



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 12:24 PM JST

PDB ID : 9IL9 / pdb_00009il9
Title : Crystal Structure of SME-1 carbapenemase in complex with Avibactam.
Authors : Dhankhar, K.; Hazra, S.
Deposited on : 2024-06-29
Resolution : 2.28 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

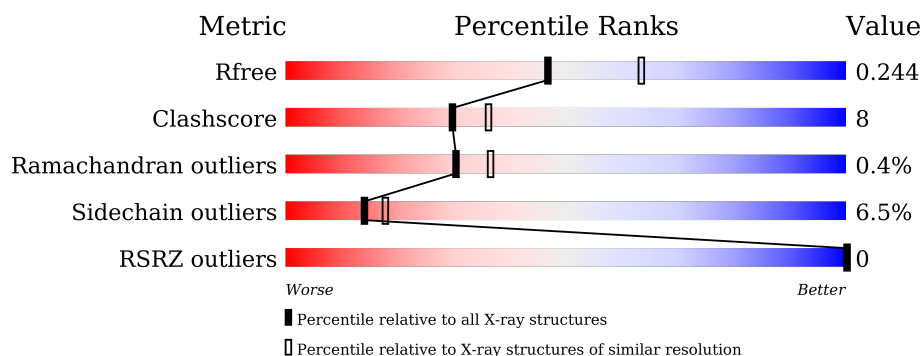
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.28 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}	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	275	
1	B	275	

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
3	PEG	A	302	-	-	X	-
4	PO4	A	303	-	-	X	-
5	CL	A	304	-	-	X	-
5	CL	A	305	-	-	X	-
7	EDO	B	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4400 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.

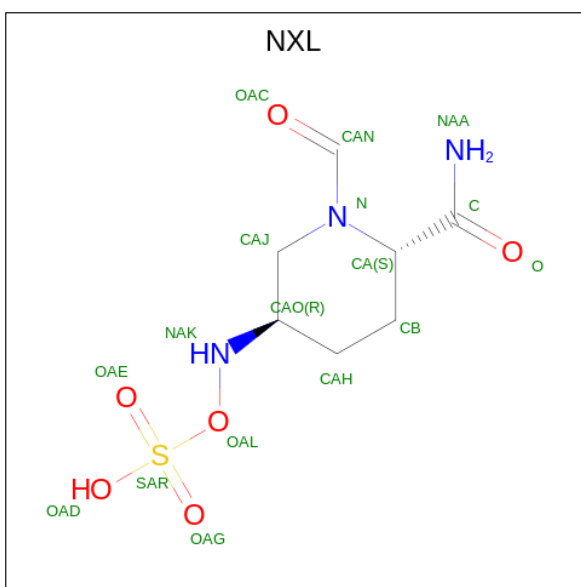
- Molecule 1 is a protein called beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	2	0
			2075	1299	368	401	7			
1	B	267	Total	C	N	O	S	0	2	0
			2077	1300	367	403	7			

There are 16 discrepancies between the modelled and reference sequences:

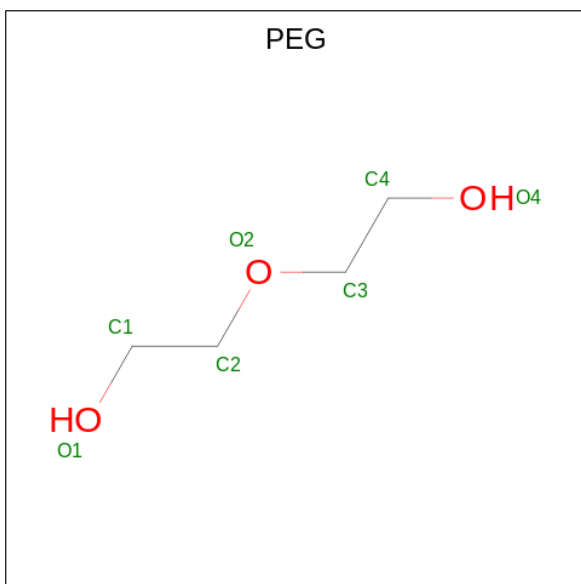
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q54488
A	0	GLY	-	expression tag	UNP Q54488
A	268	HIS	-	expression tag	UNP Q54488
A	269	HIS	-	expression tag	UNP Q54488
A	270	HIS	-	expression tag	UNP Q54488
A	271	HIS	-	expression tag	UNP Q54488
A	272	HIS	-	expression tag	UNP Q54488
A	273	HIS	-	expression tag	UNP Q54488
B	-1	MET	-	initiating methionine	UNP Q54488
B	0	GLY	-	expression tag	UNP Q54488
B	268	HIS	-	expression tag	UNP Q54488
B	269	HIS	-	expression tag	UNP Q54488
B	270	HIS	-	expression tag	UNP Q54488
B	271	HIS	-	expression tag	UNP Q54488
B	272	HIS	-	expression tag	UNP Q54488
B	273	HIS	-	expression tag	UNP Q54488

- Molecule 2 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (CCD ID: NXL) (formula: C₇H₁₃N₃O₆S) (labeled as "Ligand of Interest" by depositor).



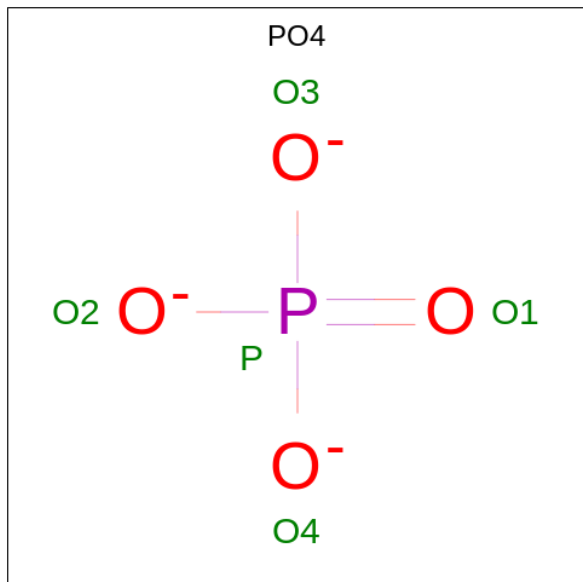
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 17	C 7	N 3	O 6	S 1	0	0
2	B	1	Total 17	C 7	N 3	O 6	S 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

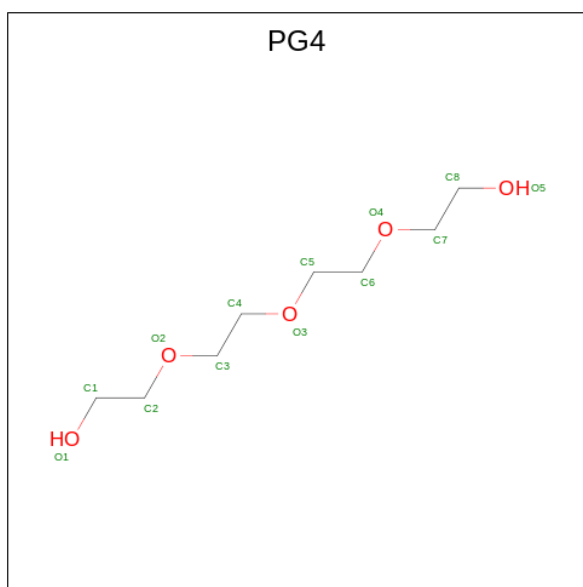


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

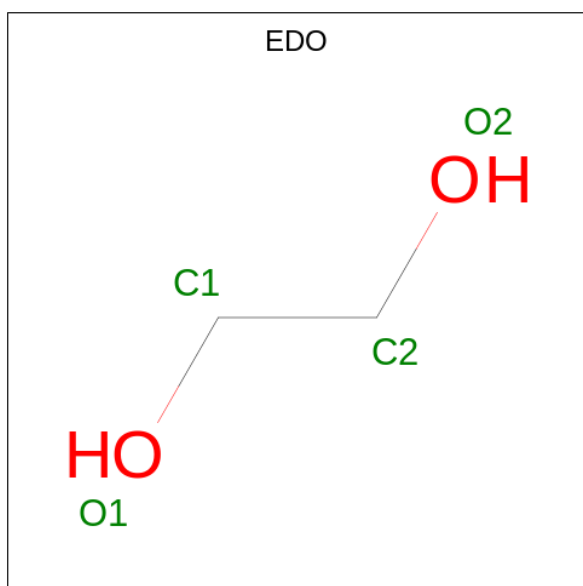
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is water.

