



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:59 AM UTC

PDB ID : 7UNI / pdb_00007uni
Title : De novo designed chlorophyll dimer protein with Zn pheophorbide a methyl ester, SP2-ZnPPaM
Authors : Kennedy, M.A.; Stoddard, B.L.; Ennist, N.M.
Deposited on : 2022-04-11
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

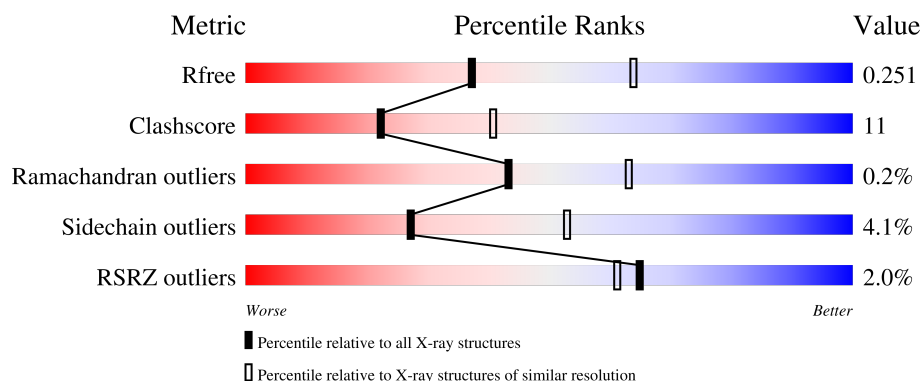
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	250	
1	B	250	
1	C	250	
1	D	250	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OE9	A	301	X	-	-	-
2	OE9	B	301	X	-	-	-
2	OE9	C	301	X	-	-	-
2	OE9	D	301	X	-	-	-

2 Entry composition [i](#)

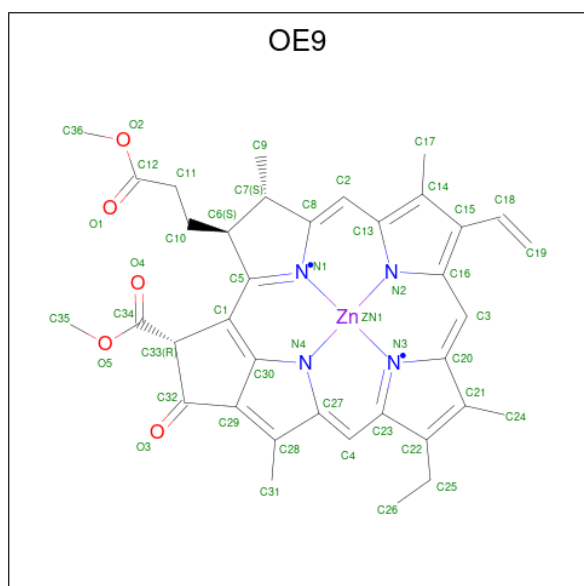
There are 6 unique types of molecules in this entry. The entry contains 6899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SP2-ZnPPaM designed chlorophyll dimer protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1739	1127	292	314	6			
1	C	242	Total	C	N	O	S	0	0	0
			1662	1068	281	307	6			
1	B	245	Total	C	N	O	S	0	0	0
			1771	1136	300	329	6			
1	D	237	Total	C	N	O	S	0	0	0
			1512	968	260	280	4			

- Molecule 2 is [methyl 9-ethenyl-14-ethyl-3-(3-methoxy-3-oxopropyl)-4,8,13,18-tetramethyl-2-oxophorbine-21-carboxylato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26]zinc (CCD ID: OE9) (formula: C₃₆H₃₆N₄O₅Zn) (labeled as "Ligand of Interest" by depositor).



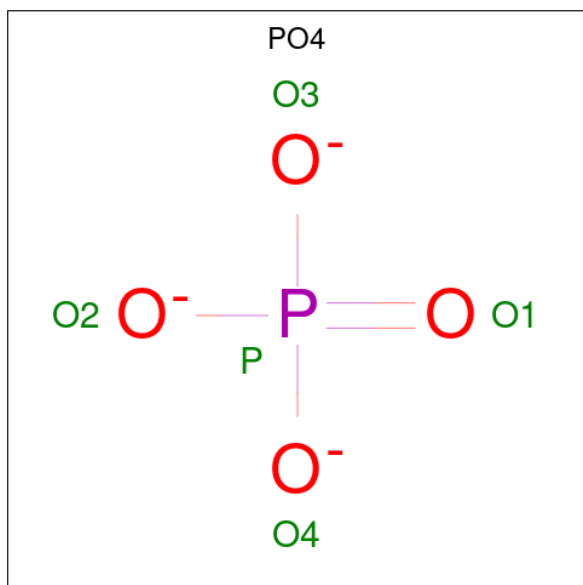
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Zn	0	0
			45	35	4	5	1		

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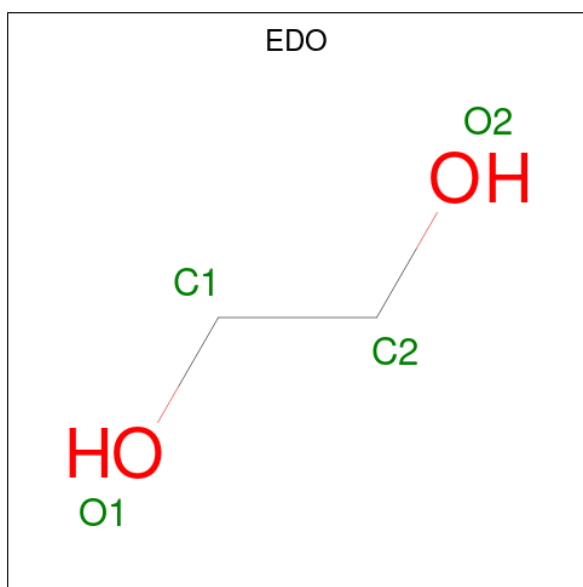
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	Zn	0	0
			38	30	4	3	1		
2	B	1	Total	C	N	O	Zn	0	0
			45	35	4	5	1		
2	D	1	Total	C	N	O	Zn	0	0
			40	32	4	3	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



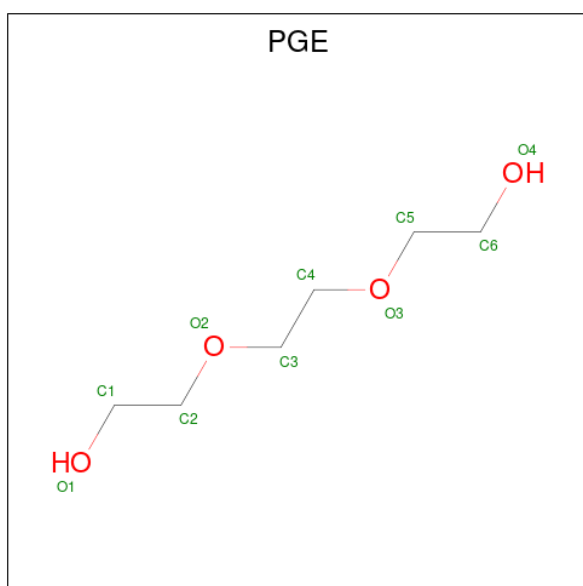
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

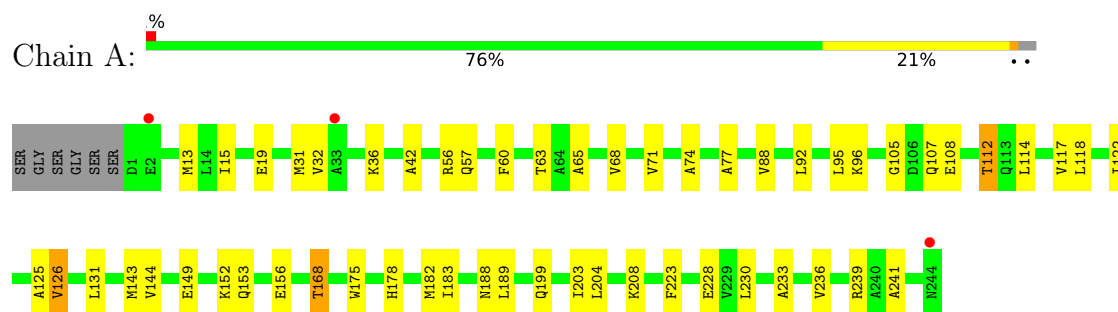
- Molecule 6 is water.

