



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2026 – 02:16 PM JST

PDB ID : 9UJ7 / pdb_00009uj7
Title : Crystal Structure of SME-1 E166A in complex with cefoperazone
Authors : Dhankhar, K.; Hazra, S.
Deposited on : 2025-04-17
Resolution : 2.20 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 : 1.8.5 (274361), CSD as541be (2020)
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

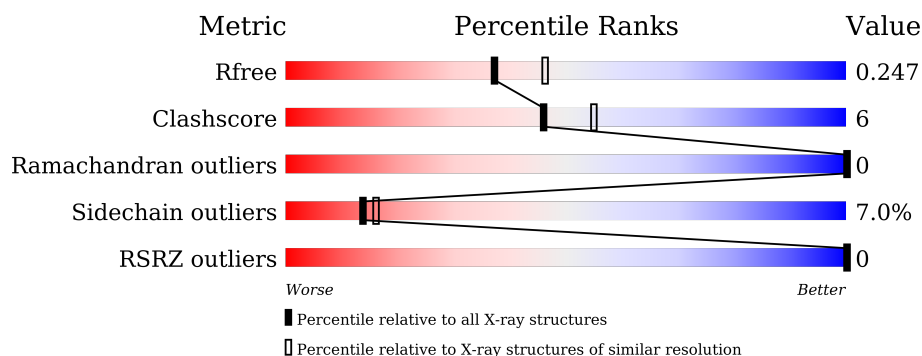
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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
2	DGK	A	301	X	-	-	-
2	DGK	B	301	X	-	-	-
4	CL	A	304	-	-	X	-
4	CL	A	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4313 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.

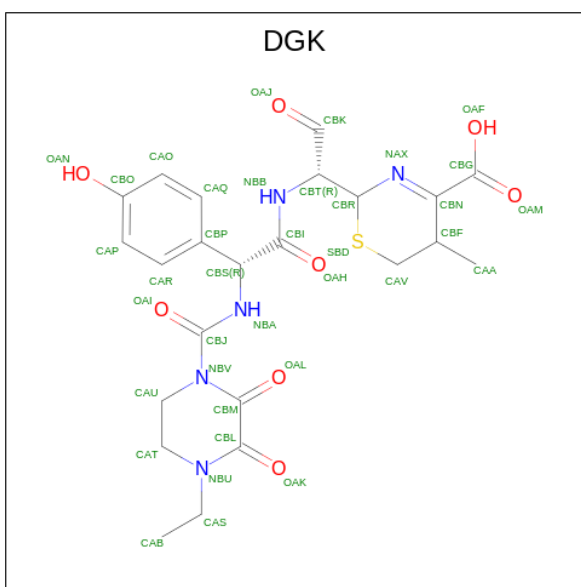
- Molecule 1 is a protein called Beta-lactamase SME-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	267	Total	C	N	O	S	0	0	0
			2057	1288	365	397	7			
1	A	267	Total	C	N	O	S	0	0	0
			2057	1288	365	397	7			

There are 18 discrepancies between the modelled and reference sequences:

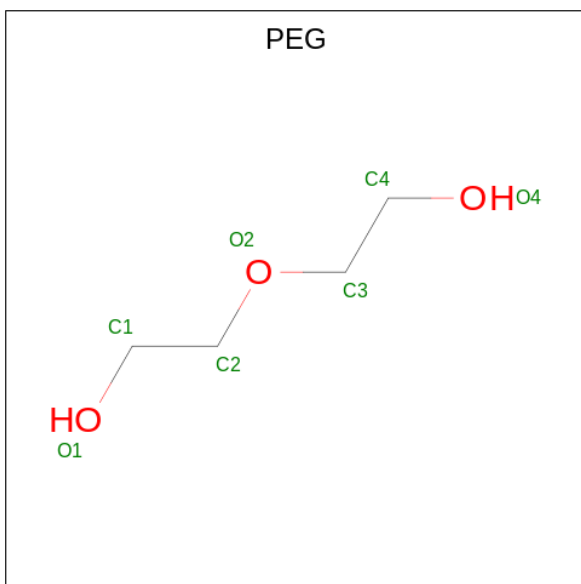
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP P52682
B	0	GLY	-	expression tag	UNP P52682
B	143	ALA	GLU	engineered mutation	UNP P52682
B	268	HIS	-	expression tag	UNP P52682
B	269	HIS	-	expression tag	UNP P52682
B	270	HIS	-	expression tag	UNP P52682
B	271	HIS	-	expression tag	UNP P52682
B	272	HIS	-	expression tag	UNP P52682
B	273	HIS	-	expression tag	UNP P52682
A	-1	MET	-	initiating methionine	UNP P52682
A	0	GLY	-	expression tag	UNP P52682
A	143	ALA	GLU	engineered mutation	UNP P52682
A	268	HIS	-	expression tag	UNP P52682
A	269	HIS	-	expression tag	UNP P52682
A	270	HIS	-	expression tag	UNP P52682
A	271	HIS	-	expression tag	UNP P52682
A	272	HIS	-	expression tag	UNP P52682
A	273	HIS	-	expression tag	UNP P52682