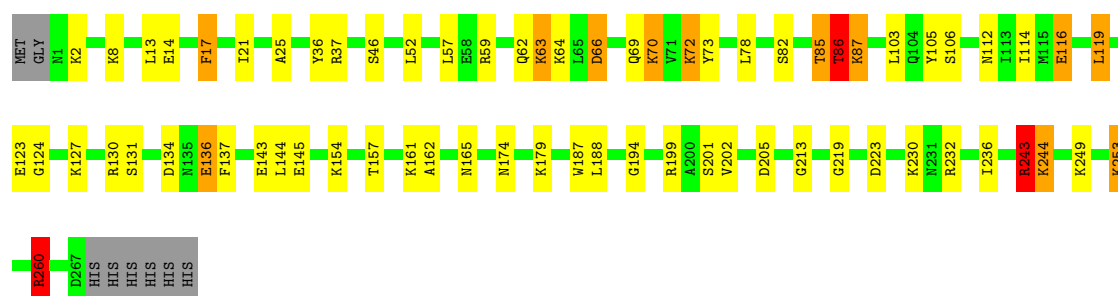
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	88	Total 88	O 88	0	0
8	B	95	Total 95	O 95	0	0

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: beta-lactamase

Chain A: 



- Molecule 1: beta-lactamase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 51.87Å 77.43Å 90.00° 114.11° 90.00°	Depositor
Resolution (Å)	23.18 – 2.28 23.18 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.18-2.28) 99.8 (23.18-2.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.155 , 0.241 0.154 , 0.244	Depositor DCC
R_{free} test set	1154 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	1.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4400	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.69% 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: CL, EDO, PG4, NXL, PEG, PO4

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	0.92	1/2116 (0.0%)	1.70	36/2851 (1.3%)
1	B	0.84	0/2121	1.65	42/2859 (1.5%)
All	All	0.88	1/4237 (0.0%)	1.67	78/5710 (1.4%)

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	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ARG	NE-CZ	5.56	1.39	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	CD-NE-CZ	11.98	141.17	124.40
1	A	144	LEU	N-CA-CB	11.59	128.07	111.15
1	A	243	ARG	NE-CZ-NH1	9.87	131.37	121.50
1	A	144	LEU	N-CA-C	-9.71	102.52	114.75
1	B	174	ASN	CA-CB-CG	-9.28	103.32	112.60
1	B	123	GLU	CB-CG-CD	8.59	127.21	112.60
1	A	244	LYS	CG-CD-CE	8.40	130.62	111.30
1	A	243	ARG	NE-CZ-NH2	-8.16	111.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ARG	CD-NE-CZ	-8.16	112.98	124.40
1	B	254	THR	CA-CB-OG1	-8.03	97.56	109.60
1	B	174	ASN	CB-CA-C	-7.97	97.25	110.72
1	B	86	THR	N-CA-CB	7.25	121.52	110.28
1	A	244	LYS	CB-CG-CD	7.25	127.96	111.30
1	B	74	GLU	CB-CG-CD	7.16	124.77	112.60
1	A	243	ARG	CG-CD-NE	-7.08	96.42	112.00
1	A	86	THR	CA-CB-OG1	7.07	120.21	109.60
1	B	41	ARG	CG-CD-NE	-7.04	96.52	112.00
1	B	163	VAL	N-CA-CB	7.01	119.55	110.57
1	A	179	LYS	CB-CG-CD	6.81	126.97	111.30
1	B	205	ASP	CB-CA-C	6.75	121.36	110.09
1	A	244	LYS	N-CA-CB	6.67	119.92	110.12
1	B	58	GLU	CB-CG-CD	6.65	123.91	112.60
1	B	267	ASP	CB-CA-C	-6.55	97.66	110.10
1	B	66	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	87	LYS	N-CA-CB	6.42	120.87	110.40
1	A	13	LEU	N-CA-CB	-6.40	100.71	110.12
1	A	72	LYS	CB-CG-CD	6.36	125.93	111.30
1	A	105	TYR	N-CA-CB	-6.35	101.34	110.80
1	A	199	ARG	N-CA-CB	6.34	119.57	110.06
1	B	45	CYS	CB-CA-C	-6.30	108.29	115.79
1	B	20	ARG	CD-NE-CZ	6.28	133.19	124.40
1	B	41	ARG	CD-NE-CZ	6.19	133.07	124.40
1	B	87	LYS	N-CA-CB	6.15	120.60	110.39
1	B	20	ARG	CB-CG-CD	-6.04	97.41	111.30
1	B	153	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	242	THR	OG1-CB-CG2	-5.99	97.31	109.30
1	B	249	LYS	CB-CA-C	5.99	120.47	109.46
1	B	63	LYS	CB-CA-C	5.90	121.11	111.26
1	B	1	ASN	CB-CA-C	5.83	121.18	110.10
1	A	136	GLU	CG-CD-OE1	-5.78	105.12	118.40
1	A	116	GLU	N-CA-CB	5.74	118.65	110.16
1	A	86	THR	N-CA-CB	5.73	119.16	110.28
1	B	116	GLU	CB-CG-CD	5.68	122.26	112.60
1	A	253	LYS	CG-CD-CE	-5.64	98.33	111.30
1	A	174	ASN	CB-CA-C	-5.63	101.89	111.02
1	B	244	LYS	CB-CG-CD	5.62	124.22	111.30
1	B	231	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	202	VAL	N-CA-CB	5.57	118.00	111.87
1	A	66	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	205	ASP	CB-CA-C	5.53	119.96	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	132	ILE	N-CA-C	-5.48	107.41	112.83
1	B	84	ILE	N-CA-C	-5.46	106.37	111.45
1	A	85	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	249	LYS	CB-CA-C	5.41	118.77	109.51
1	B	230	LYS	CB-CA-C	-5.38	101.77	109.84
1	B	130	ARG	CD-NE-CZ	5.36	131.90	124.40
1	B	20	ARG	CA-CB-CG	5.33	124.76	114.10
1	B	151	PRO	N-CA-CB	-5.32	98.48	103.27
1	A	260[A]	ARG	N-CA-CB	5.29	117.67	110.01
1	A	260[B]	ARG	N-CA-CB	5.29	117.67	110.01
1	A	131	SER	CA-C-N	-5.28	114.78	122.28
1	A	131	SER	C-N-CA	-5.28	114.78	122.28
1	B	229	PRO	N-CA-C	-5.27	103.50	111.41
1	A	63	LYS	CB-CA-C	5.22	119.98	111.26
1	B	8	LYS	N-CA-CB	5.20	117.77	110.12
1	A	59	ARG	N-CA-CB	5.19	117.75	110.12
1	B	234	PRO	N-CA-C	5.18	119.34	111.11
1	A	157	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	2	LYS	CB-CG-CD	5.12	123.07	111.30
1	B	192	THR	OG1-CB-CG2	5.11	119.52	109.30
1	B	131	SER	CA-C-N	-5.09	114.51	122.09
1	B	131	SER	C-N-CA	-5.09	114.51	122.09
1	B	244	LYS	N-CA-CB	5.08	117.68	110.16
1	B	203	PRO	N-CA-CB	5.08	107.83	103.31
1	A	188	LEU	CA-C-O	-5.06	115.50	120.82
1	B	41	ARG	CB-CA-C	-5.04	101.20	109.53
1	A	165	ASN	CA-CB-CG	-5.03	107.57	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Mainchain,Peptide
1	A	260[A]	ARG	Sidechain
1	A	260[B]	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	20	ARG	Sidechain
1	B	232	ARG	Sidechain
1	B	243	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2075	0	2076	35	0
1	B	2077	0	2071	26	0
2	A	17	0	11	1	0
2	B	17	0	11	0	0
3	A	7	0	10	4	0
4	A	5	0	0	4	0
5	A	2	0	0	4	0
6	B	13	0	18	6	0
7	B	4	0	5	4	0
8	A	88	0	0	5	0
8	B	95	0	0	1	0
All	All	4400	0	4202	69	0