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

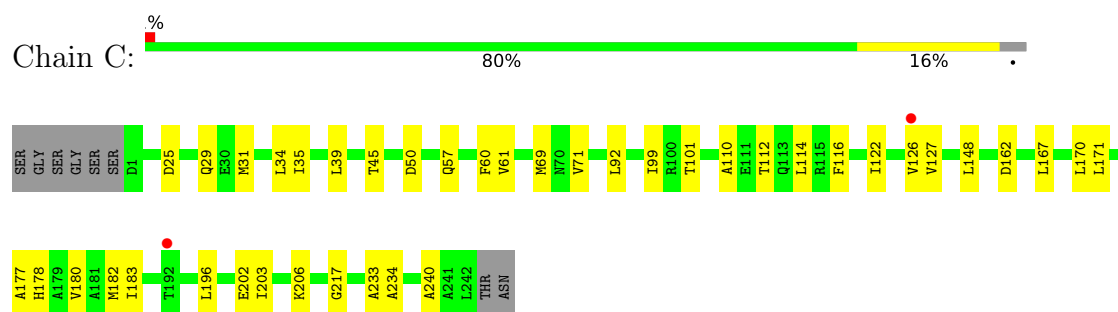
3 Residue-property plots

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.

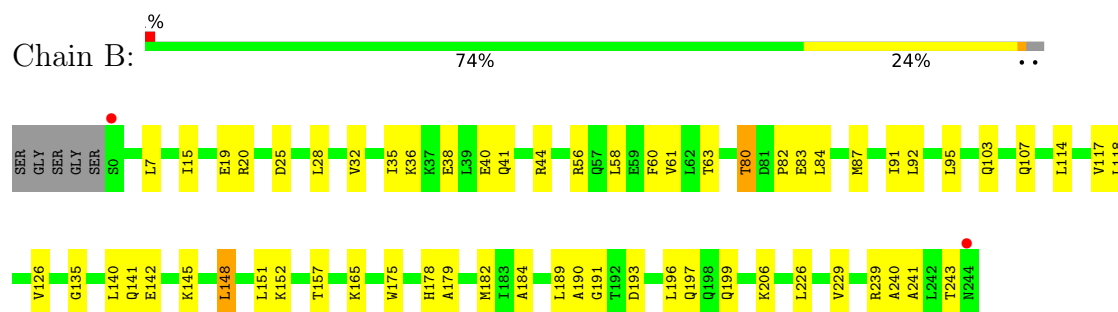
- Molecule 1: SP2-ZnPPaM designed chlorophyll dimer protein



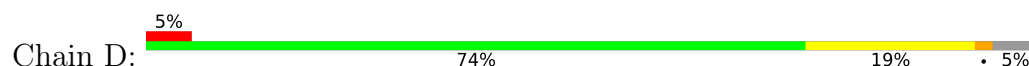
- Molecule 1: SP2-ZnPPaM designed chlorophyll dimer protein

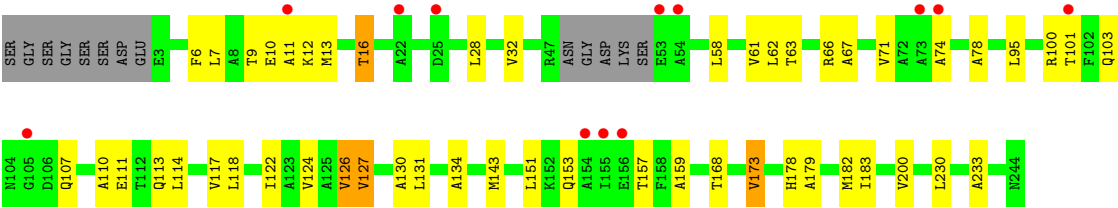


- Molecule 1: SP2-ZnPPaM designed chlorophyll dimer protein



- Molecule 1: SP2-ZnPPaM designed chlorophyll dimer protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.85Å 54.96Å 89.36Å 87.83° 84.06° 69.45°	Depositor
Resolution (Å)	49.26 – 2.50 49.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.26-2.50) 93.4 (49.26-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.199 , 0.252 0.199 , 0.251	Depositor DCC
R_{free} test set	2008 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6899	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PO4, OE9, EDO

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	0/1755	0.51	0/2384
1	B	0.40	0/1787	0.57	0/2426
1	C	0.29	0/1678	0.43	0/2291
1	D	0.29	0/1525	0.44	0/2094
All	All	0.35	0/6745	0.49	0/9195

