:HE2	2.02	0.41
1:D:110:MET:HG2	1:D:110:MET:O	2.20	0.41
1:A:8:PRO:HB3	1:A:74:MET:HE1	2.03	0.41
1:A:71:SER:HA	2:A:201:COA:H61	2.03	0.41
1:C:8:PRO:HB3	1:C:74:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:CG1	1:B:93:VAL:HG13	2.49	0.41
2:A:201:COA:H61	2:A:201:COA:H32	1.84	0.41
1:D:6:ILE:HG23	1:D:86:LEU:HD13	2.03	0.41
1:C:119:MET:HG2	1:D:117:PHE:CE2	2.55	0.41
1:A:29:PHE:HE2	1:A:87:ILE:HD11	1.85	0.41
1:A:116:VAL:HG13	1:B:116:VAL:HG13	2.03	0.40
1:E:8:PRO:HB3	1:E:74:MET:HE3	2.03	0.40
1:A:8:PRO:HB3	1:A:74:MET:CE	2.52	0.40
2:A:201:COA:O2A	2:A:201:COA:O4A	2.39	0.40
1:F:159:LYS:HG3	1:F:159:LYS:O	2.21	0.40
1:B:44:PRO:HD2	6:E:358:HOH:O	2.21	0.40
1:C:90:LEU:HD21	1:C:117:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

## 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	157/166 (95%)	157 (100%)	0	0	100	100
1	B	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	C	157/166 (95%)	152 (97%)	5 (3%)	0	100	100
1	D	157/166 (95%)	154 (98%)	3 (2%)	0	100	100
1	E	157/166 (95%)	154 (98%)	3 (2%)	0	100	100
1	F	161/166 (97%)	159 (99%)	2 (1%)	0	100	100
All	All	953/996 (96%)	938 (98%)	15 (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	134/138 (97%)	134 (100%)	0	100	100
1	B	138/138 (100%)	138 (100%)	0	100	100
1	C	134/138 (97%)	134 (100%)	0	100	100
1	D	134/138 (97%)	134 (100%)	0	100	100
1	E	134/138 (97%)	134 (100%)	0	100	100
1	F	136/138 (99%)	136 (100%)	0	100	100
All	All	810/828 (98%)	810 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	81	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	201	-	3,3,3	0.22	0	2,2,2	0.38	0
3	PAE	B	203	-	7,7,7	1.48	1 (14%)	9,10,10	1.87	1 (11%)
5	GOL	F	201	-	5,5,5	0.13	0	5,5,5	0.30	0
2	COA	E	202	-	41,50,50	0.66	0	52,75,75	1.35	6 (11%)
3	PAE	A	202	-	7,7,7	1.06	1 (14%)	9,10,10	1.34	1 (11%)
3	PAE	F	202	-	7,7,7	1.25	1 (14%)	9,10,10	1.95	3 (33%)
3	PAE	D	201	-	7,7,7	1.04	0	9,10,10	1.67	3 (33%)
3	PAE	E	201	-	7,7,7	1.62	2 (28%)	9,10,10	1.91	3 (33%)
2	COA	A	201	-	41,50,50	0.70	1 (2%)	52,75,75	1.06	4 (7%)
5	GOL	B	202	-	5,5,5	0.15	0	5,5,5	0.46	0
3	PAE	C	201	-	7,7,7	2.17	3 (42%)	9,10,10	1.25	1 (11%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	201	-	-	1/1/1/1	-
3	PAE	B	203	-	-	0/5/5/5	-
5	GOL	F	201	-	-	4/4/4/4	-
2	COA	E	202	-	-	20/44/64/64	0/3/3/3
3	PAE	A	202	-	-	0/5/5/5	-
3	PAE	F	202	-	-	0/5/5/5	-
3	PAE	D	201	-	-	2/5/5/5	-
3	PAE	E	201	-	-	2/5/5/5	-
2	COA	A	201	-	-	23/44/64/64	0/3/3/3
5	GOL	B	202	-	-	2/4/4/4	-
3	PAE	C	201	-	-	3/5/5/5	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	PAE	C1P-C1	3.69	1.55	1.51
3	C	201	PAE	P-C1P	3.07	1.84	1.79
2	A	201	COA	P3B-O3B	2.57	1.64	1.59
3	B	203	PAE	P-O3P	2.48	1.55	1.50
3	E	201	PAE	P-C1P	2.48	1.83	1.79
3	F	202	PAE	O1-C1	-2.38	1.22	1.30
3	E	201	PAE	P-O1P	-2.15	1.50	1.54
3	C	201	PAE	P-O1P	-2.03	1.50	1.54
3	A	202	PAE	O1-C1	-2.02	1.23	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	PAE	O3P-P-C1P	-4.50	100.67	110.94
2	E	202	COA	C7P-C6P-C5P	4.32	119.55	112.36
3	F	202	PAE	O1P-P-C1P	3.99	115.21	106.84
3	E	201	PAE	O1P-P-C1P	3.56	114.31	106.84
2	E	202	COA	C7P-N8P-C9P	3.16	128.23	122.59
3	F	202	PAE	O2P-P-C1P	-3.14	100.24	106.84
2	E	202	COA	CEP-CBP-CCP	3.05	113.21	108.23
3	E	201	PAE	O3P-P-C1P	-2.98	104.14	110.94
2	E	202	COA	CDP-CBP-CAP	2.87	113.79	108.82
2	A	201	COA	O5A-P2A-O4A	2.71	125.66	112.24
3	D	201	PAE	O2-C1-C1P	-2.68	116.31	122.53
2	A	201	COA	O2B-C2B-C3B	2.63	118.64	111.17
3	A	202	PAE	O3P-P-C1P	-2.43	105.40	110.94
3	D	201	PAE	O3P-P-C1P	-2.42	105.43	110.94
3	E	201	PAE	O2-C1-C1P	-2.34	117.09	122.53
2	E	202	COA	CAP-C9P-N8P	2.32	121.21	116.58
2	A	201	COA	O6A-CCP-CBP	-2.30	106.86	110.55
3	F	202	PAE	O3P-P-C1P	-2.29	105.72	110.94
2	E	202	COA	C5A-C6A-N6A	2.24	123.75	120.35
3	D	201	PAE	O2P-P-C1P	2.17	111.40	106.84
2	A	201	COA	C5A-C6A-N6A	2.16	123.64	120.35
3	C	201	PAE	O2P-P-C1P	2.00	111.04	106.84