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

All (69) 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)
6:B:302:PG4:H72	7:B:303:EDO:H12	1.18	1.08
1:A:82:SER:O	1:A:86:THR:HG23	1.52	1.04
6:B:302:PG4:C7	7:B:303:EDO:H12	1.90	1.00
1:A:112:ASN:O	1:A:116:GLU:HG3	1.65	0.95
1:B:82:SER:O	1:B:86:THR:HG23	1.65	0.94
6:B:302:PG4:H72	7:B:303:EDO:C1	2.09	0.80
1:B:112:ASN:O	1:B:116:GLU:HG3	1.81	0.80
1:B:267:ASP:C	6:B:302:PG4:H12	2.06	0.79
1:A:66:ASP:H	1:A:69:GLN:HE21	1.33	0.76
3:A:302:PEG:H12	4:A:303:PO4:O2	1.92	0.68
3:A:302:PEG:C1	4:A:303:PO4:O2	2.42	0.68
1:B:66:ASP:H	1:B:69:GLN:NE2	1.92	0.67
1:A:253:LYS:HG3	8:A:404:HOH:O	1.94	0.67
1:B:66:ASP:H	1:B:69:GLN:HE21	1.43	0.66
3:A:302:PEG:H21	4:A:303:PO4:O2	1.99	0.63
3:A:302:PEG:C2	4:A:303:PO4:O2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:HB2	1:A:260[A]:ARG:HG3	1.82	0.59
1:A:17:PHE:CE2	1:A:243:ARG:HD2	2.37	0.59
1:B:57:LEU:HB3	1:B:180:VAL:HG13	1.86	0.58
1:B:267:ASP:C	6:B:302:PG4:C1	2.78	0.57
1:A:223:ASP:OD2	5:A:305:CL:CL	2.61	0.56
1:A:57:LEU:HD11	1:A:187:TRP:CZ3	2.42	0.55
1:A:134:ASP:OD2	5:A:304:CL:CL	2.62	0.55
1:A:260[B]:ARG:NH2	8:A:404:HOH:O	2.40	0.55
1:B:123:GLU:HG2	8:B:468:HOH:O	2.07	0.55
1:A:66:ASP:H	1:A:69:GLN:NE2	2.02	0.55
1:A:82:SER:O	1:A:86:THR:CG2	2.40	0.54
1:A:62:GLN:OE1	1:A:64:LYS:HE3	2.07	0.54
1:B:17:PHE:CE2	1:B:243:ARG:HD2	2.43	0.53
1:A:194:GLY:O	5:A:305:CL:CL	2.65	0.52
1:A:112:ASN:O	1:A:116:GLU:CG	2.49	0.51
1:A:161:LYS:CE	8:A:408:HOH:O	2.59	0.50
1:B:46:SER:HB2	1:B:213:GLY:HA2	1.94	0.49
1:A:103:LEU:C	1:A:103:LEU:HD23	2.37	0.49
1:A:137:PHE:HB2	5:A:304:CL:CL	2.49	0.49
1:A:52:LEU:C	1:A:52:LEU:HD23	2.39	0.48
1:A:82:SER:HB3	1:A:85:THR:OG1	2.15	0.46
1:B:112:ASN:O	1:B:116:GLU:CG	2.57	0.46
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.67	0.46
1:B:177:ASN:OD1	1:B:177:ASN:C	2.59	0.46
1:B:17:PHE:CD2	1:B:243:ARG:HD2	2.50	0.46
1:B:264:GLN:O	1:B:267:ASP:HB2	2.16	0.45
1:B:57:LEU:HB3	1:B:180:VAL:CG1	2.46	0.45
1:B:167:LEU:HD21	1:B:226:VAL:HG23	1.97	0.45
1:A:63:LYS:HB3	1:A:63:LYS:HE2	1.50	0.45
1:A:70:LYS:HE3	1:A:70:LYS:HA	1.99	0.44
1:A:136:GLU:HG3	1:A:162:ALA:HB2	1.98	0.44
6:B:302:PG4:H71	7:B:303:EDO:H12	1.91	0.44
1:A:36:TYR:CE2	1:A:37:ARG:HG3	2.53	0.44
1:B:27:ASP:HB2	1:B:266:ILE:HD12	1.99	0.44
1:A:201:SER:HB2	1:A:260[B]:ARG:HG2	2.00	0.43
1:B:23:VAL:HG11	1:B:262:ALA:HB2	2.01	0.43
1:A:46:SER:HB2	1:A:213:GLY:HA2	2.01	0.43
1:B:82:SER:HB3	1:B:85:THR:OG1	2.19	0.43
1:A:119:LEU:O	1:A:124:GLY:HA3	2.18	0.43
1:A:154:LYS:NZ	8:A:409:HOH:O	2.50	0.43
1:A:219:GLY:HA3	1:A:243:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB3	2:A:301:NXL:H3	2.00	0.42
1:B:74:GLU:H	1:B:74:GLU:CD	2.25	0.42
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.91	0.41
1:A:14:GLU:HB3	1:A:21:ILE:HD12	2.02	0.41
1:A:25:ALA:HA	1:A:236:ILE:O	2.20	0.41
1:B:100:SER:HB3	1:B:187:TRP:CE2	2.55	0.41
1:A:161:LYS:NZ	8:A:408:HOH:O	2.48	0.41
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.86	0.41
1:A:114:ILE:HG22	1:A:119:LEU:HD22	2.02	0.41
1:B:38:SER:HB2	1:B:161:LYS:HB2	2.03	0.41
1:B:137:PHE:CD1	1:B:137:PHE:C	2.98	0.41
1:B:49:LYS:HE2	1:B:111:THR:OG1	2.21	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	267/275 (97%)	258 (97%)	8 (3%)	1 (0%)	30	36
1	B	268/275 (98%)	261 (97%)	6 (2%)	1 (0%)	30	36
All	All	535/550 (97%)	519 (97%)	14 (3%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	ALA
1	A	73	TYR

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	218/224 (97%)	203 (93%)	15 (7%)	13	16
1	B	218/224 (97%)	204 (94%)	14 (6%)	14	18
All	All	436/448 (97%)	407 (93%)	29 (7%)	14	17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	17	PHE
1	A	70	LYS
1	A	72	LYS
1	A	86	THR
1	A	87	LYS
1	A	119	LEU
1	A	123	GLU
1	A	127	LYS
1	A	145[A]	GLU
1	A	145[B]	GLU
1	A	230	LYS
1	A	232	ARG
1	A	243	ARG
1	A	244	LYS
1	B	17	PHE
1	B	61	GLN
1	B	70	LYS
1	B	74	GLU
1	B	86	THR
1	B	106	SER
1	B	119	LEU
1	B	123	GLU
1	B	127	LYS
1	B	214	SER
1	B	230	LYS
1	B	249	LYS

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Mol	Chain	Res	Type
1	B	253	LYS
1	B	264	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	69	GLN
1	A	147	ASN
1	B	69	GLN
1	B	81	HIS
1	B	168	ASN
1	B	186	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	PEG	A	302	-	6,6,6	0.87	0	5,5,5	0.31	0
2	NXL	A	301	1	14,17,17	1.84	1 (7%)	17,24,24	1.52	4 (23%)
6	PG4	B	302	-	12,12,12	0.56	0	11,11,11	0.52	0
7	EDO	B	303	-	3,3,3	0.83	0	2,2,2	2.54	1 (50%)
4	PO4	A	303	-	4,4,4	1.49	1 (25%)	6,6,6	0.74	0
2	NXL	B	301	1	14,17,17	1.79	3 (21%)	17,24,24	1.92	6 (35%)