- Molecule 2 is Hydrolysed Cefoperazone (CCD ID: DGK) (formula: $C_{23}H_{27}N_5O_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 37	C 23	N 5	O 8	S 1	0	0
2	A	1	Total 37	C 23	N 5	O 8	S 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	A	5	Total 5	Cl 5	0	0

- Molecule 5 is water.

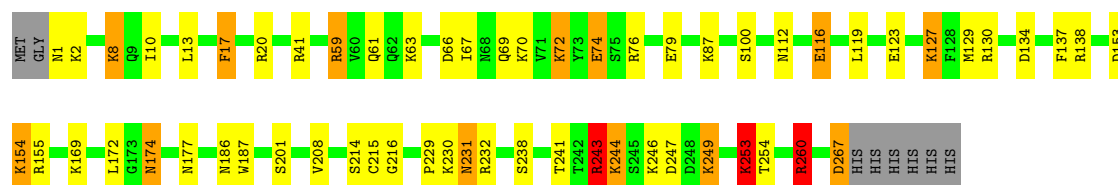
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	61	Total 61	O 61	0	0
5	A	51	Total 51	O 51	0	0

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.

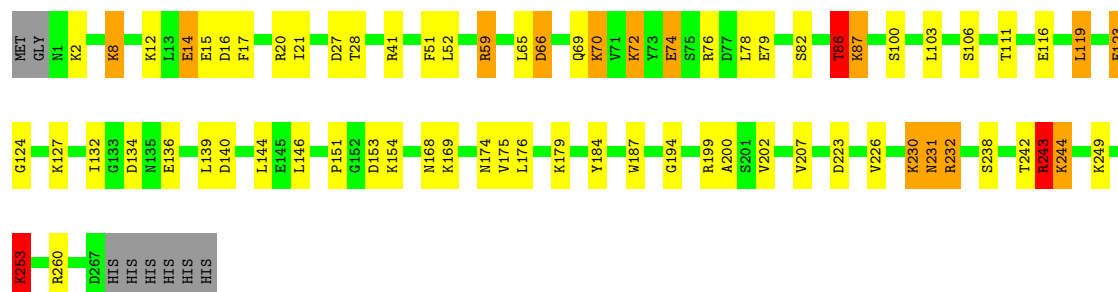
• Molecule 1: Beta-lactamase SME-1

Chain B: 



• Molecule 1: Beta-lactamase SME-1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.59Å 51.35Å 78.00Å 90.00° 114.05° 90.00°	Depositor
Resolution (Å)	23.18 – 2.20 23.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.18-2.20) 99.8 (23.18-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.162 , 0.247 0.162 , 0.247	Depositor DCC
R_{free} test set	1274 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.8	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	4313	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.38% 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: PEG, DGK, CL