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1739	0	1719	39	0
1	B	1771	0	1747	40	0
1	C	1662	0	1561	28	0
1	D	1512	0	1310	34	0
2	A	45	0	0	4	0
2	B	45	0	0	0	0
2	C	38	0	0	2	0
2	D	40	0	0	2	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
4	A	4	0	6	1	0
4	C	4	0	6	0	0
5	A	10	0	14	4	0
5	B	10	0	14	2	0
6	A	6	0	0	0	0
6	B	3	0	0	0	0
All	All	6899	0	6377	140	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 11.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:MET:HE3	1:B:151:LEU:HG	1.62	0.81
1:A:15:ILE:HG21	1:A:36:LYS:HG3	1.65	0.79
1:A:31:MET:HG3	1:A:92:LEU:HD22	1.64	0.78
1:A:183:ILE:HD11	1:A:203:ILE:HG22	1.75	0.69
1:D:182:MET:HE1	1:D:230:LEU:HG	1.76	0.68
1:A:42:ALA:HB2	1:A:57:GLN:HG2	1.76	0.68
1:A:199:GLN:OE1	1:A:239:ARG:NH2	2.27	0.68
1:D:179:ALA:HA	1:D:182:MET:HE2	1.76	0.68
1:C:171:LEU:HG	1:D:13:MET:HE1	1.77	0.66
1:D:67:ALA:O	1:D:71:VAL:HG23	1.96	0.65
1:C:116:PHE:CE2	1:C:170:LEU:HD22	2.32	0.64
1:B:178:HIS:ND1	5:B:302:PGE:H2	2.13	0.63
1:A:63:THR:HG23	1:A:118:LEU:HD22	1.81	0.63
1:C:127:VAL:HG11	1:C:148:LEU:HD13	1.80	0.62
1:D:63:THR:HG23	1:D:118:LEU:HD22	1.81	0.62
1:D:12:LYS:O	1:D:16:THR:HG23	1.98	0.62
1:A:122:ILE:O	1:A:126:VAL:HG23	2.01	0.61
1:A:68:VAL:HA	1:A:71:VAL:HG12	1.84	0.59
1:C:202:GLU:O	1:C:206:LYS:HG3	2.03	0.59
1:B:135:GLY:O	1:B:141:GLN:NE2	2.36	0.59
1:B:179:ALA:HA	1:B:182:MET:HE3	1.85	0.59
1:A:31:MET:CE	1:A:96:LYS:HB2	2.33	0.58
1:A:182:MET:HE2	2:A:301:OE9:C3	2.33	0.58
1:C:196:LEU:HD21	1:C:240:ALA:HA	1.86	0.58
1:C:39:LEU:HB2	1:C:61:VAL:HG11	1.86	0.57
1:D:183:ILE:HG23	1:D:200:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:HB3	1:B:28:LEU:HB2	1.86	0.56
1:B:80:THR:O	1:B:82:PRO:HD3	2.06	0.56
1:C:126:VAL:HG22	2:C:301:OE9:O5	2.06	0.56
1:D:182:MET:HE3	1:D:233:ALA:HB3	1.87	0.55
1:B:179:ALA:HA	1:B:182:MET:CE	2.36	0.55
1:B:60:PHE:CE2	1:B:114:LEU:HD22	2.41	0.55
1:C:182:MET:HE1	1:C:234:ALA:HB2	1.90	0.54
1:B:157:THR:HG21	1:B:165:LYS:HG2	1.89	0.54
1:A:13:MET:HE2	1:B:175:TRP:CD2	2.41	0.54
1:A:95:LEU:HB2	1:A:117:VAL:HG11	1.90	0.54
1:A:178:HIS:ND1	5:A:304:PGE:H5	2.23	0.54
1:C:25:ASP:O	1:C:29:GLN:HG3	2.07	0.54
1:D:182:MET:HG2	2:D:301:OE9:C15	2.38	0.53
1:A:31:MET:HE3	1:A:96:LYS:HB2	1.90	0.53
1:B:189:LEU:HD13	1:B:241:ALA:HB2	1.90	0.53
1:A:77:ALA:HB2	4:A:303:EDO:H11	1.90	0.53
1:B:95:LEU:HB2	1:B:117:VAL:HG11	1.91	0.52
1:C:183:ILE:HD11	1:C:203:ILE:HG22	1.91	0.52
1:B:60:PHE:CZ	1:B:114:LEU:HD22	2.45	0.52
1:D:124:VAL:HA	1:D:127:VAL:HG13	1.92	0.52
1:B:199:GLN:OE1	1:B:239:ARG:NH2	2.38	0.52
1:D:122:ILE:O	1:D:126:VAL:HG13	2.10	0.51
1:B:7:LEU:HB2	1:B:58:LEU:HD21	1.92	0.51
1:D:11:ALA:HB2	1:D:62:LEU:HD13	1.93	0.51
2:A:301:OE9:C35	5:A:304:PGE:H32	2.40	0.50
1:C:31:MET:HG2	1:C:92:LEU:HD22	1.92	0.50
1:C:177:ALA:HA	1:C:180:VAL:HG12	1.92	0.50
1:D:113:GLN:O	1:D:117:VAL:HG23	2.10	0.50
1:C:182:MET:HB2	1:C:233:ALA:HB1	1.92	0.50
1:A:175:TRP:CZ2	5:A:304:PGE:H6	2.46	0.50
1:C:182:MET:CE	1:C:234:ALA:HB2	2.42	0.50
1:B:19:GLU:HB2	1:B:32:VAL:HG11	1.93	0.49
1:B:15:ILE:HD11	1:B:35:ILE:HG22	1.94	0.49
1:D:143:MET:HE2	1:D:143:MET:HB2	1.68	0.49
1:D:107:GLN:O	1:D:111:GLU:N	2.42	0.48
1:C:178:HIS:O	1:C:182:MET:HG2	2.14	0.48
1:B:193:ASP:O	1:B:197:GLN:HG3	2.13	0.48
1:D:130:ALA:O	1:D:134:ALA:N	2.40	0.48
1:B:56:ARG:NH2	1:B:107:GLN:HB2	2.29	0.47
1:A:74:ALA:HB2	1:A:125:ALA:HA	1.96	0.47
1:B:63:THR:HG23	1:B:118:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HB3	3:A:302:PO4:O3	2.13	0.47
1:C:31:MET:O	1:C:35:ILE:HD12	2.15	0.47
1:B:36:LYS:O	1:B:40:GLU:HG3	2.14	0.47
1:B:191:GLY:O	1:B:197:GLN:NE2	2.36	0.47
2:A:301:OE9:C35	2:A:301:OE9:C1	2.92	0.47
1:D:101:THR:HB	1:D:110:ALA:HB2	1.96	0.47
1:A:31:MET:HE1	1:A:96:LYS:HB2	1.97	0.47
1:C:170:LEU:HD12	1:C:170:LEU:HA	1.74	0.46
1:A:71:VAL:CG2	1:A:88:VAL:HG13	2.46	0.46
1:A:228:GLU:HG2	1:B:20:ARG:NH2	2.30	0.46
5:A:304:PGE:H52	5:A:304:PGE:H3	1.76	0.46
1:D:100:ARG:HA	1:D:103:GLN:HG2	1.98	0.46
1:D:58:LEU:HA	1:D:61:VAL:HG22	1.98	0.46
1:A:152:LYS:O	1:A:156:GLU:HG3	2.15	0.46
1:A:168:THR:HG22	1:A:223:PHE:CZ	2.50	0.46
1:A:19:GLU:CG	1:A:32:VAL:HG11	2.46	0.45
1:A:189:LEU:HD13	1:A:241:ALA:HB2	1.97	0.45
1:B:196:LEU:HD11	1:B:243:THR:HG21	1.97	0.45
1:A:108:GLU:O	1:A:112:THR:HG22	2.16	0.45
1:C:45:THR:HG22	1:C:50:ASP:O	2.17	0.45
1:A:168:THR:HG22	1:A:223:PHE:HZ	1.81	0.45
1:A:71:VAL:HG23	1:A:88:VAL:HG13	1.99	0.44
1:B:142:GLU:O	1:B:145:LYS:HG2	2.17	0.44
1:C:162:ASP:OD2	1:C:162:ASP:N	2.50	0.44
1:B:84:LEU:HD23	1:B:84:LEU:HA	1.63	0.44
1:A:182:MET:HG2	2:A:301:OE9:C18	2.48	0.44
1:C:34:LEU:HD21	1:C:99:ILE:HG21	1.98	0.44
1:D:74:ALA:O	1:D:78:ALA:N	2.50	0.44
1:B:206:LYS:HB3	1:B:229:VAL:HG22	1.99	0.44
1:D:182:MET:HG2	2:D:301:OE9:C18	2.47	0.44
1:A:204:LEU:HG	1:A:208:LYS:HE2	2.00	0.44
1:D:151:LEU:HD13	1:D:173:VAL:HG11	2.00	0.43
1:B:87:MET:O	1:B:91:ILE:HG12	2.18	0.43
1:C:60:PHE:CE1	1:C:114:LEU:HD22	2.53	0.43
1:B:83:GLU:HB3	1:B:148:LEU:HD11	1.99	0.43
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.85	0.43
1:A:143:MET:HE2	1:A:143:MET:HB3	1.77	0.43
1:D:28:LEU:O	1:D:32:VAL:HG23	2.19	0.43
1:A:178:HIS:NE2	1:A:182:MET:HE3	2.34	0.42
1:A:233:ALA:O	1:A:236:VAL:HG12	2.18	0.42
1:C:182:MET:HG2	1:C:182:MET:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:O	1:D:103:GLN:HG2	2.19	0.42
1:B:190:ALA:HB2	1:B:196:LEU:HB3	2.00	0.42
1:B:140:LEU:HD13	1:B:184:ALA:HB2	2.01	0.42
1:D:153:GLN:O	1:D:157:THR:OG1	2.32	0.42
1:D:178:HIS:ND1	1:D:230:LEU:HD11	2.34	0.42
1:A:143:MET:SD	1:A:204:LEU:HD11	2.60	0.42
1:C:69:MET:HE2	1:C:69:MET:HB3	1.81	0.42
1:B:41:GLN:OE1	1:B:44:ARG:NH2	2.51	0.42
1:D:95:LEU:HB2	1:D:117:VAL:HG11	2.02	0.42
1:D:114:LEU:HD23	1:D:114:LEU:HA	1.81	0.42
1:A:131:LEU:HD13	1:A:144:VAL:HG11	2.02	0.41
1:B:38:GLU:CD	1:B:103:GLN:HE21	2.26	0.41
1:D:10:GLU:HG2	1:D:62:LEU:HD11	2.02	0.41
1:C:171:LEU:CG	1:D:13:MET:HE1	2.49	0.41
1:D:6:PHE:O	1:D:9:THR:OG1	2.34	0.41
1:D:182:MET:HE1	1:D:230:LEU:O	2.21	0.41
1:B:175:TRP:CZ2	5:B:302:PGE:H1	2.55	0.41
1:B:239:ARG:O	1:B:243:THR:HG23	2.20	0.41
1:C:182:MET:SD	2:C:301:OE9:C16	3.08	0.41
1:A:60:PHE:CE2	1:A:114:LEU:HD22	2.55	0.41
1:C:101:THR:HG22	1:C:110:ALA:HB2	2.02	0.41
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.78	0.41
1:D:100:ARG:HA	1:D:103:GLN:CG	2.51	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.88	0.41
1:D:7:LEU:CB	1:D:58:LEU:HD21	2.51	0.41
1:A:65:ALA:HA	1:A:68:VAL:HG12	2.01	0.41
1:A:105:GLY:O	1:A:107:GLN:N	2.54	0.41
1:B:87:MET:HE1	1:B:152:LYS:HA	2.03	0.41
1:B:38:GLU:HB3	1:B:61:VAL:HG22	2.02	0.40
1:B:190:ALA:N	1:B:240:ALA:HB1	2.36	0.40
1:C:122:ILE:O	1:C:126:VAL:HG23	2.20	0.40
1:C:71:VAL:HG11	1:C:92:LEU:HG	2.03	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	242/250 (97%)	239 (99%)	3 (1%)	0	100	100
1	B	243/250 (97%)	240 (99%)	3 (1%)	0	100	100
1	C	240/250 (96%)	229 (95%)	10 (4%)	1 (0%)	30	49
1	D	233/250 (93%)	228 (98%)	4 (2%)	1 (0%)	30	49
All	All	958/1000 (96%)	936 (98%)	20 (2%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	ALA
1	C	217	GLY