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
3	PEG	A	302	-	-	2/4/4/4	-
2	NXL	A	301	1	-	0/5/25/25	0/1/1/1
6	PG4	B	302	-	-	7/10/10/10	-
7	EDO	B	303	-	-	0/1/1/1	-
2	NXL	B	301	1	-	0/5/25/25	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NXL	C-NAA	6.39	1.49	1.32
2	B	301	NXL	C-NAA	4.99	1.45	1.32
2	B	301	NXL	O-C	-3.18	1.17	1.23
4	A	303	PO4	P-O2	2.75	1.62	1.54
2	B	301	NXL	CAJ-CAO	2.34	1.55	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NXL	OAL-SAR-OAG	4.36	117.12	103.29
2	B	301	NXL	C-CA-N	-3.48	102.93	111.27
7	B	303	EDO	O1-C1-C2	-3.10	89.63	111.91
2	A	301	NXL	CB-CAH-CAO	2.77	114.55	111.48
2	A	301	NXL	CA-C-NAA	2.52	122.70	116.55
2	A	301	NXL	CAO-CAJ-N	-2.35	106.80	110.11
2	B	301	NXL	CB-CAH-CAO	2.31	114.04	111.48
2	B	301	NXL	CAJ-CAO-NAK	2.11	117.02	109.02
2	A	301	NXL	CAH-CB-CA	2.08	114.66	110.30
2	B	301	NXL	O-C-NAA	-2.06	119.42	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NXL	CB-CA-N	2.03	113.24	110.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

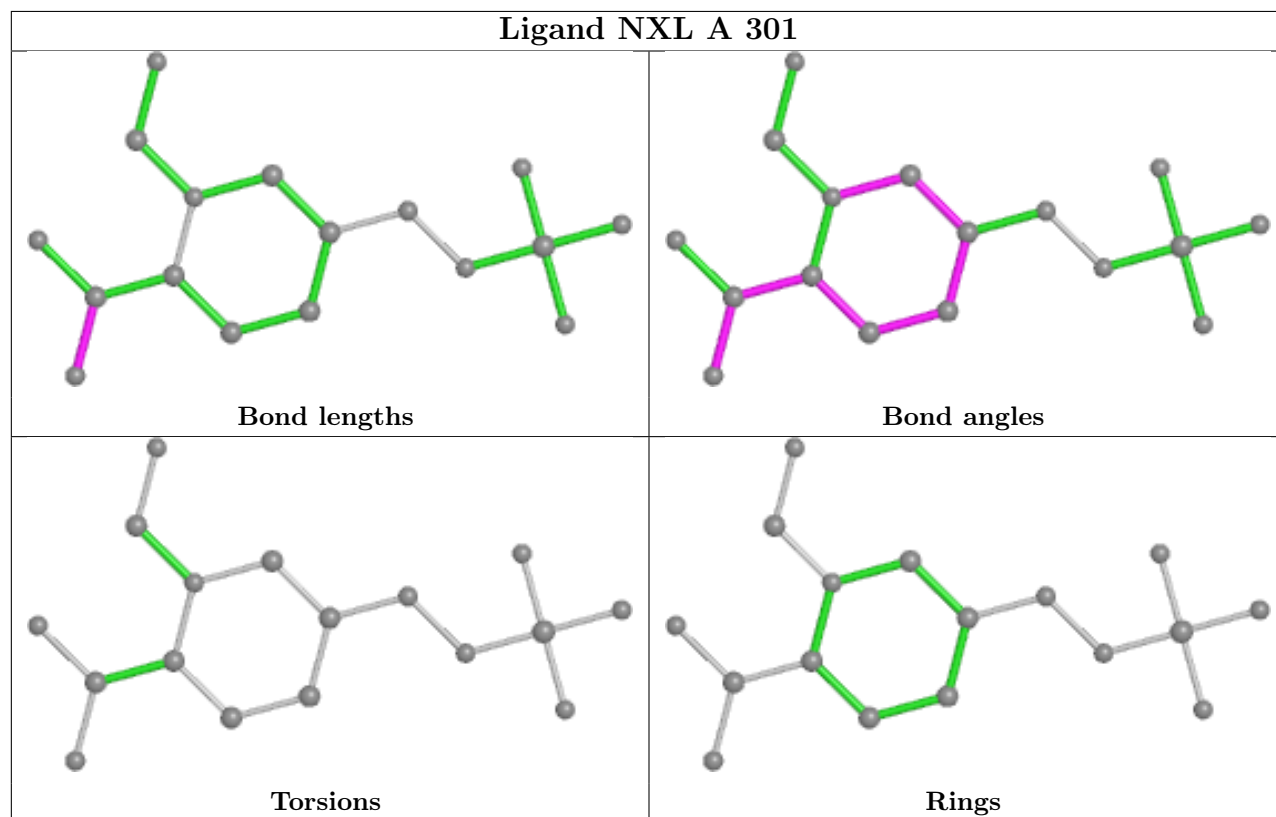
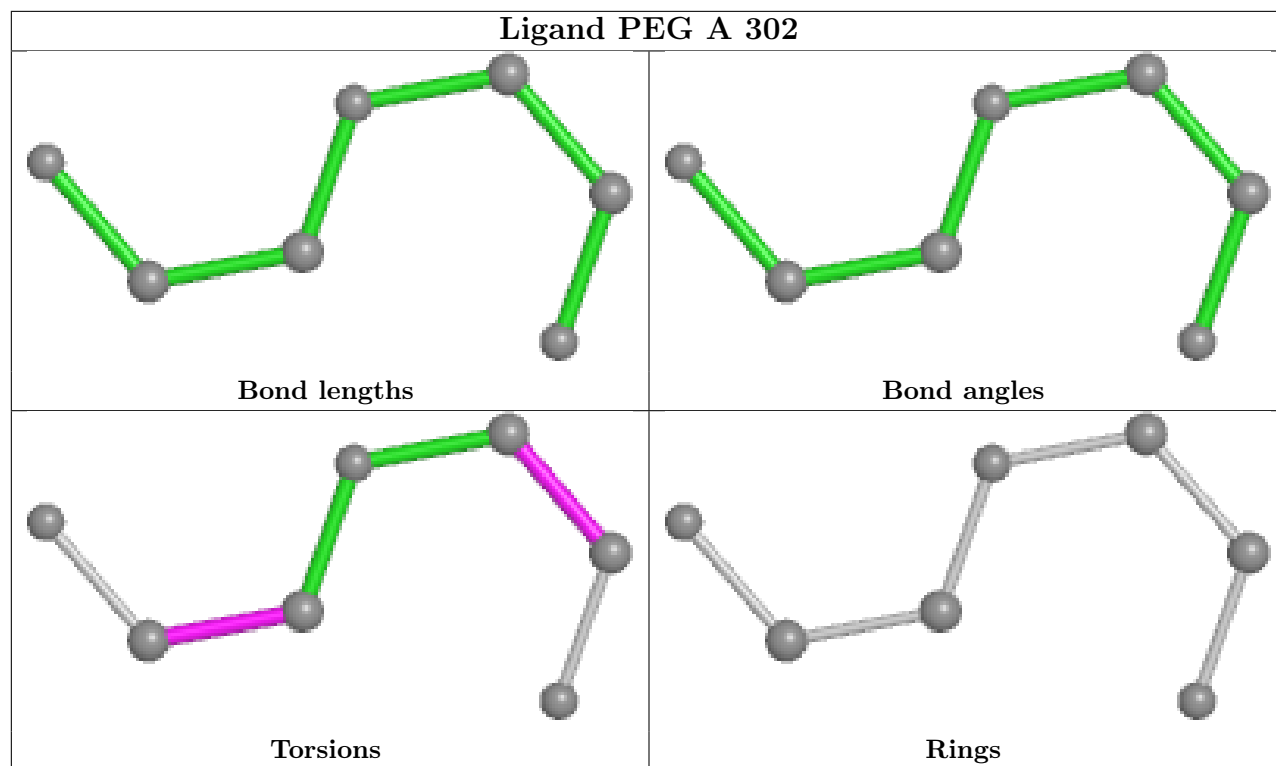
Mol	Chain	Res	Type	Atoms
6	B	302	PG4	O4-C7-C8-O5
3	A	302	PEG	O1-C1-C2-O2
6	B	302	PG4	C3-C4-O3-C5
3	A	302	PEG	O2-C3-C4-O4
6	B	302	PG4	C8-C7-O4-C6
6	B	302	PG4	C4-C3-O2-C2
6	B	302	PG4	C6-C5-O3-C4
6	B	302	PG4	C5-C6-O4-C7
6	B	302	PG4	O3-C5-C6-O4