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	1.12	3/2092 (0.1%)	1.86	57/2820 (2.0%)
1	B	1.10	1/2092 (0.0%)	1.90	51/2820 (1.8%)
All	All	1.11	4/4184 (0.1%)	1.88	108/5640 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ARG	NE-CZ	8.76	1.42	1.33
1	A	151	PRO	CA-CB	5.65	1.61	1.53
1	B	243	ARG	CZ-NH2	5.32	1.40	1.33
1	A	15	GLU	CD-OE2	5.20	1.35	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	ARG	CD-NE-CZ	12.62	142.07	124.40
1	B	244	LYS	N-CA-CB	12.38	127.97	110.01
1	B	230	LYS	CB-CA-C	12.26	130.25	109.53
1	A	244	LYS	N-CA-CB	12.02	127.43	110.01
1	B	123	GLU	CB-CG-CD	10.83	131.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ASN	CA-CB-CG	-10.34	102.27	112.60
1	A	179	LYS	CB-CG-CD	9.65	133.50	111.30
1	A	244	LYS	CG-CD-CE	9.01	132.01	111.30
1	B	41	ARG	CD-NE-CZ	8.95	136.93	124.40
1	B	246	LYS	CD-CE-NZ	-8.84	83.61	111.90
1	B	127	LYS	CB-CG-CD	8.84	131.63	111.30
1	B	244	LYS	CA-CB-CG	8.56	131.21	114.10
1	B	267	ASP	CB-CA-C	-8.54	93.87	110.10
1	B	249	LYS	CB-CG-CD	8.48	130.81	111.30
1	A	253	LYS	CG-CD-CE	8.37	130.56	111.30
1	A	244	LYS	CB-CG-CD	8.24	130.26	111.30
1	A	202	VAL	N-CA-CB	8.00	118.47	111.67
1	A	8	LYS	CG-CD-CE	7.77	129.16	111.30
1	B	260	ARG	CB-CG-CD	7.59	128.76	111.30
1	A	72	LYS	CD-CE-NZ	7.56	136.08	111.90
1	A	41	ARG	CD-NE-CZ	7.54	134.96	124.40
1	B	244	LYS	CB-CA-C	-7.50	99.11	110.88
1	B	87	LYS	CB-CA-C	-7.34	97.05	110.63
1	B	169	LYS	CG-CD-CE	7.32	128.12	111.30
1	B	41	ARG	CA-CB-CG	-7.31	99.48	114.10
1	A	243	ARG	CD-NE-CZ	7.30	134.63	124.40
1	B	243	ARG	NE-CZ-NH2	7.25	125.72	119.20
1	B	76	ARG	CD-NE-CZ	-7.24	114.26	124.40
1	B	79	GLU	CB-CG-CD	7.24	124.90	112.60
1	A	86	THR	CA-CB-OG1	7.24	120.45	109.60
1	A	86	THR	CA-CB-CG2	7.23	122.79	110.50
1	A	207	VAL	N-CA-CB	-7.20	102.35	110.99
1	B	63	LYS	CB-CA-C	7.18	123.25	111.26
1	B	72	LYS	CD-CE-NZ	7.15	134.77	111.90
1	A	70	LYS	CB-CG-CD	7.13	127.69	111.30
1	B	8	LYS	CG-CD-CE	-7.07	95.03	111.30
1	B	232	ARG	CB-CG-CD	-6.99	95.22	111.30
1	B	244	LYS	CB-CG-CD	6.97	127.33	111.30
1	B	1	ASN	CB-CA-C	6.88	123.17	110.10
1	A	123	GLU	CA-C-N	6.86	127.55	120.00
1	A	123	GLU	C-N-CA	6.86	127.55	120.00
1	B	231	ASN	CA-CB-CG	6.83	119.42	112.60
1	A	59	ARG	NE-CZ-NH2	-6.78	113.10	119.20
1	B	246	LYS	CG-CD-CE	6.75	126.83	111.30
1	B	243	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	A	249	LYS	CB-CG-CD	6.68	126.66	111.30
1	A	12	LYS	CB-CG-CD	6.59	126.46	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	20	ARG	CD-NE-CZ	6.51	133.52	124.40
1	B	260	ARG	CG-CD-NE	-6.48	97.75	112.00
1	A	153	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	74	GLU	CB-CA-C	-6.41	96.91	110.31
1	A	232	ARG	CA-CB-CG	-6.26	101.57	114.10
1	A	168	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	253	LYS	CA-CB-CG	-6.05	102.00	114.10