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	COA	C3B-C4B-C5B-O5B
2	A	201	COA	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	201	COA	C5B-O5B-P1A-O1A
2	A	201	COA	CCP-O6A-P2A-O3A
2	A	201	COA	CAP-C9P-N8P-C7P
2	A	201	COA	C6P-C5P-N4P-C3P
2	A	201	COA	O5P-C5P-N4P-C3P
2	E	202	COA	C5B-O5B-P1A-O1A
2	E	202	COA	C5B-O5B-P1A-O2A
2	E	202	COA	CCP-O6A-P2A-O4A
2	E	202	COA	CCP-O6A-P2A-O5A
2	E	202	COA	CAP-CBP-CCP-O6A
2	E	202	COA	OAP-CAP-CBP-CCP
2	E	202	COA	OAP-CAP-CBP-CDP
2	E	202	COA	CAP-C9P-N8P-C7P
3	C	201	PAE	C1-C1P-P-O1P
3	C	201	PAE	C1-C1P-P-O2P
3	C	201	PAE	C1-C1P-P-O3P
3	D	201	PAE	O1-C1-C1P-P
2	E	202	COA	O9P-C9P-N8P-C7P
2	A	201	COA	C4B-C5B-O5B-P1A
2	A	201	COA	C2B-C3B-O3B-P3B
2	E	202	COA	CDP-CBP-CCP-O6A
2	E	202	COA	CEP-CBP-CCP-O6A
5	F	201	GOL	O1-C1-C2-C3
5	F	201	GOL	C1-C2-C3-O3
5	F	201	GOL	O1-C1-C2-O2
2	E	202	COA	C3B-C4B-C5B-O5B
4	B	201	EDO	O1-C1-C2-O2
2	A	201	COA	O9P-C9P-N8P-C7P
2	A	201	COA	OAP-CAP-CBP-CDP
2	A	201	COA	OAP-CAP-CBP-CEP
2	E	202	COA	OAP-CAP-CBP-CEP
2	A	201	COA	C4B-C3B-O3B-P3B
5	F	201	GOL	O2-C2-C3-O3
2	E	202	COA	C3B-O3B-P3B-O9A
5	B	202	GOL	O2-C2-C3-O3
2	A	201	COA	P2A-O3A-P1A-O2A
2	E	202	COA	C4B-C5B-O5B-P1A
2	A	201	COA	C5B-O5B-P1A-O2A
2	A	201	COA	CCP-O6A-P2A-O4A
2	E	202	COA	O4B-C4B-C5B-O5B
2	A	201	COA	OAP-CAP-CBP-CCP
3	D	201	PAE	O2-C1-C1P-P

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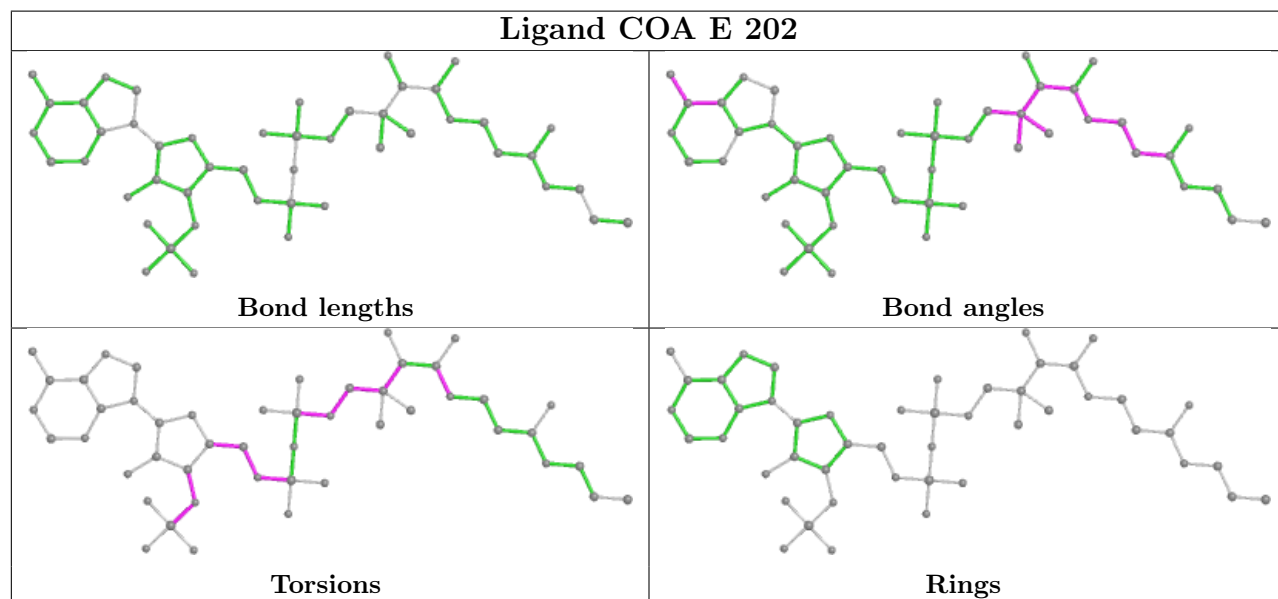
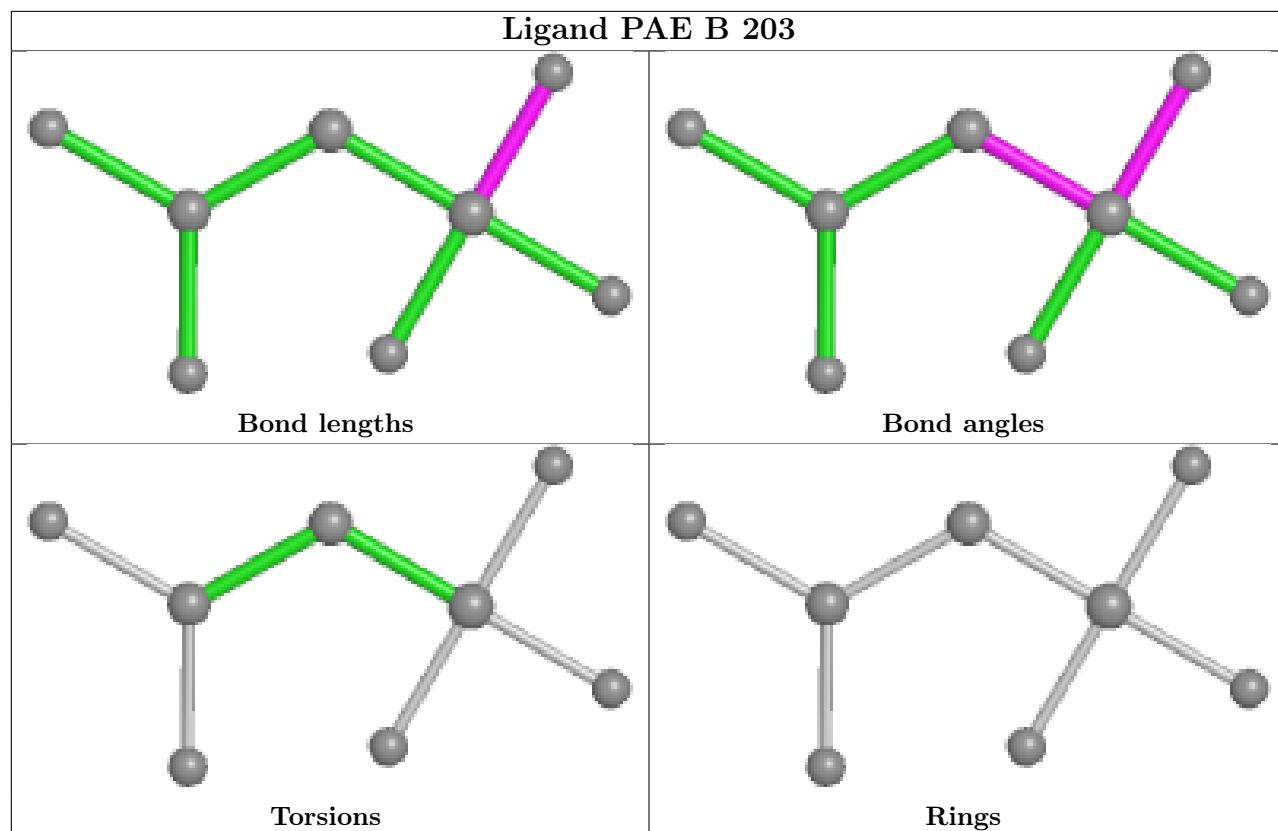
Mol	Chain	Res	Type	Atoms
3	E	201	PAE	O2-C1-C1P-P
2	E	202	COA	C4B-C3B-O3B-P3B
5	B	202	GOL	C1-C2-C3-O3
2	A	201	COA	C9P-CAP-CBP-CDP
2	A	201	COA	C9P-CAP-CBP-CEP
2	A	201	COA	O5P-C5P-C6P-C7P
2	A	201	COA	C5B-O5B-P1A-O3A
2	E	202	COA	C5B-O5B-P1A-O3A
2	E	202	COA	CCP-O6A-P2A-O3A
2	A	201	COA	P2A-O3A-P1A-O1A
2	E	202	COA	CBP-CCP-O6A-P2A
2	A	201	COA	C9P-CAP-CBP-CCP
3	E	201	PAE	O1-C1-C1P-P