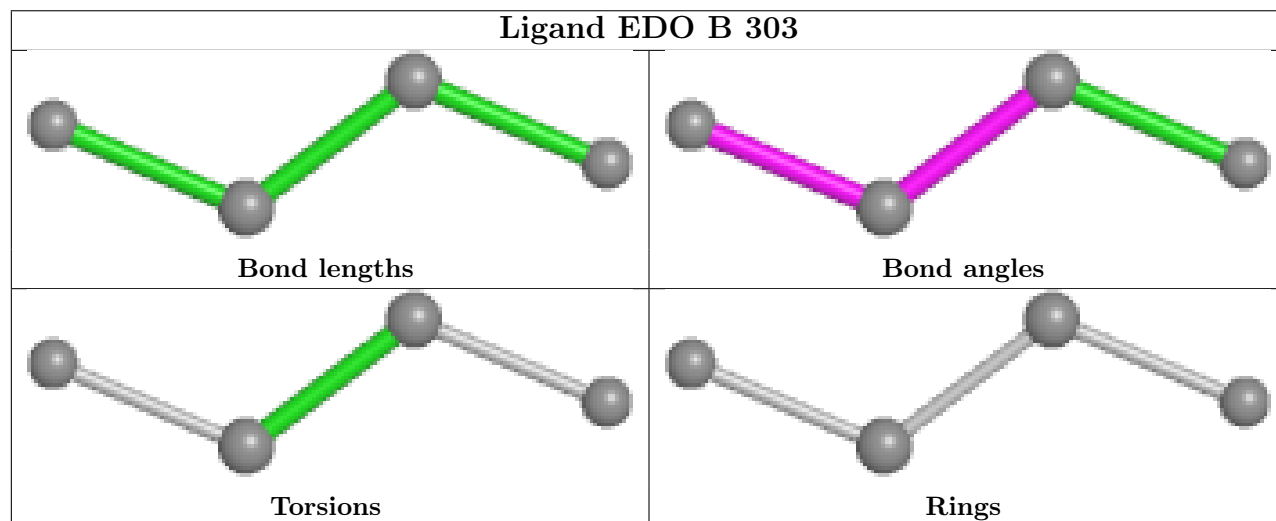
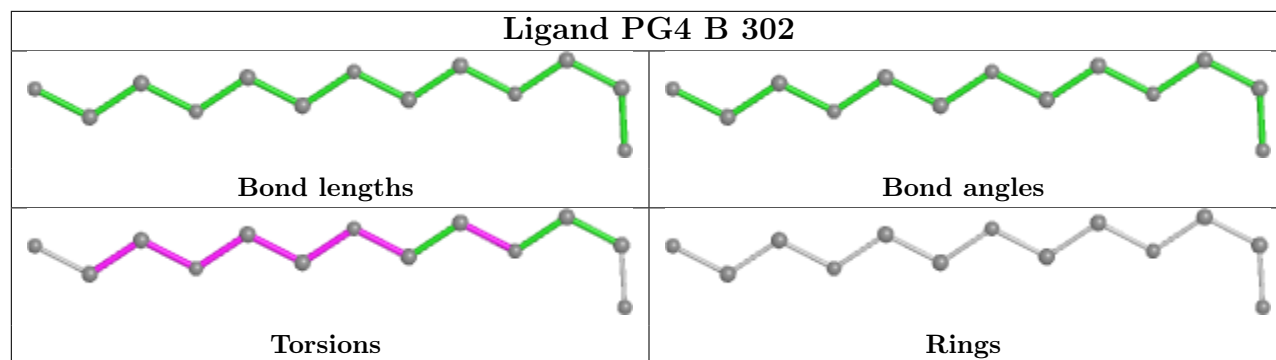
There are no ring outliers.

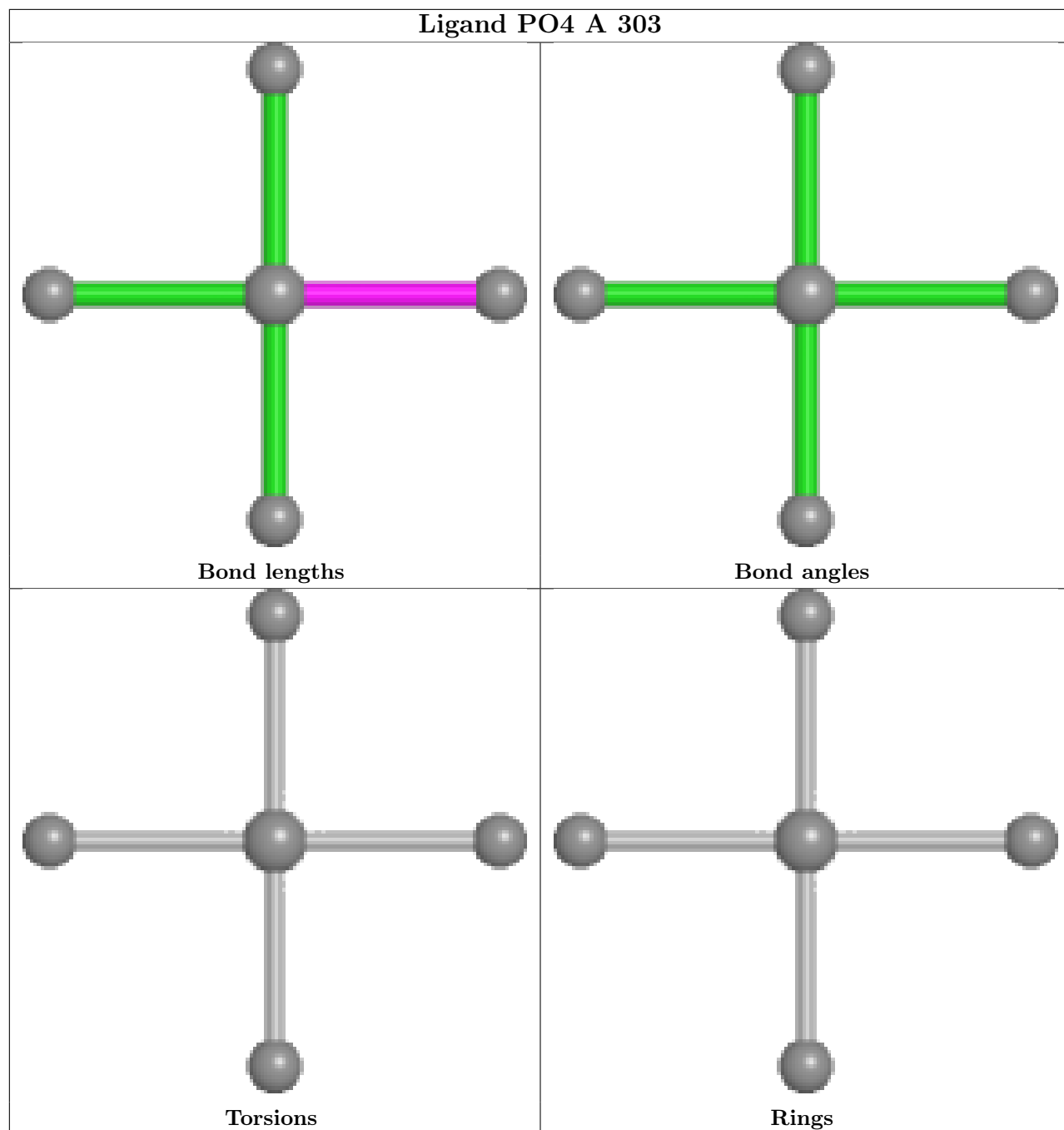
5 monomers are involved in 11 short contacts:

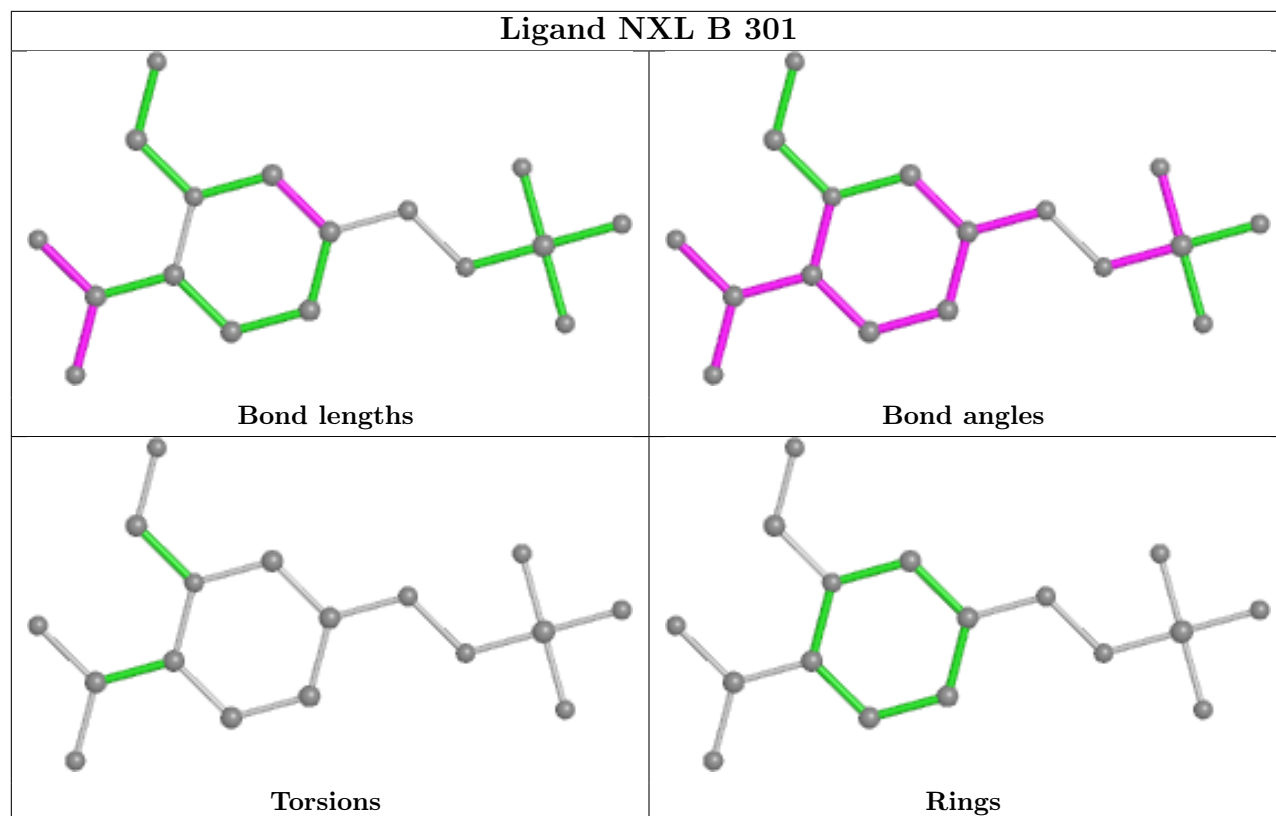
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	PEG	4	0
2	A	301	NXL	1	0
6	B	302	PG4	6	0
7	B	303	EDO	4	0
4	A	303	PO4	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	267/275 (97%)	-1.05	0 100 100	7, 14, 29, 51	2 (0%)
1	B	267/275 (97%)	-1.06	0 100 100	7, 14, 31, 48	2 (0%)
All	All	534/550 (97%)	-1.06	0 100 100	7, 14, 30, 51	4 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	PO4	A	303	5/5	0.87	0.14	56,59,67,73	0
6	PG4	B	302	13/13	0.88	0.09	26,29,36,40	0
3	PEG	A	302	7/7	0.93	0.08	33,39,44,45	0
7	EDO	B	303	4/4	0.93	0.07	26,27,29,30	0
2	NXL	B	301	17/17	0.97	0.06	12,14,24,29	0
2	NXL	A	301	17/17	0.98	0.04	12,15,21,23	0
5	CL	A	305	1/1	0.98	0.10	42,42,42,42	0

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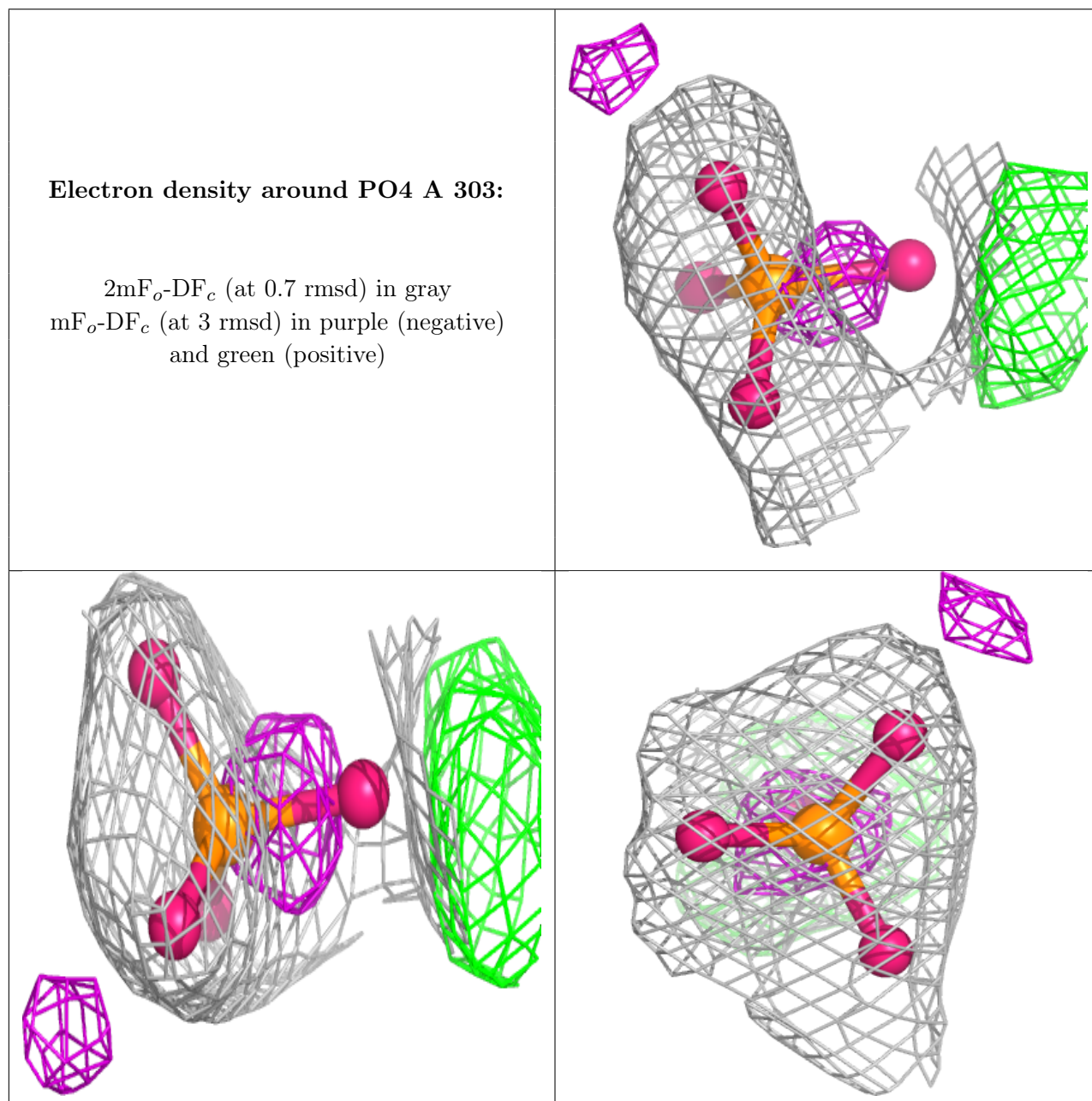
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	A	304	1/1	0.99	0.11	46,46,46,46	0

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.