1	A	140	ASP	N-CA-C	-6.04	106.56	114.04
1	A	2	LYS	N-CA-C	-6.00	105.45	112.89
1	A	243	ARG	CA-CB-CG	-5.99	102.13	114.10
1	B	229	PRO	N-CA-C	-5.98	102.84	111.22
1	A	140	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	63	LYS	CB-CG-CD	5.92	124.92	111.30
1	A	79	GLU	CB-CG-CD	5.86	122.56	112.60
1	B	172	LEU	N-CA-CB	5.86	118.69	110.90
1	B	8	LYS	N-CA-CB	5.78	119.19	110.30
1	B	2	LYS	CG-CD-CE	5.76	124.55	111.30
1	A	66	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	132	ILE	N-CA-C	-5.67	106.79	112.17
1	B	253	LYS	CD-CE-NZ	5.65	129.99	111.90
1	B	2	LYS	CD-CE-NZ	5.64	129.94	111.90
1	A	260	ARG	N-CA-CB	5.61	118.37	110.12
1	B	216	GLY	O-C-N	-5.60	114.90	122.35
1	A	66	ASP	N-CA-CB	-5.58	101.80	110.57
1	A	66	ASP	CB-CA-C	5.57	119.35	109.72
1	A	8	LYS	N-CA-CB	5.54	118.37	110.16
1	B	10	ILE	N-CA-CB	5.54	117.66	110.57
1	A	116	GLU	CB-CG-CD	5.53	122.01	112.60
1	A	169	LYS	CG-CD-CE	5.52	124.00	111.30
1	A	16	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	174	ASN	CB-CA-C	-5.46	99.23	109.72
1	A	14	GLU	CG-CD-OE2	-5.44	105.89	118.40
1	A	51	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	247	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	238	SER	N-CA-CB	-5.41	102.28	110.77
1	B	215	CYS	CA-C-N	-5.40	109.35	121.18
1	B	215	CYS	C-N-CA	-5.40	109.35	121.18
1	A	41	ARG	CB-CG-CD	-5.32	99.07	111.30
1	A	86	THR	N-CA-CB	5.31	118.52	110.28
1	A	230	LYS	CB-CA-C	5.30	118.16	109.90
1	B	154	LYS	CG-CD-CE	5.29	123.48	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ASN	CA-CB-CG	-5.28	107.32	112.60
1	A	154	LYS	CB-CA-C	5.28	118.83	109.65
1	A	200	ALA	N-CA-C	-5.22	106.86	113.18
1	A	28	THR	CA-CB-OG1	-5.20	101.80	109.60
1	B	208	VAL	N-CA-CB	-5.18	102.94	111.44
1	A	87	LYS	N-CA-CB	5.18	118.31	110.28
1	B	116	GLU	CB-CA-C	5.17	120.79	109.99
1	B	241	THR	CA-CB-CG2	5.15	119.25	110.50
1	B	238	SER	N-CA-CB	-5.14	102.69	110.77
1	B	87	LYS	CB-CG-CD	-5.10	99.56	111.30
1	B	130	ARG	N-CA-CB	5.09	118.06	110.22
1	A	2	LYS	N-CA-CB	5.08	118.69	110.40
1	A	226	VAL	CB-CA-C	-5.08	103.93	110.84
1	A	27	ASP	CA-CB-CG	5.05	117.66	112.60
1	A	136	GLU	CG-CD-OE1	-5.03	106.82	118.40
1	B	116	GLU	CB-CG-CD	5.03	121.14	112.60
1	A	184	TYR	N-CA-C	-5.03	105.71	111.14
1	A	74	GLU	CB-CG-CD	-5.02	104.07	112.60
1	A	116	GLU	CB-CA-C	5.01	120.61	110.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	B	138	ARG	Sidechain
1	B	155	ARG	Sidechain
1	B	243	ARG	Sidechain
1	B	260	ARG	Sidechain
1	B	59	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	2057	0	2054	32	0
1	B	2057	0	2054	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	37	0	0	2	0
2	B	37	0	0	0	0
3	B	7	0	10	0	0
4	A	5	0	0	7	0
4	B	1	0	0	1	0
5	A	51	0	0	2	0
5	B	61	0	0	2	0