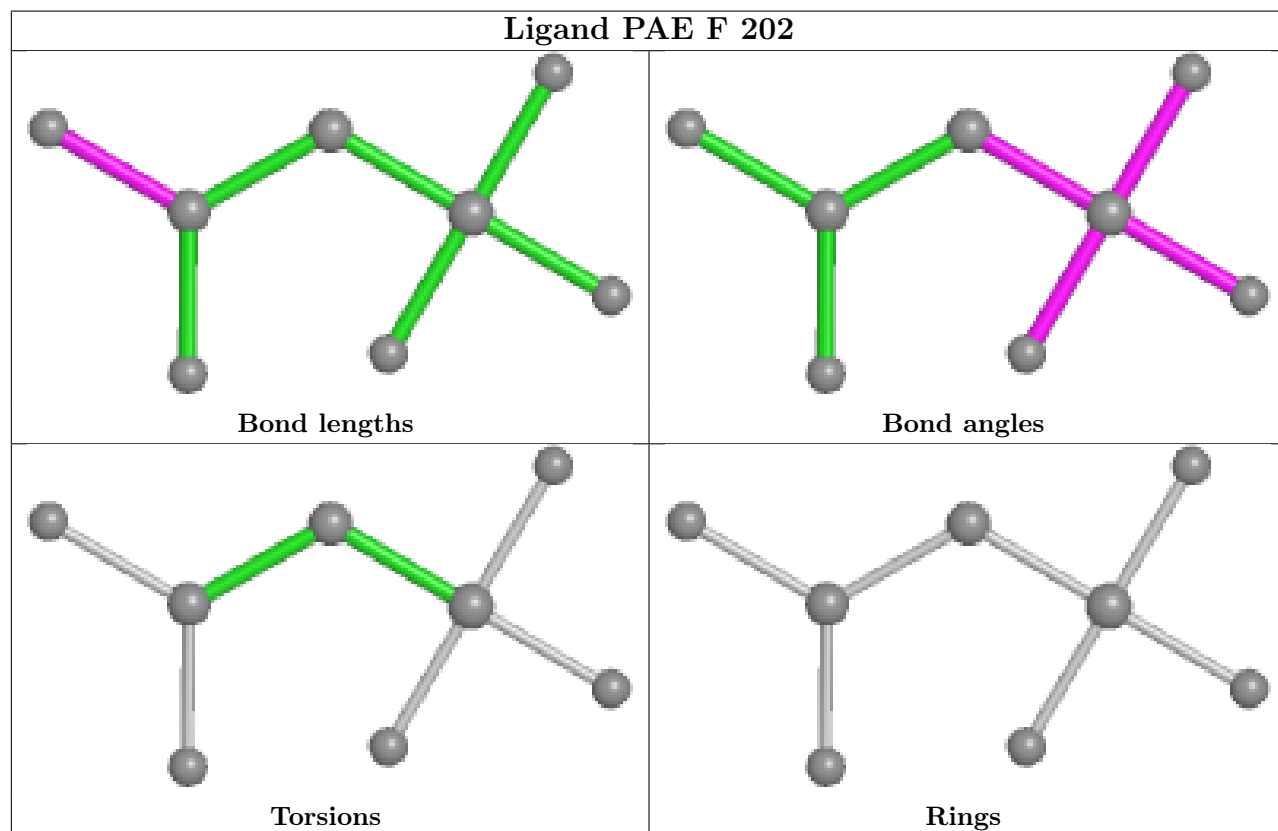
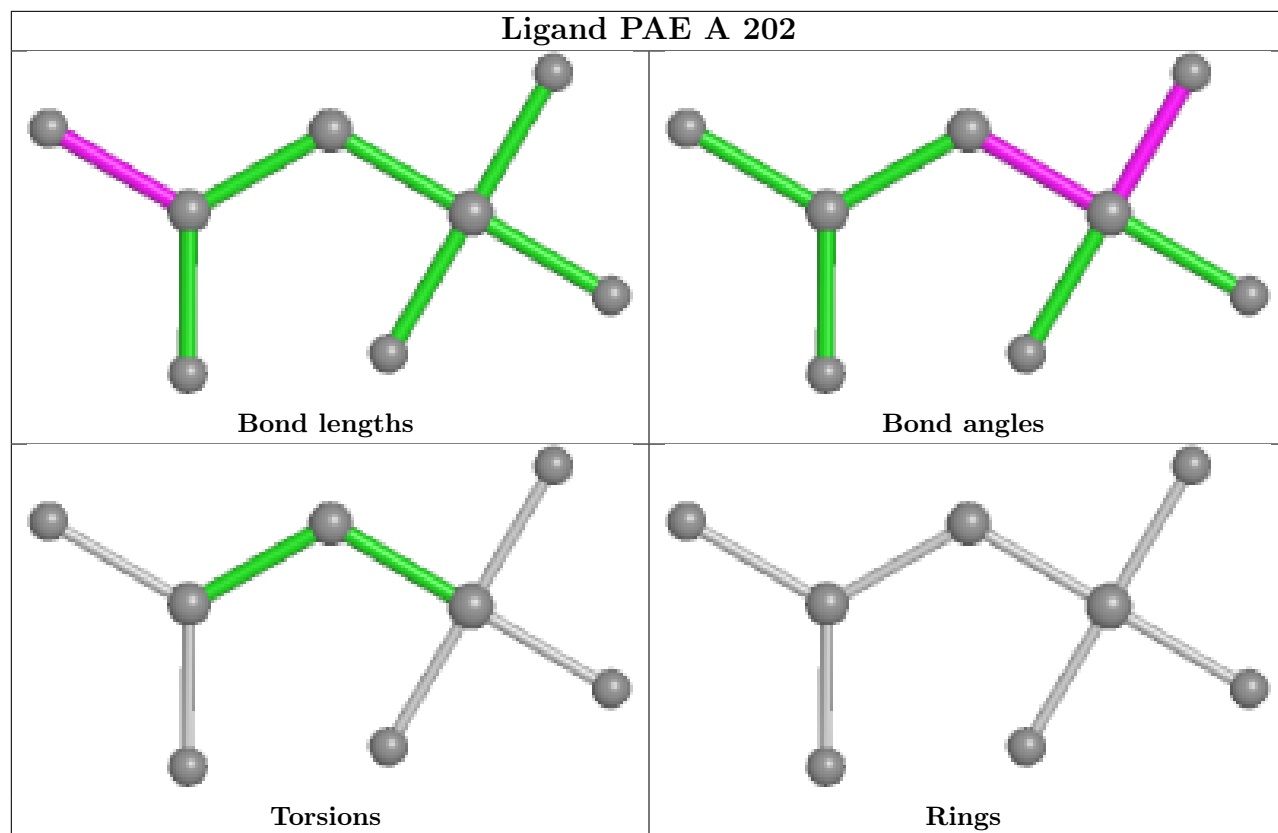
There are no ring outliers.