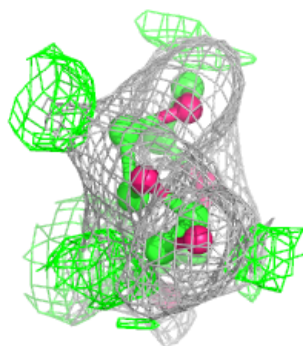
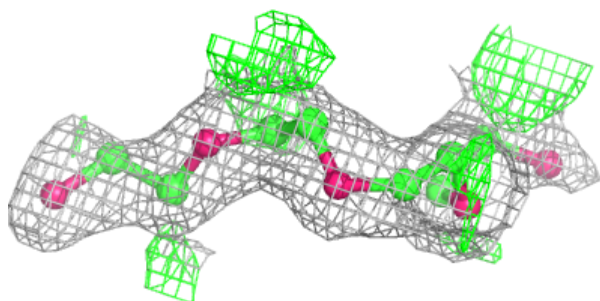
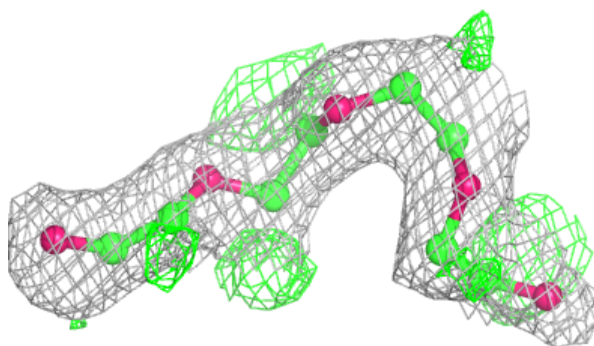
Electron density around PO4 A 303:

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

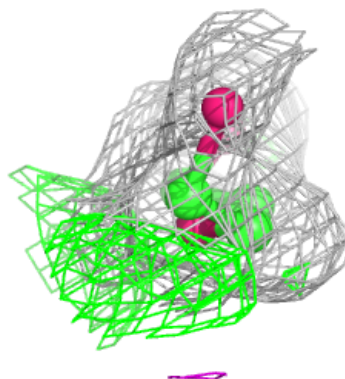
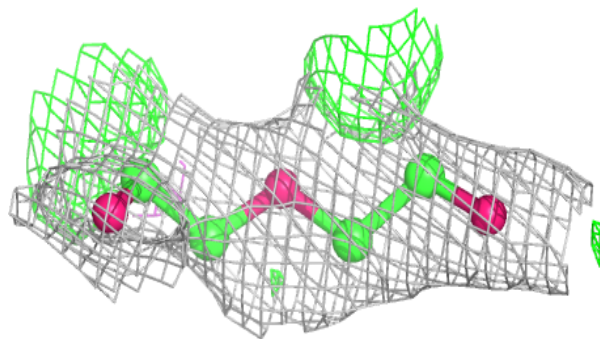
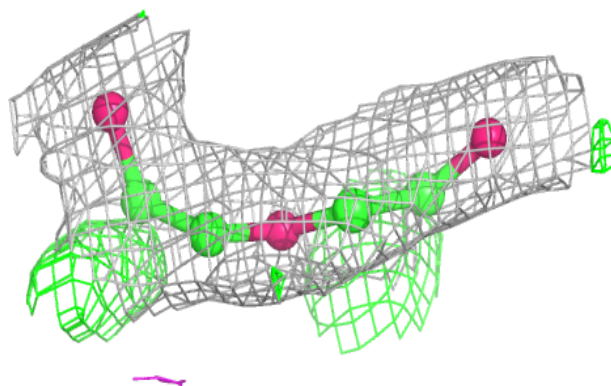


Electron density around PG4 B 302:

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

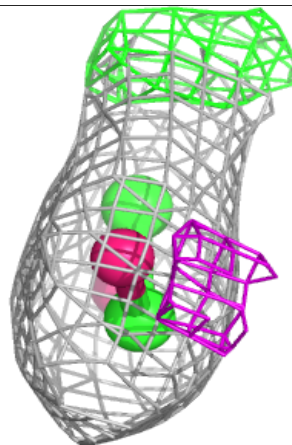
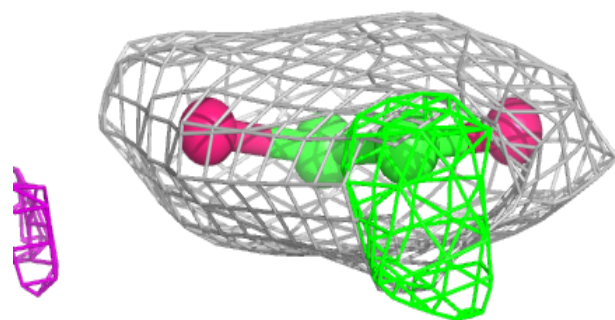
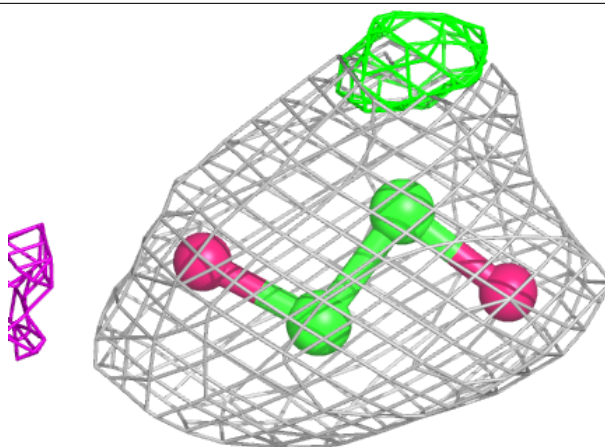
**Electron density around PEG A 302:**

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

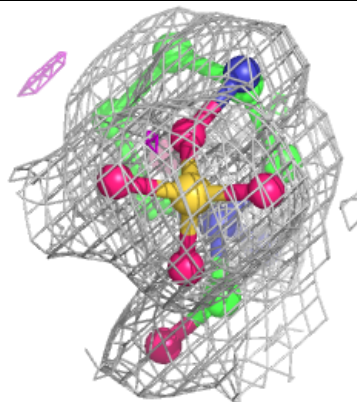
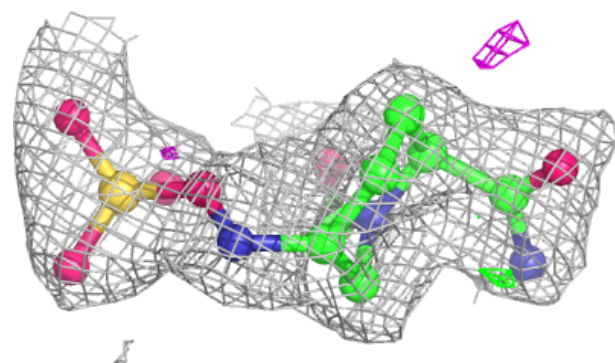
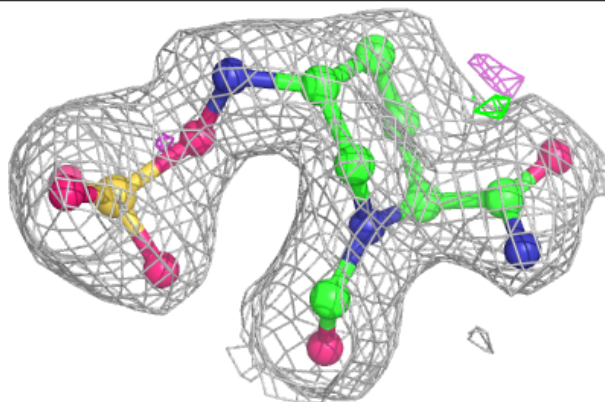


Electron density around EDO B 303:

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

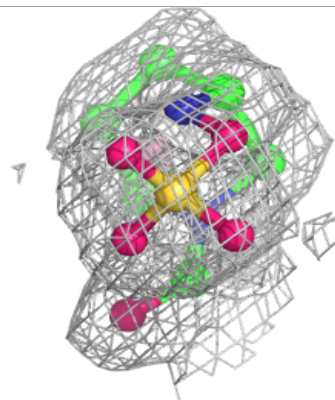
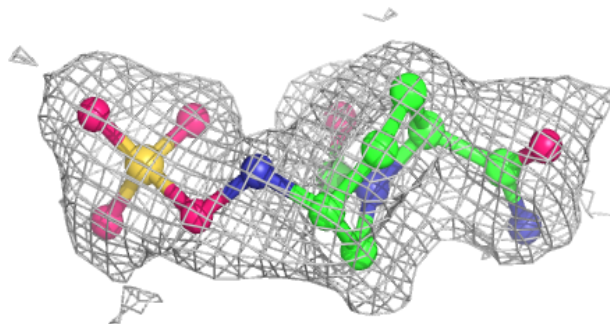
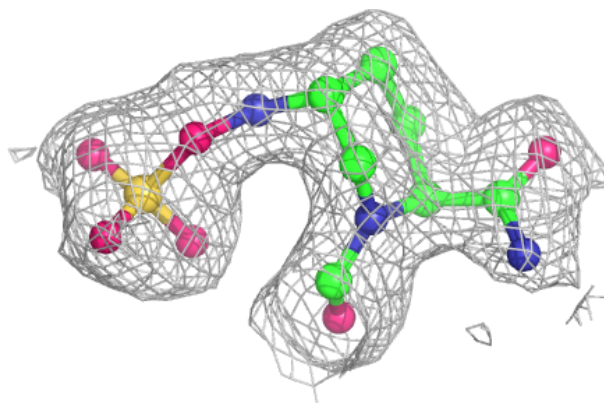
**Electron density around NXL B 301:**