All	All	4313	0	4118	47	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 (47) 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:253:LYS:CD	1:A:253:LYS:H	1.51	1.19
1:A:253:LYS:H	1:A:253:LYS:HD2	1.13	1.06
1:A:253:LYS:HD2	1:A:253:LYS:N	1.72	0.98
1:A:253:LYS:CD	1:A:253:LYS:N	2.23	0.97
1:A:253:LYS:H	1:A:253:LYS:HD3	1.34	0.93
1:A:82:SER:O	1:A:86:THR:HG23	1.69	0.91
1:A:199:ARG:HG3	4:A:306:CL:CL	2.19	0.79
1:B:134:ASP:OD2	4:B:303:CL:CL	2.39	0.77
1:A:66:ASP:H	1:A:69:GLN:HE21	1.34	0.75
1:B:66:ASP:H	1:B:69:GLN:HE21	1.32	0.74
1:B:66:ASP:H	1:B:69:GLN:NE2	1.86	0.73
1:B:253:LYS:CE	5:B:434:HOH:O	2.41	0.68
4:A:302:CL:CL	5:A:413:HOH:O	2.49	0.67
1:A:194:GLY:O	4:A:306:CL:CL	2.49	0.67
1:A:144:LEU:HB3	2:A:301:DGK:CAT	2.25	0.66
1:A:144:LEU:HD22	2:A:301:DGK:CAT	2.29	0.63
1:B:253:LYS:HE3	5:B:434:HOH:O	1.99	0.61
1:B:74:GLU:H	1:B:74:GLU:CD	2.12	0.58
1:A:76:ARG:HH11	1:A:76:ARG:HG3	1.70	0.56
1:A:231:ASN:O	1:A:232:ARG:HG3	2.06	0.55
1:A:176:LEU:N	4:A:304:CL:CL	2.61	0.54
1:A:14:GLU:HB3	1:A:21:ILE:HD12	1.87	0.54
1:B:17:PHE:CE2	1:B:243:ARG:HD2	2.43	0.53
1:A:66:ASP:H	1:A:69:GLN:NE2	2.02	0.53
1:B:201:SER:HB2	1:B:260:ARG:HG2	1.92	0.51
1:A:119:LEU:O	1:A:124:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLN:HG3	1:B:177:ASN:ND2	2.28	0.49
1:A:175:VAL:N	4:A:304:CL:CL	2.84	0.48
1:B:59:ARG:HD3	1:B:59:ARG:HA	1.59	0.47
1:A:78:LEU:HD13	1:A:86:THR:HG22	1.96	0.46
1:A:59:ARG:HB2	1:A:65:LEU:HD12	1.96	0.46
1:B:13:LEU:HG	1:B:254:THR:HG23	1.97	0.46
1:A:134:ASP:OD2	4:A:305:CL:CL	2.70	0.46
1:A:76:ARG:HG3	1:A:76:ARG:NH1	2.31	0.45
1:A:74:GLU:HG3	5:A:402:HOH:O	2.17	0.44
1:A:223:ASP:OD2	4:A:306:CL:CL	2.73	0.43
1:A:76:ARG:HD3	1:A:78:LEU:HD23	2.00	0.43
1:A:103:LEU:C	1:A:103:LEU:HD23	2.44	0.43
1:A:139:LEU:HD11	1:A:146:LEU:HD22	2.01	0.43
1:B:100:SER:HB3	1:B:187:TRP:CE2	2.54	0.42
1:A:242:THR:C	1:A:243:ARG:HG3	2.44	0.41
1:B:112:ASN:O	1:B:116:GLU:HG2	2.21	0.41
1:B:129:MET:HG3	1:B:137:PHE:CD1	2.56	0.41
1:A:59:ARG:CB	1:A:65:LEU:HD12	2.51	0.41
1:A:52:LEU:HD13	1:A:111:THR:HG23	2.03	0.40
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.84	0.40
1:A:100:SER:HB3	1:A:187:TRP:CE2	2.56	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	265/275 (96%)	259 (98%)	6 (2%)	0	100	100
1	B	265/275 (96%)	256 (97%)	9 (3%)	0	100	100
All	All	530/550 (96%)	515 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/223 (96%)	201 (94%)	14 (6%)	15	18
1	B	215/223 (96%)	199 (93%)	16 (7%)	13	14
All	All	430/446 (96%)	400 (93%)	30 (7%)	14	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LYS
1	B	17	PHE
1	B	67	ILE
1	B	70	LYS
1	B	72	LYS
1	B	74	GLU
1	B	119	LEU
1	B	127	LYS
1	B	154	LYS
1	B	174	ASN
1	B	214	SER
1	B	231	ASN
1	B	244	LYS
1	B	249	LYS
1	B	253	LYS
1	B	267	ASP
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	106	SER
1	A	119	LEU
1	A	123	GLU