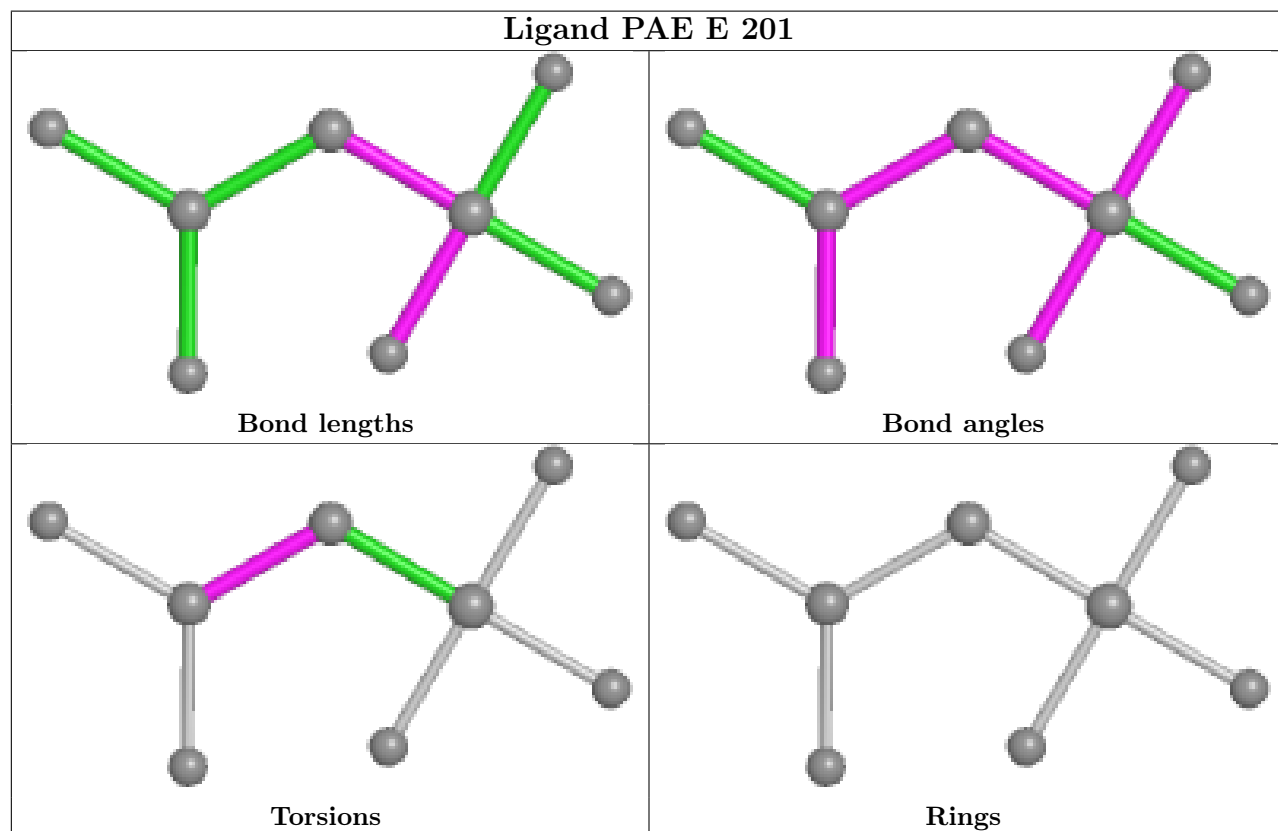
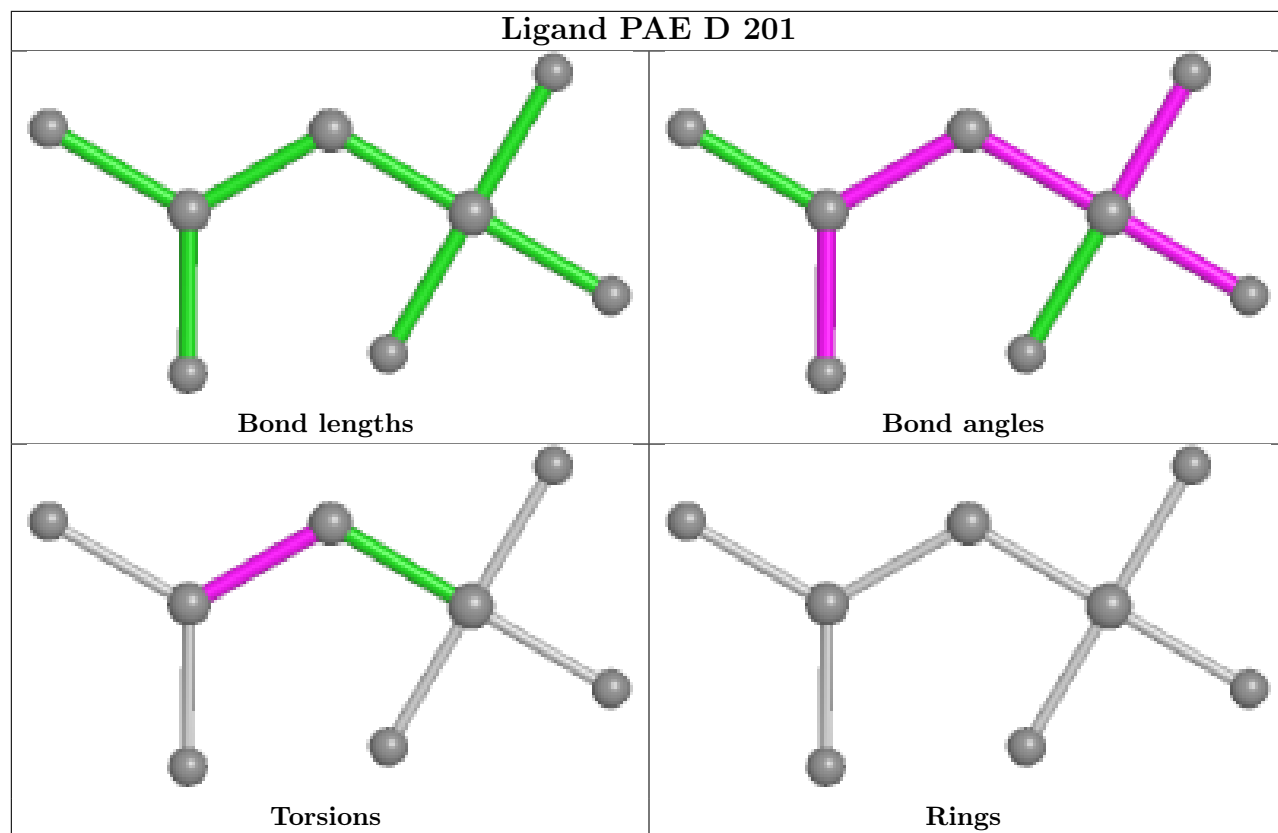
5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	PAE	2	0
2	E	202	COA	7	0
3	F	202	PAE	1	0
2	A	201	COA	12	0
5	B	202	GOL	1	0