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



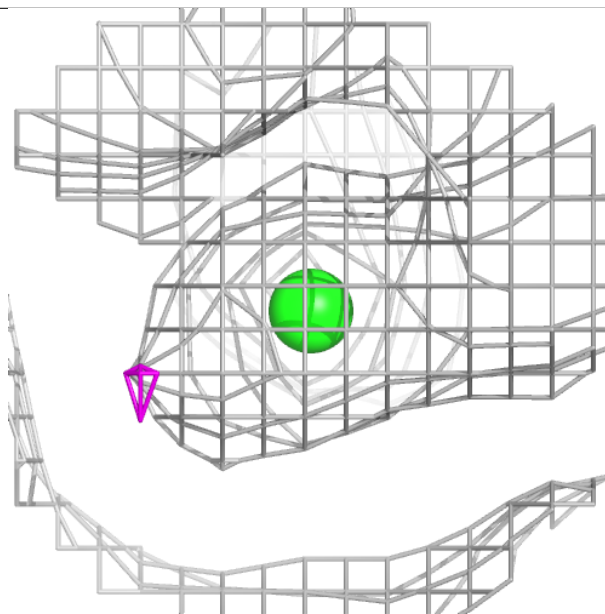
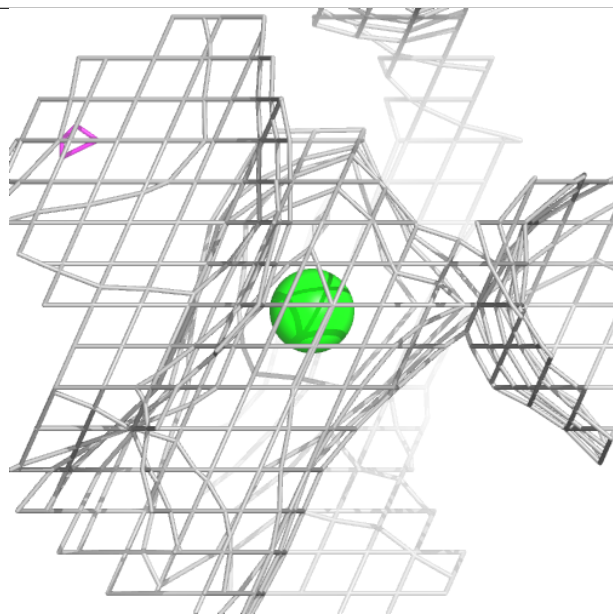
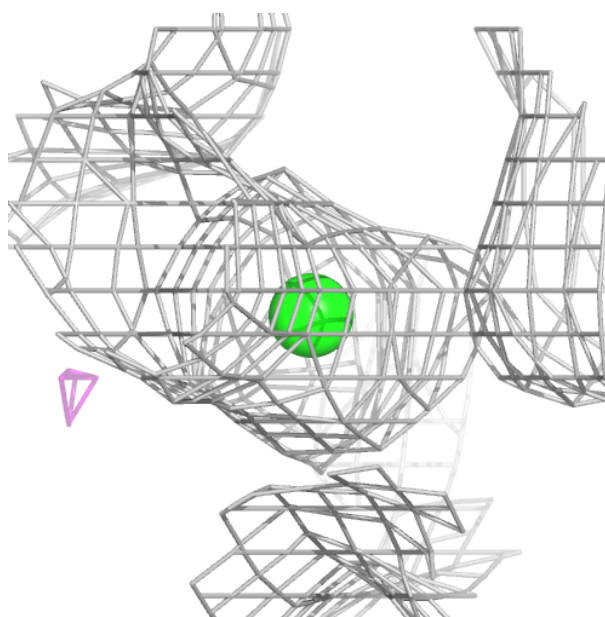
Electron density around NXL A 301:

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



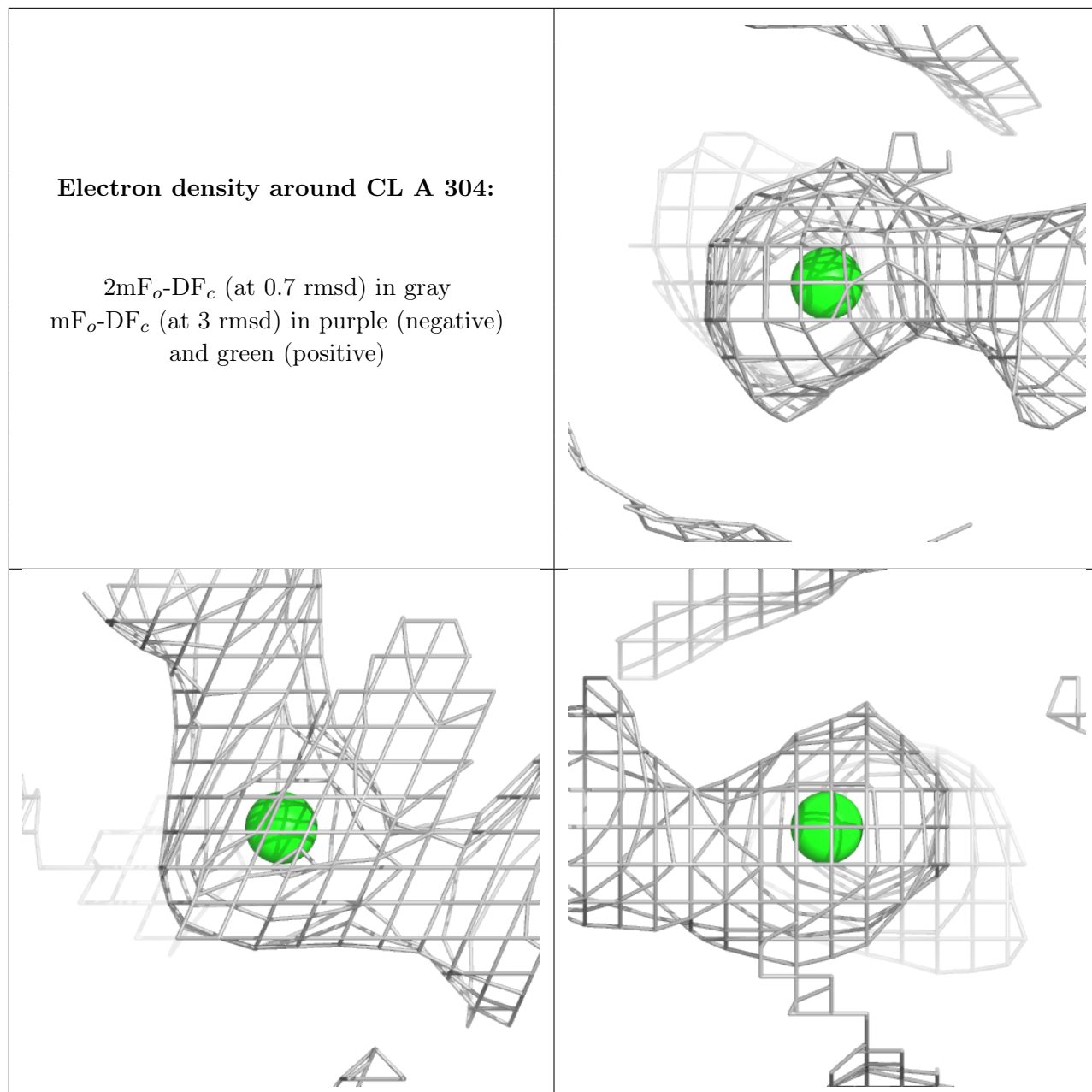
Electron density around CL A 305:

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



Electron density around CL A 304:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.