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Mol	Chain	Res	Type
1	A	127	LYS
1	A	230	LYS
1	A	231	ASN
1	A	244	LYS
1	A	253	LYS

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

Mol	Chain	Res	Type
1	B	62	GLN
1	B	69	GLN
1	B	168	ASN
1	B	250	HIS
1	A	69	GLN
1	A	168	ASN
1	A	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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	B	302	-	6,6,6	1.30	0	5,5,5	0.75	0
2	DGK	B	301	1	33,39,39	2.70	6 (18%)	37,55,55	2.66	17 (45%)
2	DGK	A	301	1	33,39,39	3.51	5 (15%)	37,55,55	3.96	14 (37%)

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	B	302	-	-	1/4/4/4	-
2	DGK	B	301	1	2/2/12/15	4/25/62/62	0/2/3/3
2	DGK	A	301	1	3/3/12/15	6/25/62/62	0/2/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	DGK	CBN-NAX	18.73	1.44	1.28
2	B	301	DGK	CBN-NAX	12.66	1.39	1.28
2	B	301	DGK	CBF-CBN	-5.15	1.44	1.51
2	A	301	DGK	CBT-NBB	-3.58	1.41	1.46
2	B	301	DGK	CAT-CAU	3.11	1.63	1.51
2	A	301	DGK	OAF-CBG	-2.93	1.22	1.30
2	A	301	DGK	CAA-CBF	-2.88	1.43	1.52
2	B	301	DGK	CAA-CBF	-2.72	1.43	1.52
2	B	301	DGK	CAU-NBV	2.61	1.52	1.48
2	B	301	DGK	CAS-NBU	2.41	1.57	1.48
2	A	301	DGK	CBL-NBU	-2.04	1.32	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DGK	CBT-NBB-CBI	14.82	139.31	123.12
2	A	301	DGK	CAA-CBF-CBN	11.18	126.95	109.96
2	B	301	DGK	CAA-CBF-CBN	9.49	124.39	109.96
2	A	301	DGK	OAJ-CBK-CBT	-7.76	103.19	124.83
2	A	301	DGK	OAH-CBI-NBB	-5.64	112.48	122.93
2	B	301	DGK	OAI-CBJ-NBV	5.19	125.60	119.78
2	B	301	DGK	OAJ-CBK-CBT	-4.69	111.75	124.83
2	A	301	DGK	CBI-CBS-NBA	-4.54	94.52	108.44
2	A	301	DGK	CAV-CBF-CBN	4.36	119.62	108.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DGK	OAL-CBM-NBV	4.26	127.20	119.98
2	B	301	DGK	OAK-CBL-NBU	3.96	127.78	123.66
2	A	301	DGK	CBS-CBI-NBB	3.60	126.14	116.82
2	A	301	DGK	CBP-CBS-CBI	3.43	115.88	108.16
2	A	301	DGK	CBG-CBN-NAX	-3.36	108.21	116.45
2	B	301	DGK	OAL-CBM-NBV	3.21	125.44	119.98
2	B	301	DGK	CAU-CAT-NBU	3.18	117.26	110.44
2	B	301	DGK	NBA-CBJ-NBV	-3.05	109.60	114.04
2	B	301	DGK	CBI-CBS-NBA	-2.91	99.52	108.44
2	A	301	DGK	OAI-CBJ-NBV	2.87	123.00	119.78
2	B	301	DGK	CBG-CBN-NAX	-2.85	109.46	116.45
2	B	301	DGK	CAV-CBF-CBN	2.75	115.61	108.72
2	B	301	DGK	CAT-CAU-NBV	2.61	113.70	108.78
2	A	301	DGK	CAU-CAT-NBU	2.55	115.90	110.44
2	B	301	DGK	CAT-NBU-CAS	2.54	121.50	116.79
2	B	301	DGK	OAL-CBM-CBL	-2.42	114.60	118.83
2	B	301	DGK	OAF-CBG-OAM	2.34	128.97	123.61
2	B	301	DGK	OAK-CBL-CBM	-2.30	114.81	118.83
2	B	301	DGK	CBT-NBB-CBI	2.26	125.59	123.12
2	A	301	DGK	CBS-NBA-CBJ	2.24	125.40	121.17
2	B	301	DGK	OAH-CBI-CBS	2.21	124.48	120.64
2	A	301	DGK	CAT-CAU-NBV	2.15	112.83	108.78

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	301	DGK	CBF
2	B	301	DGK	CBR
2	A	301	DGK	CBF
2	A	301	DGK	CBR
2	A	301	DGK	CBT

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	DGK	OAF-CBG-CBN-CBF
2	B	301	DGK	CAB-CAS-NBU-CAT
2	B	301	DGK	CAB-CAS-NBU-CBL
2	A	301	DGK	OAH-CBI-NBB-CBT
2	A	301	DGK	CBS-CBI-NBB-CBT
2	A	301	DGK	CAB-CAS-NBU-CAT
3	B	302	PEG	O2-C3-C4-O4

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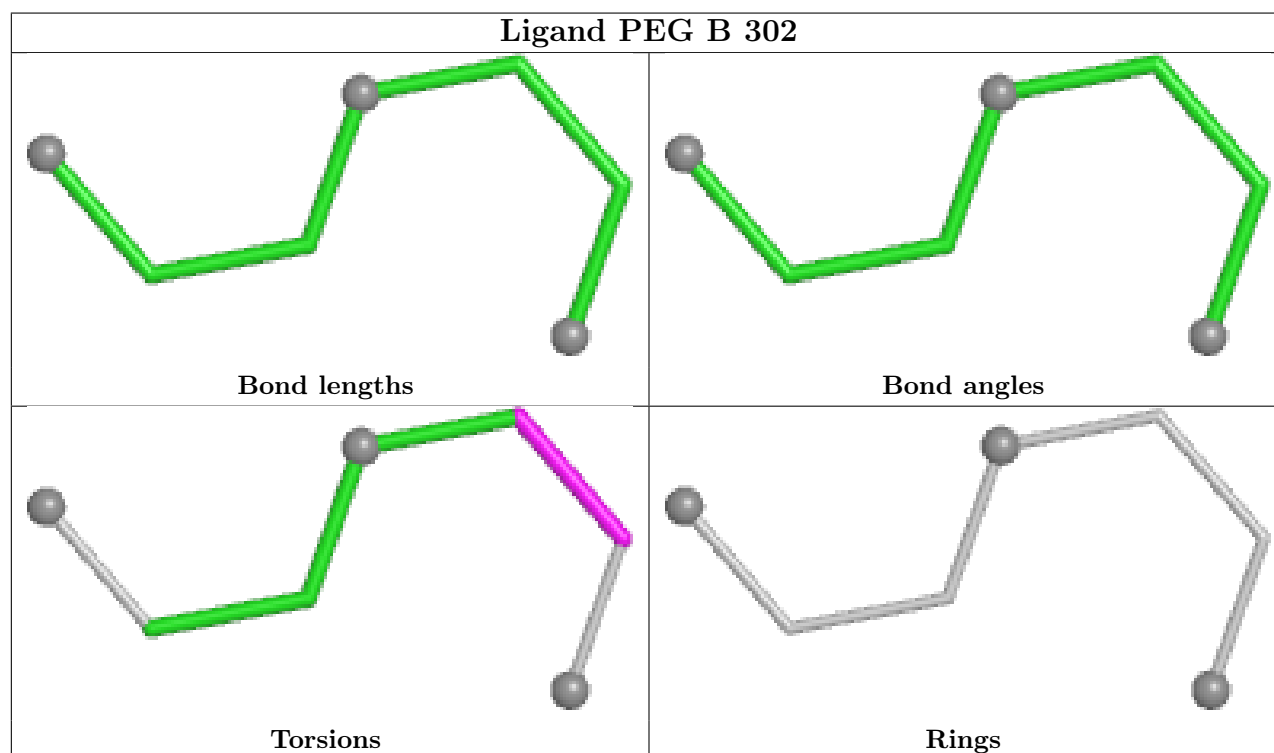
Mol	Chain	Res	Type	Atoms
2	A	301	DGK	CAB-CAS-NBU-CBL
2	A	301	DGK	CBK-CBT-NBB-CBI
2	A	301	DGK	CBR-CBT-NBB-CBI
2	B	301	DGK	CBR-CBT-NBB-CBI