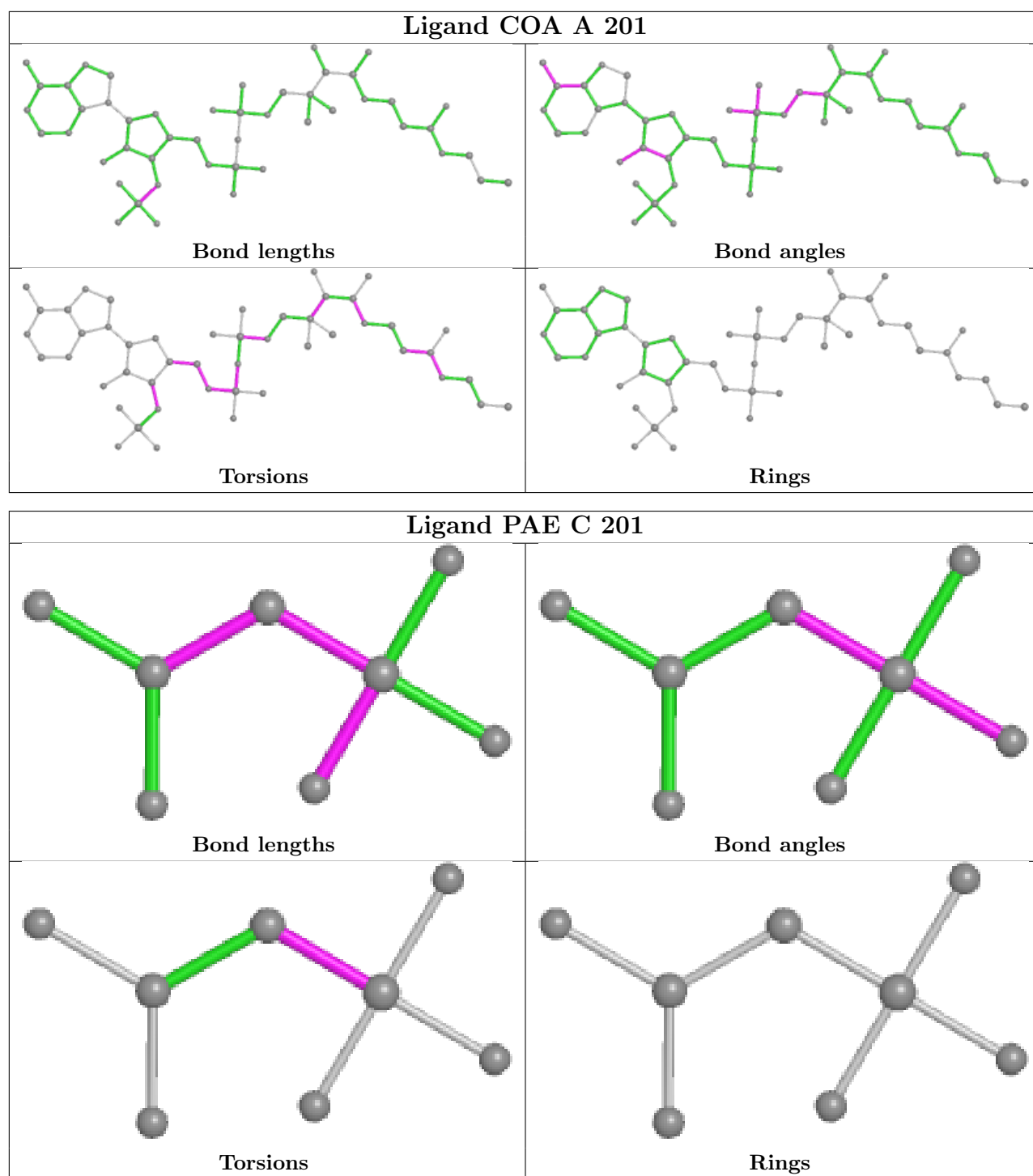
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	159/166 (95%)	0.10	5 (3%) 49 49	25, 38, 67, 95	0
1	B	166/166 (100%)	-0.13	2 (1%) 79 80	21, 31, 59, 86	0
1	C	159/166 (95%)	1.32	43 (27%) 0 0	41, 73, 113, 147	0
1	D	159/166 (95%)	0.67	18 (11%) 5 4	34, 57, 100, 163	0
1	E	159/166 (95%)	0.12	3 (1%) 66 68	22, 37, 71, 108	0
1	F	163/166 (98%)	-0.16	0 100 100	22, 33, 60, 80	0
All	All	965/996 (96%)	0.32	71 (7%) 14 14	21, 44, 92, 163	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	8.1
1	D	40	PRO	7.9
1	E	1	MET	6.7
1	C	126	PHE	6.6
1	C	136	ALA	5.6
1	D	39	SER	5.5
1	D	41	SER	5.3
1	C	39	SER	5.1
1	C	45	MET	5.1
1	C	148	ALA	4.6
1	C	44	PRO	4.6
1	C	147	PRO	4.5
1	C	155	MET	4.5
1	C	38	ALA	4.3
1	C	151	HIS	4.3
1	C	121	SER	4.2
1	C	41	SER	4.0
1	C	141	ASP	3.9
1	C	135	VAL	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	58	ALA	3.7
1	D	43	LYS	3.7
1	D	158	LEU	3.7
1	C	159	LYS	3.7
1	C	138	HIS	3.6
1	D	156	GLU	3.6
1	C	56	THR	3.6
1	C	156	GLU	3.5
1	D	75	ALA	3.4
1	C	139	ALA	3.4
1	D	48	LEU	3.4
1	D	74	MET	3.3
1	C	61	HIS	3.3
1	C	149	ASN	3.2
1	C	46	PHE	3.2
1	C	74	MET	3.2
1	D	73	LEU	3.2
1	B	-4	VAL	3.2
1	C	43	LYS	3.1
1	C	146	LEU	3.0
1	D	44	PRO	3.0
1	C	144	HIS	2.9
1	D	155	MET	2.7
1	D	38	ALA	2.7
1	C	80	ALA	2.7
1	E	126	PHE	2.7
1	A	159	LYS	2.6
1	C	98	TYR	2.6
1	C	78	ALA	2.6
1	A	1	MET	2.5
1	C	157	LYS	2.5
1	A	139	ALA	2.4
1	C	132	VAL	2.4
1	C	69	GLY	2.4
1	C	154	LEU	2.4
1	C	49	GLU	2.3
1	D	50	GLU	2.3
1	C	143	THR	2.3
1	C	47	ASP	2.3
1	C	71	SER	2.2
1	A	94	ALA	2.2
1	A	156	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	53	ALA	2.2
1	C	50	GLU	2.2
1	D	70	PHE	2.2
1	E	158	LEU	2.2
1	D	71	SER	2.2
1	C	122	LYS	2.1
1	D	1	MET	2.1
1	B	93	VAL	2.1
1	C	42	LYS	2.0
1	C	129	SER	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.