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	142/191 (74%)	135 (95%)	7 (5%)	22	45
1	B	150/191 (78%)	146 (97%)	4 (3%)	39	67
1	C	126/191 (66%)	123 (98%)	3 (2%)	43	70
1	D	94/191 (49%)	87 (93%)	7 (7%)	13	27
All	All	512/764 (67%)	491 (96%)	21 (4%)	27	53

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	112	THR
1	A	126	VAL
1	A	149	GLU

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Mol	Chain	Res	Type
1	A	153	GLN
1	A	168	THR
1	A	230	LEU
1	C	57	GLN
1	C	112	THR
1	C	167	LEU
1	B	80	THR
1	B	126	VAL
1	B	148	LEU
1	B	226	LEU
1	D	16	THR
1	D	66	ARG
1	D	126	VAL
1	D	127	VAL
1	D	131	LEU
1	D	168	THR
1	D	173	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	198	GLN
1	A	215	GLN
1	B	29	GLN
1	B	48	ASN
1	B	188	ASN
1	B	225	GLN
1	D	141	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
2	OE9	A	301	1	52,53,54	1.15	2 (3%)	58,89,90	1.28	7 (12%)
3	PO4	C	302	-	4,4,4	0.91	0	6,6,6	0.58	0
2	OE9	D	301	1	45,48,54	1.47	6 (13%)	57,83,90	1.50	10 (17%)
5	PGE	B	302	-	9,9,9	0.51	0	8,8,8	0.38	0
4	EDO	C	303	-	3,3,3	0.46	0	2,2,2	0.32	0
2	OE9	C	301	1	44,46,54	1.60	6 (13%)	50,81,90	1.59	12 (24%)
3	PO4	A	302	-	4,4,4	0.76	0	6,6,6	0.66	0
5	PGE	A	304	-	9,9,9	0.39	0	8,8,8	0.56	0
2	OE9	B	301	1	52,53,54	1.37	3 (5%)	58,89,90	1.47	13 (22%)
4	EDO	A	303	-	3,3,3	0.55	0	2,2,2	0.32	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	OE9	A	301	1	1/1/11/15	5/15/91/93	-
2	OE9	D	301	1	1/1/10/15	5/5/81/93	-
5	PGE	B	302	-	-	6/7/7/7	-
4	EDO	C	303	-	-	0/1/1/1	-
2	OE9	C	301	1	1/1/10/15	1/4/80/93	-
5	PGE	A	304	-	-	5/7/7/7	-
2	OE9	B	301	1	1/1/11/15	4/15/91/93	-
4	EDO	A	303	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	OE9	ZN1-N1	8.23	2.30	2.03
2	B	301	OE9	ZN1-N1	8.19	2.30	2.03
2	D	301	OE9	ZN1-N1	7.30	2.27	2.03
2	A	301	OE9	ZN1-N1	5.99	2.23	2.03
2	D	301	OE9	C20-N3	2.76	1.44	1.38
2	B	301	OE9	C23-N3	-2.61	1.31	1.37
2	C	301	OE9	ZN1-N3	2.58	2.11	2.03
2	D	301	OE9	C16-N2	2.42	1.43	1.38
2	C	301	OE9	C20-N3	2.34	1.43	1.38
2	C	301	OE9	C13-N2	2.32	1.43	1.38
2	D	301	OE9	ZN1-N3	2.32	2.10	2.03
2	A	301	OE9	C23-N3	-2.22	1.32	1.37
2	C	301	OE9	C23-N3	-2.15	1.32	1.37
2	D	301	OE9	C23-N3	-2.09	1.33	1.37
2	B	301	OE9	ZN1-N3	2.08	2.10	2.03
2	D	301	OE9	C13-N2	2.07	1.42	1.38
2	C	301	OE9	C16-N2	2.06	1.42	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	OE9	C5-N1-C8	5.00	114.88	106.96
2	D	301	OE9	C5-N1-C8	4.46	114.04	106.96
2	B	301	OE9	C5-N1-C8	3.72	112.86	106.96
2	A	301	OE9	C5-N1-C8	3.60	112.66	106.96
2	C	301	OE9	C13-C14-C15	3.39	110.22	107.03
2	B	301	OE9	C35-O5-C34	-3.22	108.61	115.92
2	B	301	OE9	C9-C7-C6	-3.01	102.35	113.98
2	D	301	OE9	C21-C20-N3	-2.90	105.32	109.06
2	B	301	OE9	C16-N2-C13	2.89	110.81	106.52
2	D	301	OE9	C13-C14-C15	2.64	109.52	107.03
2	B	301	OE9	C14-C13-N2	-2.62	105.73	109.02
2	D	301	OE9	C18-C15-C16	2.61	129.39	125.42
2	C	301	OE9	C14-C13-N2	-2.61	105.75	109.02
2	D	301	OE9	C4-C27-C28	2.59	130.88	125.49
2	A	301	OE9	C4-C27-C28	2.57	130.83	125.49
2	B	301	OE9	C16-C3-C20	2.57	132.28	126.25
2	C	301	OE9	C29-C30-N4	-2.56	105.74	110.51
2	D	301	OE9	C33-C1-C5	2.48	131.13	127.38
2	D	301	OE9	C4-C27-N4	-2.43	120.79	124.82
2	D	301	OE9	C20-N3-C23	2.40	109.67	106.47
2	B	301	OE9	O2-C12-O1	-2.35	117.29	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OE9	C6-C7-C8	2.34	105.66	101.87
2	C	301	OE9	C6-C7-C8	2.33	104.32	101.59
2	B	301	OE9	C20-N3-C23	2.32	109.55	106.47
2	B	301	OE9	C2-C13-N2	2.28	128.19	124.24
2	D	301	OE9	C2-C13-N2	2.27	128.16	124.24
2	C	301	OE9	C4-C27-C28	2.25	130.17	125.49
2	A	301	OE9	C15-C14-C13	2.24	109.81	107.17
2	A	301	OE9	C9-C7-C6	-2.24	105.33	113.98
2	C	301	OE9	C6-C5-C1	2.22	127.71	123.86
2	C	301	OE9	C2-C13-N2	2.21	128.07	124.24
2	A	301	OE9	C20-N3-C23	2.15	109.33	106.47
2	C	301	OE9	C21-C20-N3	-2.14	106.29	109.06
2	C	301	OE9	C4-C27-N4	-2.10	121.34	124.82
2	B	301	OE9	C4-C27-C28	2.07	129.80	125.49
2	B	301	OE9	C29-C30-N4	-2.07	106.65	110.51
2	D	301	OE9	C29-C30-N4	-2.06	106.67	110.51
2	C	301	OE9	C18-C15-C16	2.05	128.54	125.42
2	B	301	OE9	C6-C7-C8	2.03	105.16	101.87
2	C	301	OE9	C16-N2-C13	2.03	109.53	106.52
2	A	301	OE9	C4-C27-N4	-2.02	121.48	124.82
2	B	301	OE9	C21-C20-N3	-2.02	106.45	109.06