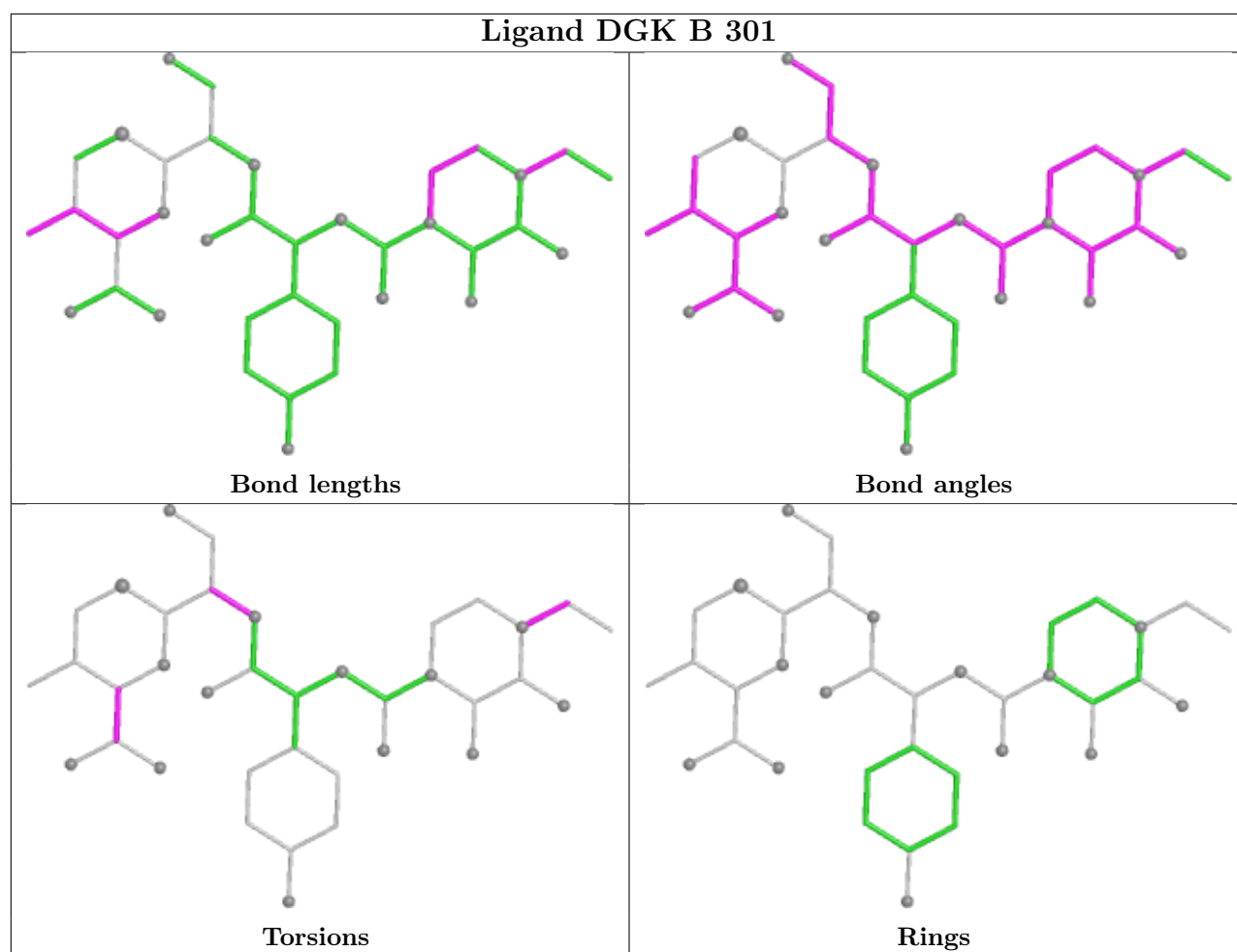
There are no ring outliers.