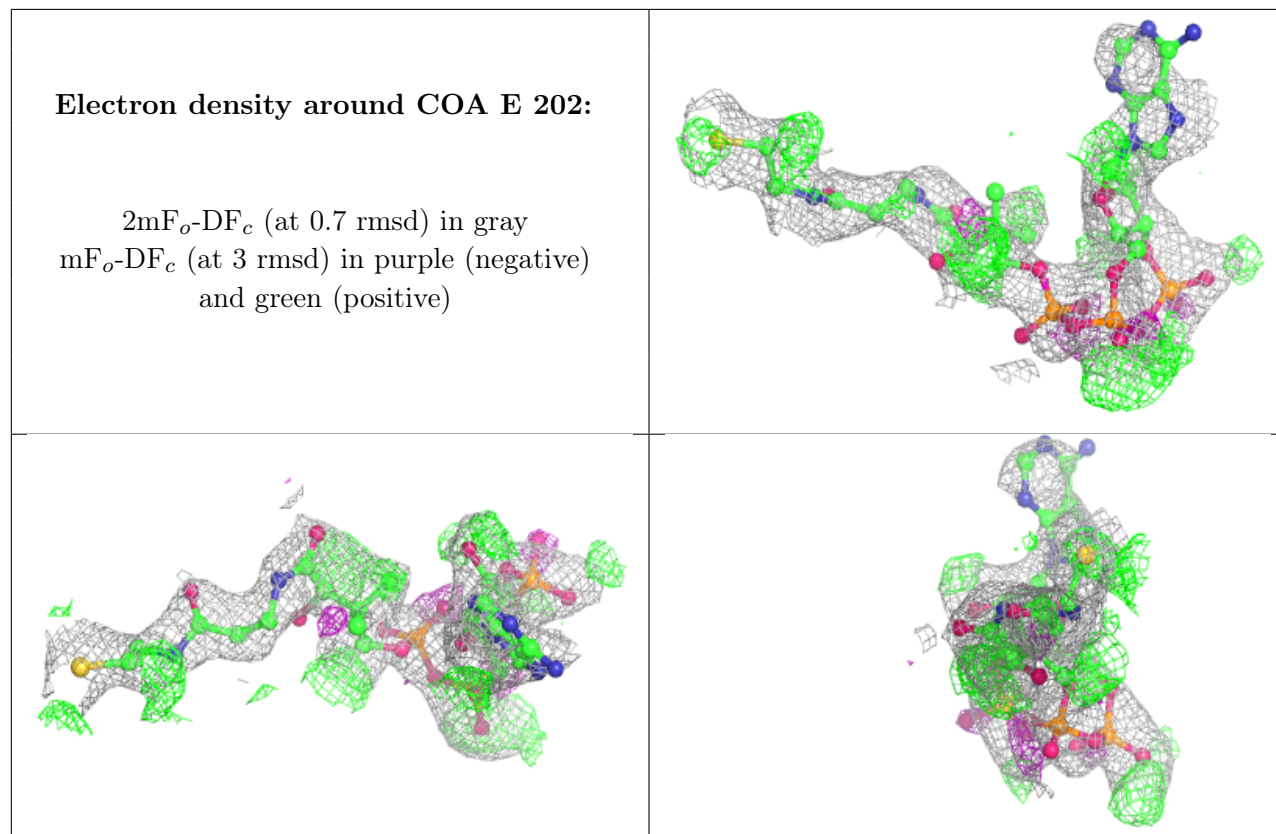
## 6.4 Ligands [i](#)

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
2	COA	E	202	48/48	0.75	0.28	35,63,82,100	48
2	COA	A	201	48/48	0.82	0.25	28,55,88,93	48
3	PAE	C	201	8/8	0.84	0.17	80,89,96,97	0
3	PAE	D	201	8/8	0.85	0.16	60,69,78,80	0
5	GOL	F	201	6/6	0.86	0.19	58,63,70,72	0
3	PAE	A	202	8/8	0.87	0.15	56,64,81,82	0
3	PAE	E	201	8/8	0.89	0.15	52,58,65,73	0
5	GOL	B	202	6/6	0.91	0.13	36,44,45,51	0
4	EDO	B	201	4/4	0.91	0.18	41,45,47,49	0
3	PAE	B	203	8/8	0.92	0.14	33,38,54,56	8
3	PAE	F	202	8/8	0.94	0.12	30,38,60,60	0

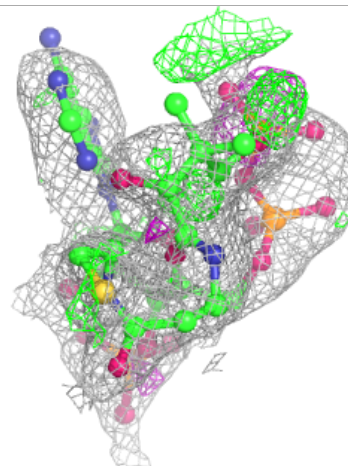
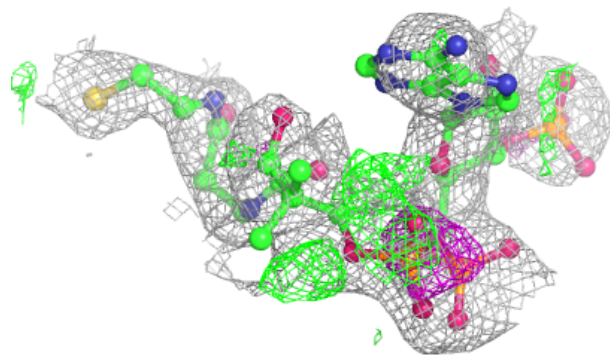
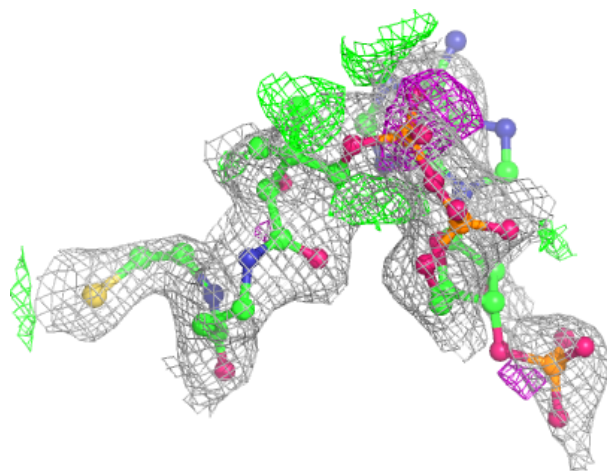
The following is a graphical depiction of the model fit to experimental electron density of all

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.