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	OE9	N4
2	C	301	OE9	N4
2	B	301	OE9	N4
2	D	301	OE9	N4

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	OE9	C1-C33-C34-O4
2	A	301	OE9	C1-C33-C34-O5
2	A	301	OE9	C33-C34-O5-C35
2	C	301	OE9	C1-C33-C34-O5
2	B	301	OE9	C1-C33-C34-O4
2	B	301	OE9	C1-C33-C34-O5
2	B	301	OE9	C33-C34-O5-C35
2	D	301	OE9	C11-C10-C6-C5
2	D	301	OE9	C11-C10-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	301	OE9	O4-C34-O5-C35
2	B	301	OE9	O4-C34-O5-C35
5	A	304	PGE	C3-C4-O3-C5
5	B	302	PGE	O3-C5-C6-O4
5	B	302	PGE	O1-C1-C2-O2
5	B	302	PGE	O2-C3-C4-O3
5	A	304	PGE	O3-C5-C6-O4
2	D	301	OE9	C6-C10-C11-C12
5	A	304	PGE	O1-C1-C2-O2
2	A	301	OE9	C21-C22-C25-C26
5	A	304	PGE	O2-C3-C4-O3
5	A	304	PGE	C1-C2-O2-C3
5	B	302	PGE	C4-C3-O2-C2
5	B	302	PGE	C3-C4-O3-C5
2	D	301	OE9	C10-C11-C12-O2
2	D	301	OE9	C10-C11-C12-O1
5	B	302	PGE	C6-C5-O3-C4

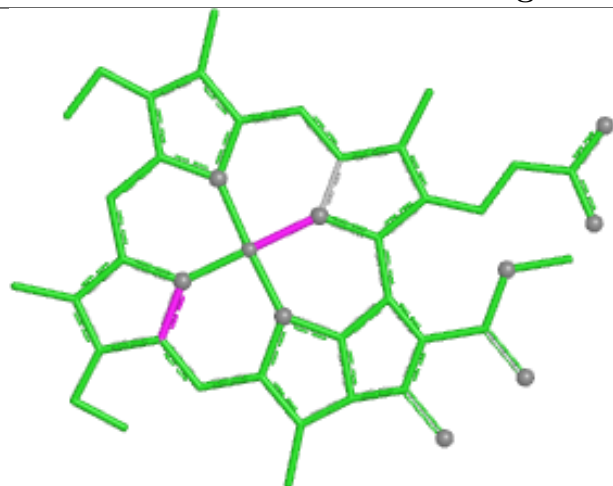
There are no ring outliers.

7 monomers are involved in 15 short contacts:

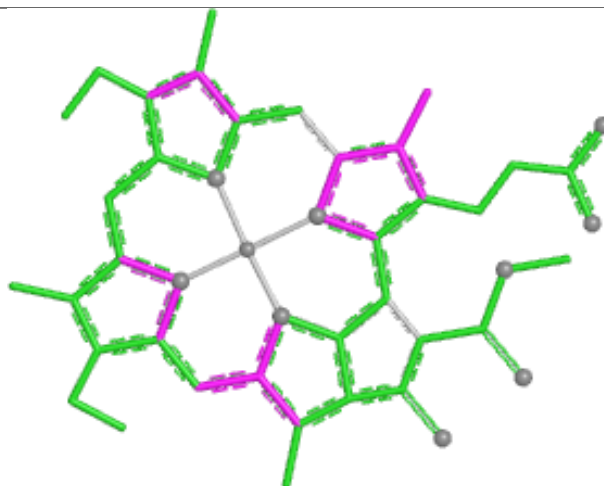
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	OE9	4	0
2	D	301	OE9	2	0
5	B	302	PGE	2	0
2	C	301	OE9	2	0
3	A	302	PO4	1	0
5	A	304	PGE	4	0
4	A	303	EDO	1	0

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.

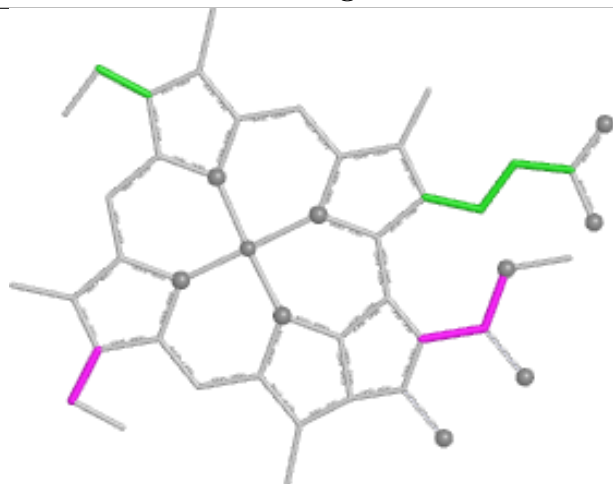
Ligand OE9 A 301



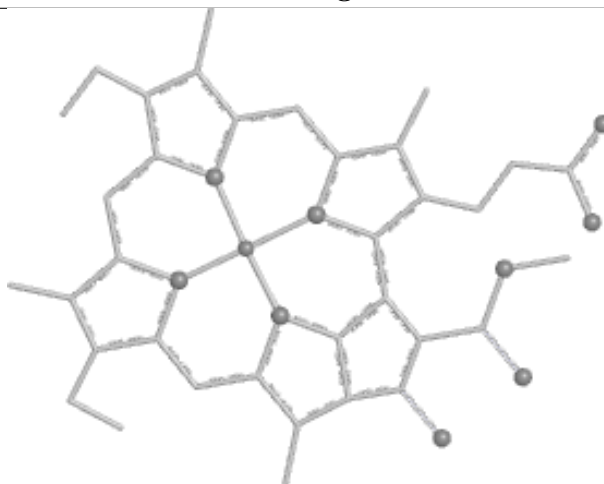
Bond lengths



Bond angles

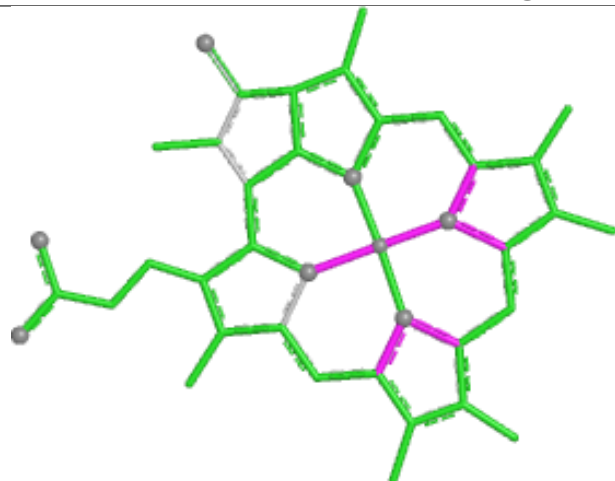


Torsions

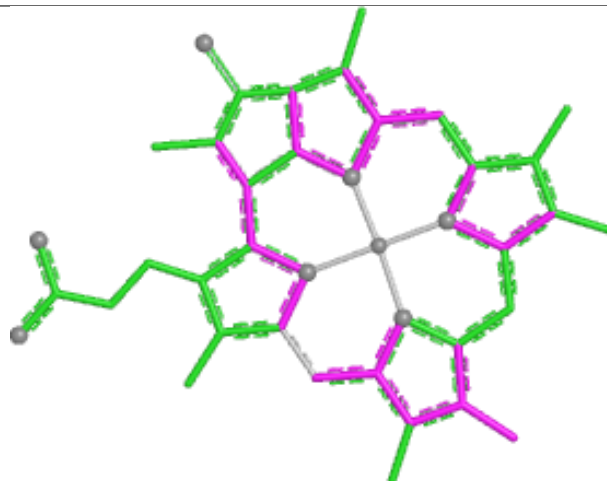


Rings

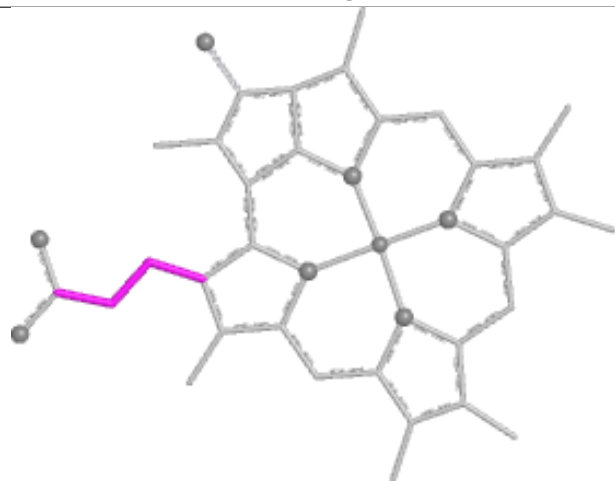
Ligand OE9 D 301



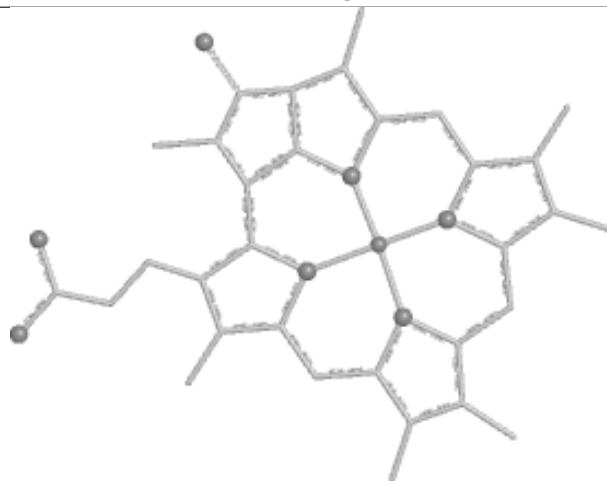
Bond lengths



Bond angles

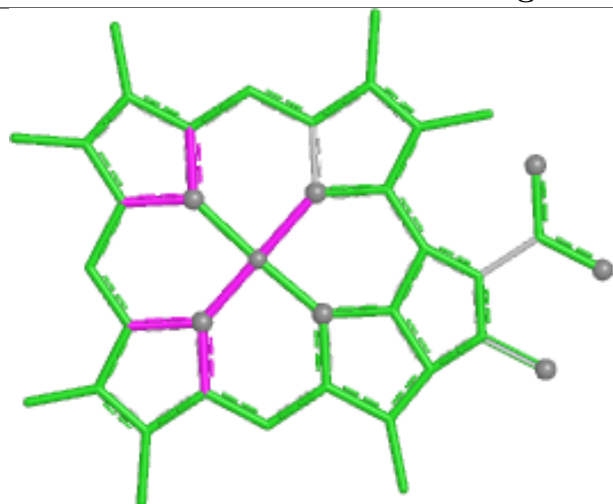


Torsions

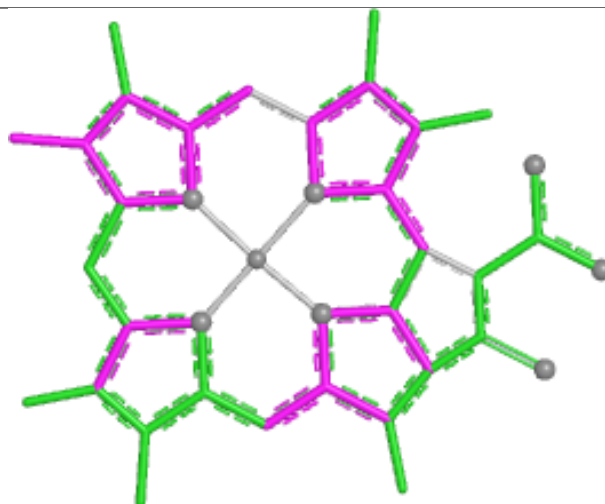


Rings

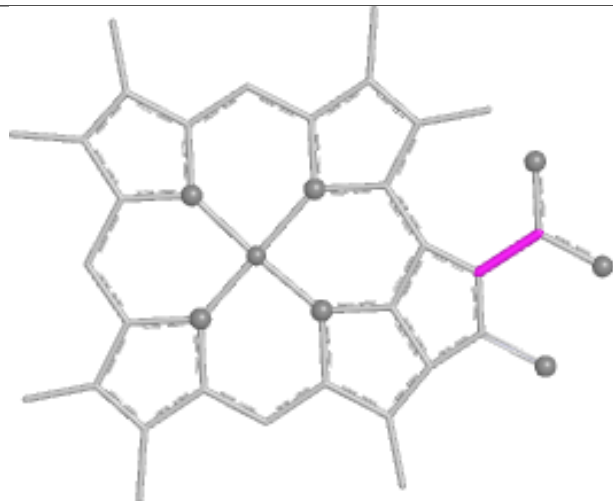
Ligand OE9 C 301



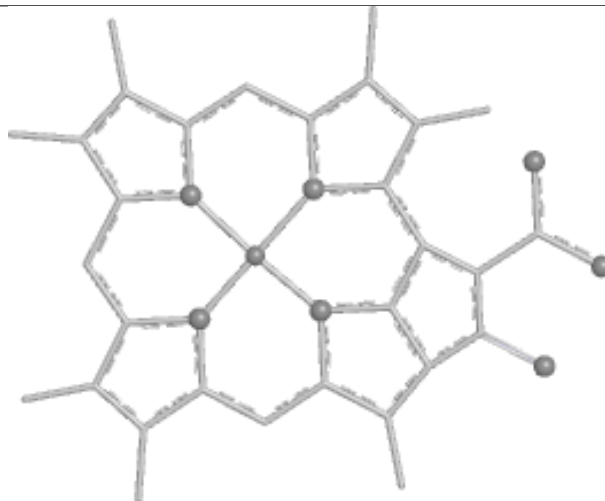
Bond lengths



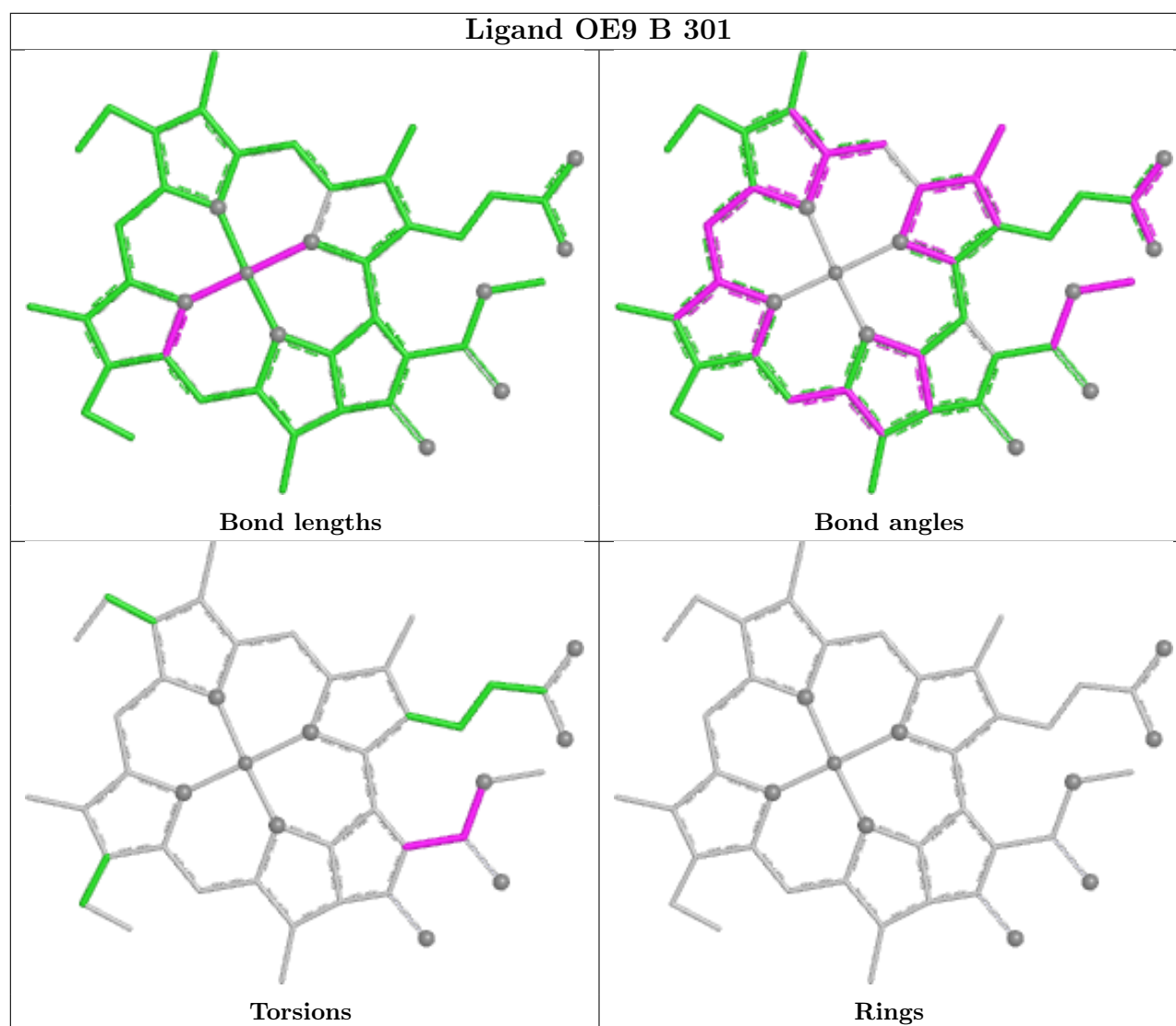
Bond angles



Torsions



Rings



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	244/250 (97%)	-0.02	3 (1%) 76 73	36, 52, 80, 115	0
1	B	245/250 (98%)	-0.15	2 (0%) 82 80	36, 50, 74, 108	0
1	C	242/250 (96%)	0.09	2 (0%) 82 80	45, 67, 103, 125	0
1	D	237/250 (94%)	0.47	12 (5%) 33 29	47, 82, 120, 141	0
All	All	968/1000 (96%)	0.09	19 (1%) 65 61	36, 59, 108, 141	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	SER	4.4
1	D	73	ALA	2.8
1	D	74	ALA	2.6
1	D	53	GLU	2.6
1	A	244	ASN	2.5
1	C	126	VAL	2.5
1	D	11	ALA	2.5
1	D	105	GLY	2.4
1	D	25	ASP	2.4
1	A	33	ALA	2.3
1	D	155	ILE	2.3
1	C	192	THR	2.3
1	B	244	ASN	2.2
1	D	54	ALA	2.1
1	D	156	GLU	2.1
1	A	2	GLU	2.0
1	D	101	THR	2.0
1	D	22	ALA	2.0
1	D	154	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