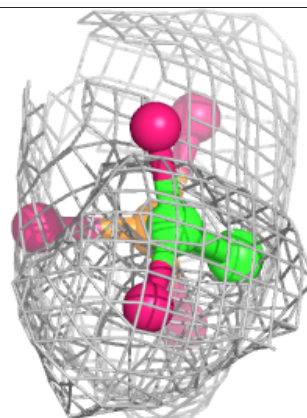
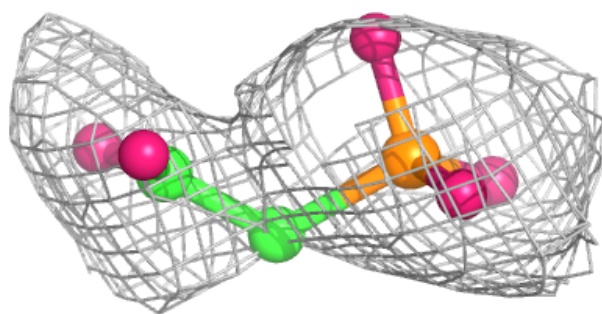
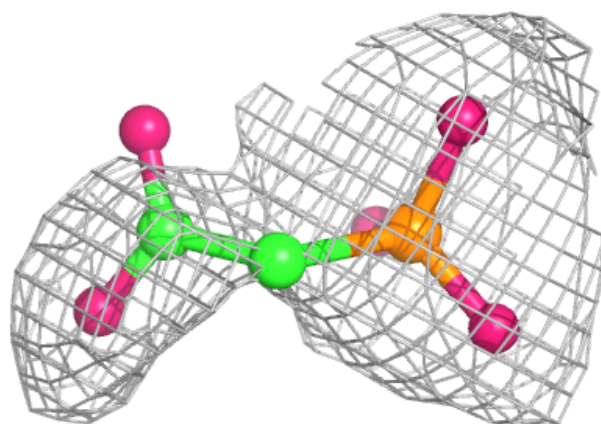
**Electron density around COA A 201:**

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



**Electron density around PAE C 201:**

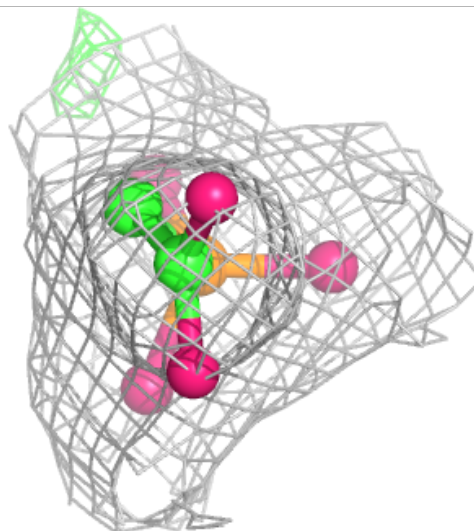
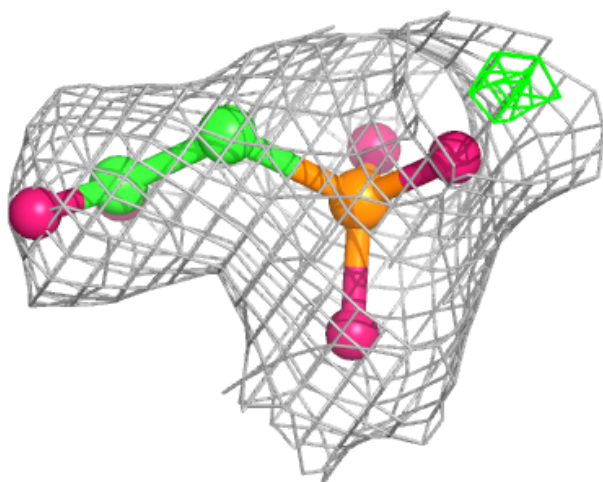
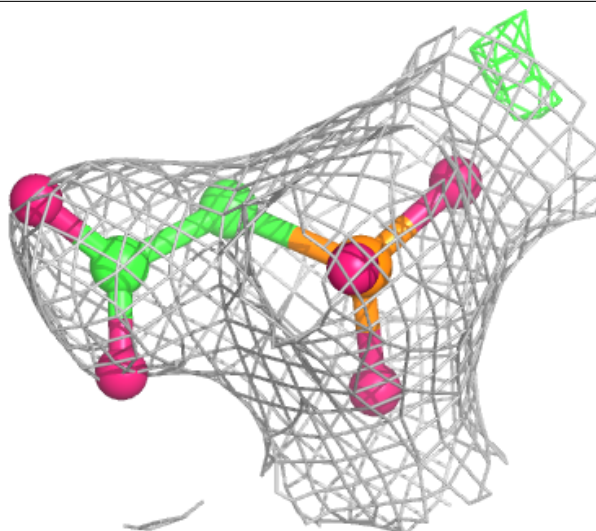
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





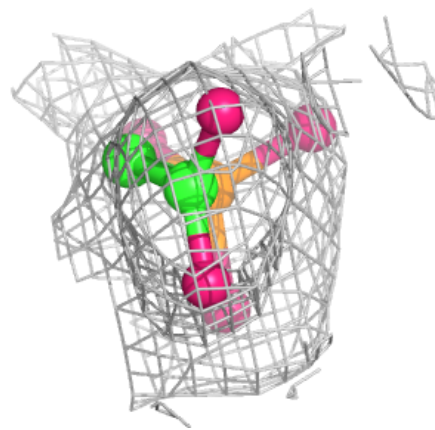
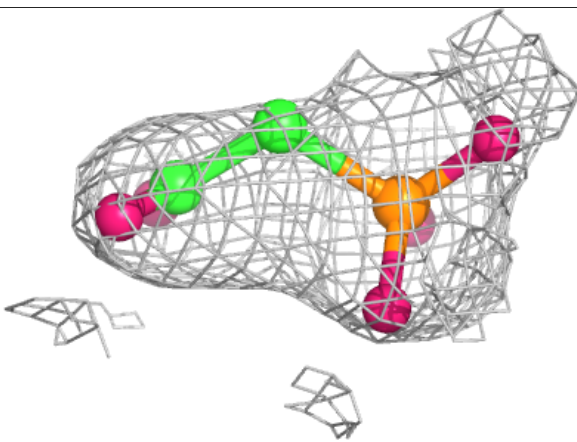
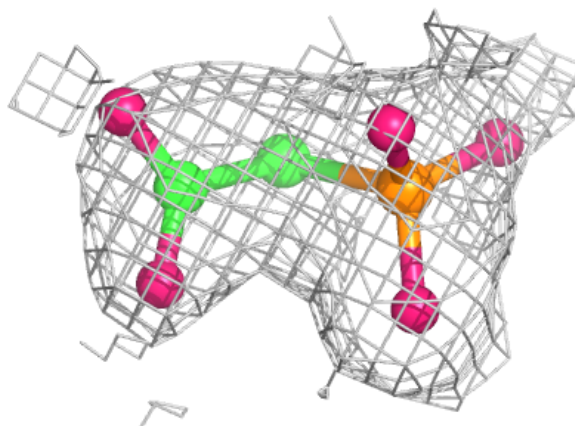
**Electron density around PAE D 201:**