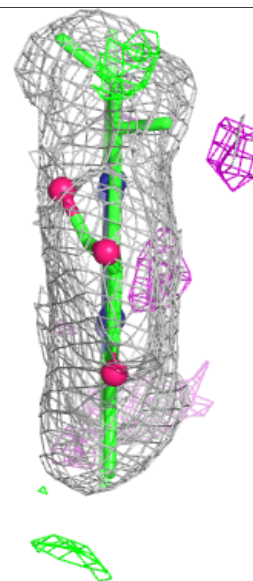
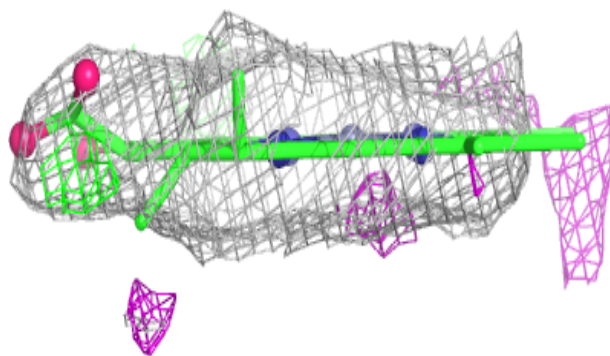
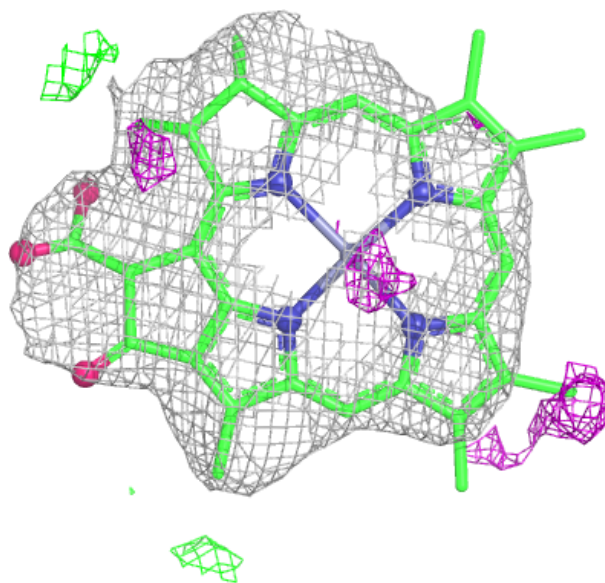
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	302	5/5	0.69	0.12	96,107,115,122	0
3	PO4	C	302	5/5	0.79	0.28	115,116,120,130	0
2	OE9	C	301	38/46	0.86	0.14	84,89,94,100	0
4	EDO	C	303	4/4	0.86	0.15	72,73,76,80	0
4	EDO	A	303	4/4	0.87	0.19	45,47,49,53	0
5	PGE	B	302	10/10	0.88	0.12	51,53,56,56	0
2	OE9	D	301	40/46	0.92	0.12	72,81,88,89	0
5	PGE	A	304	10/10	0.93	0.11	55,58,61,61	0
2	OE9	A	301	45/46	0.96	0.10	40,48,54,58	0
2	OE9	B	301	45/46	0.97	0.09	41,46,53,58	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.

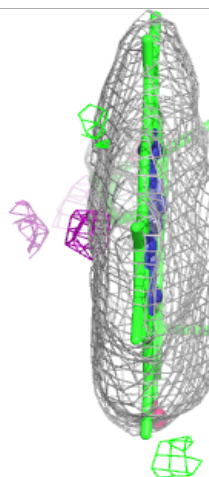
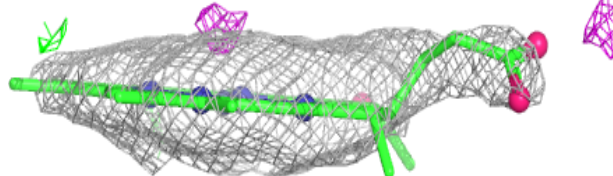
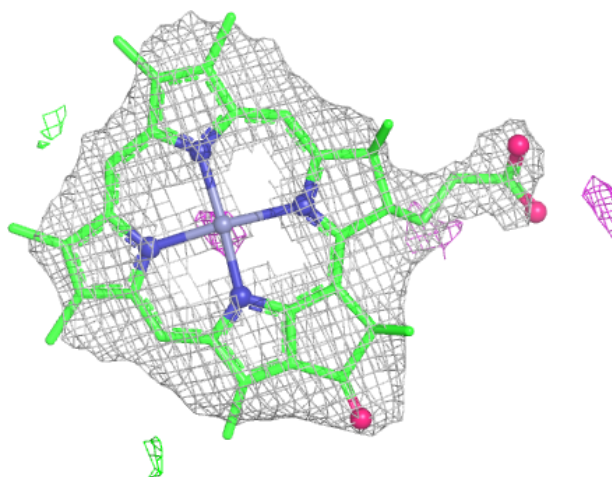
Electron density around OE9 C 301:

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



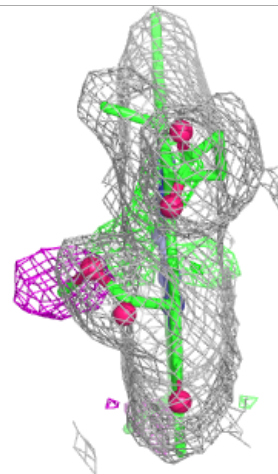
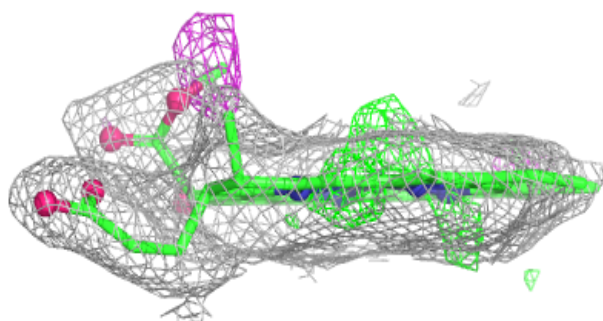
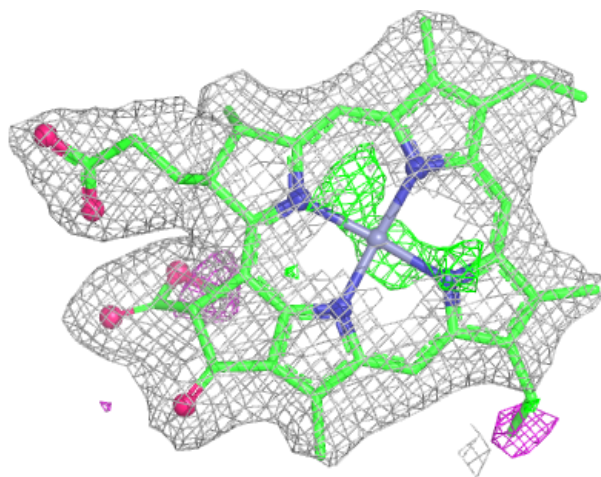
Electron density around OE9 D 301:

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



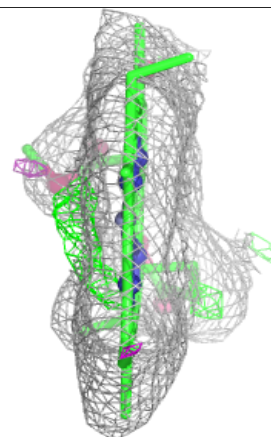
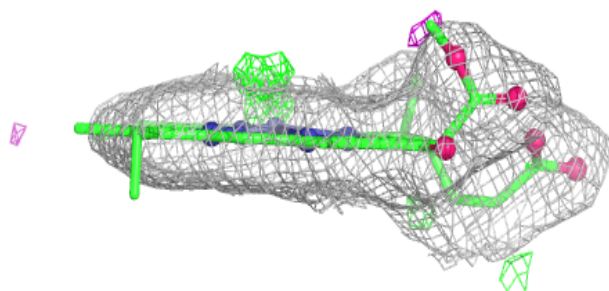
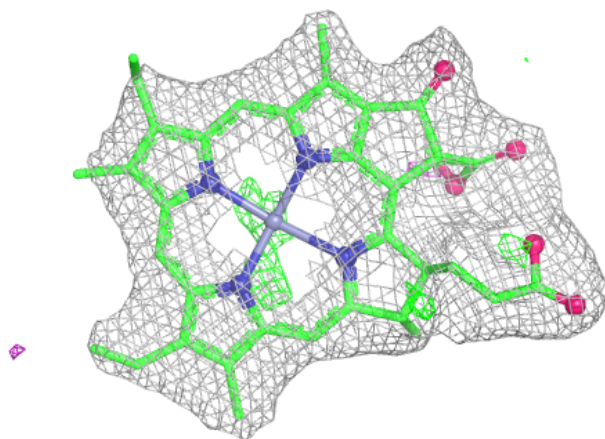
Electron density around OE9 A 301:

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



Electron density around OE9 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.