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



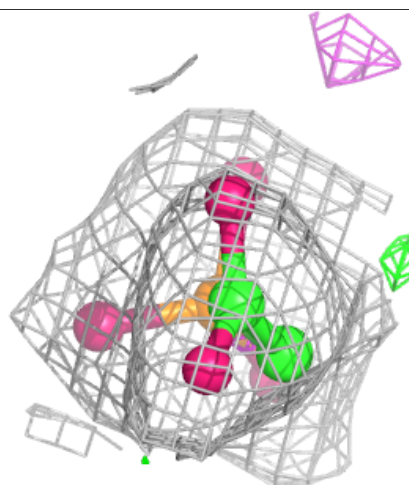
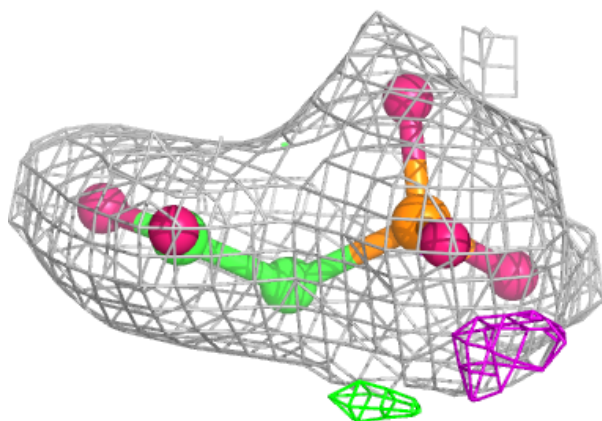
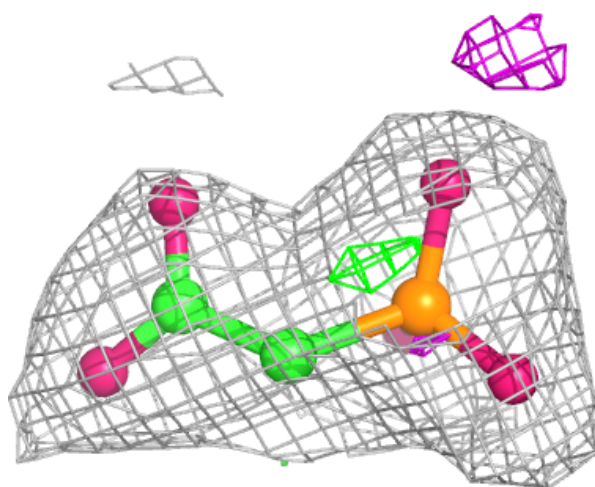
**Electron density around PAE A 202:**

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



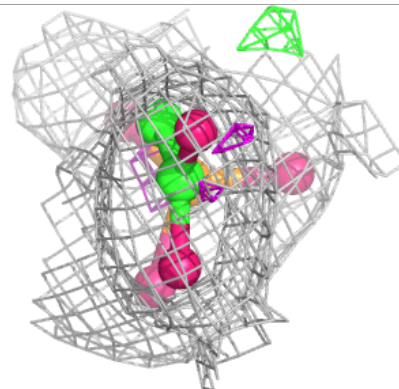
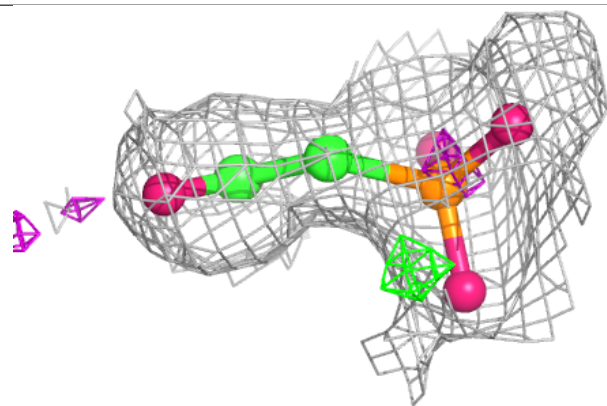
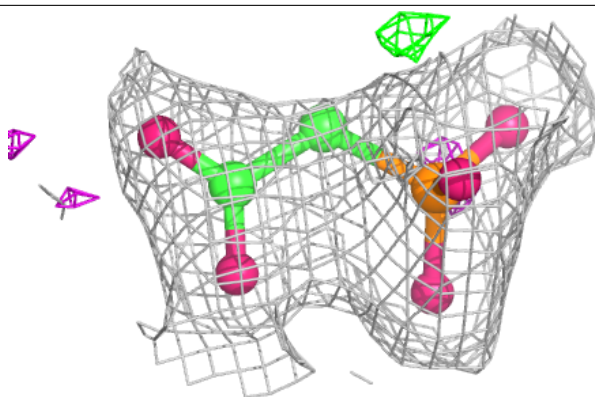
**Electron density around PAE E 201:**

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

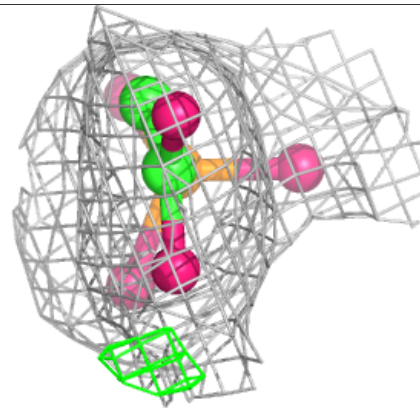
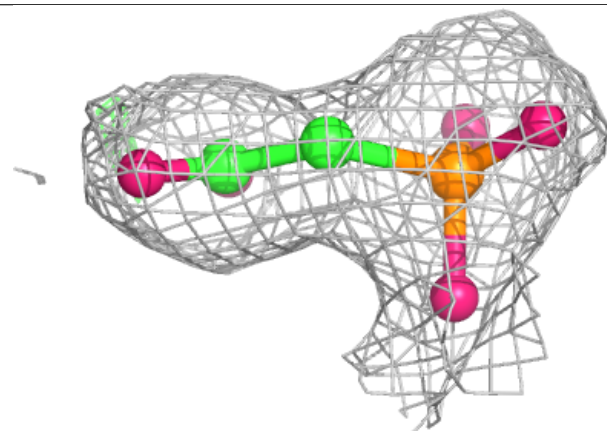
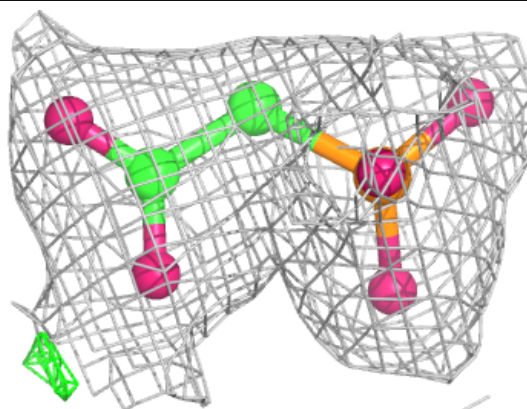


**Electron density around PAE B 203:**

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

**Electron density around PAE F 202:**

$2mF_o-DF_c$  (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.