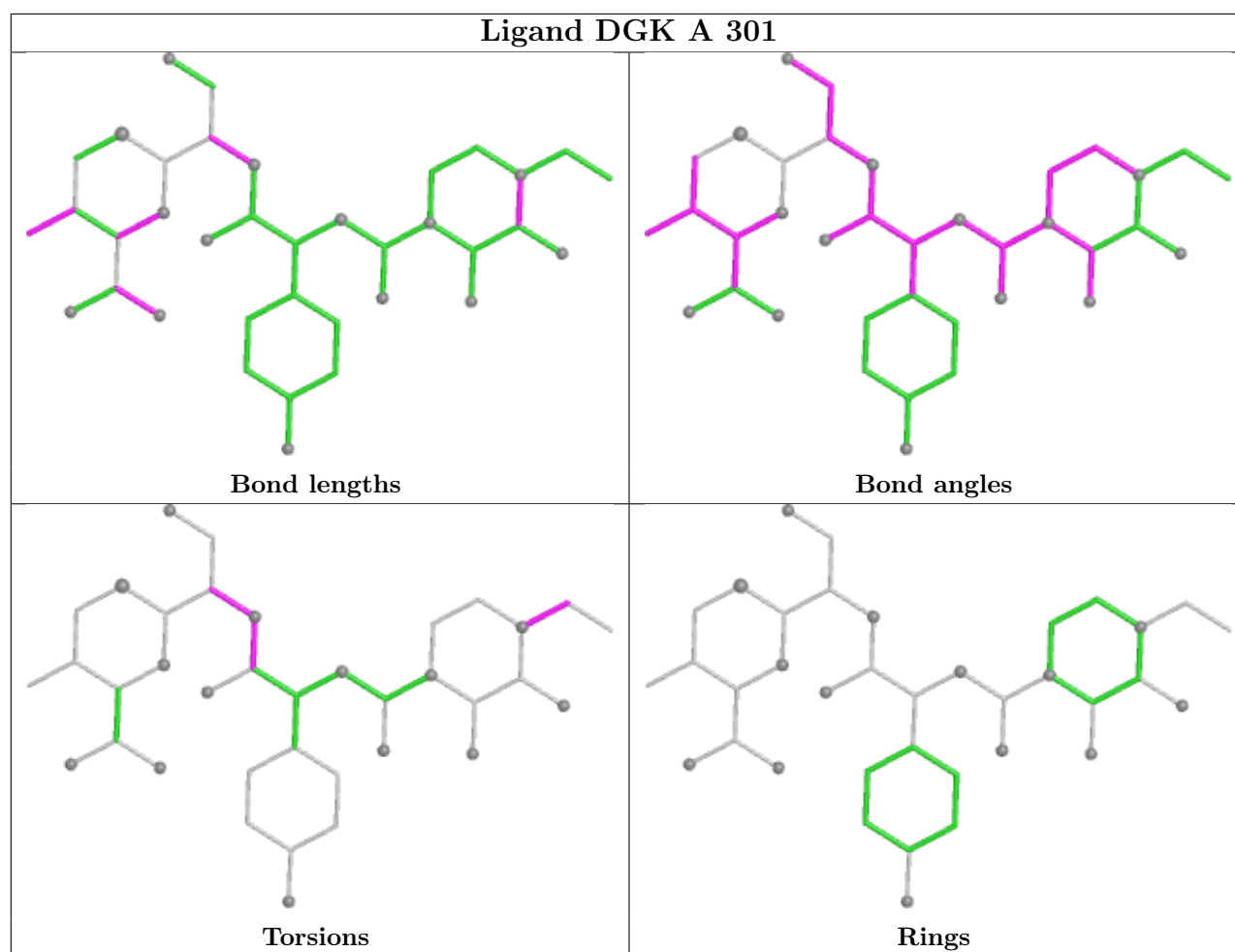
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	DGK	2	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%)	-0.89	0 100 100	11, 19, 32, 53	0
1	B	267/275 (97%)	-0.88	0 100 100	11, 19, 32, 49	0
All	All	534/550 (97%)	-0.89	0 100 100	11, 19, 32, 53	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.

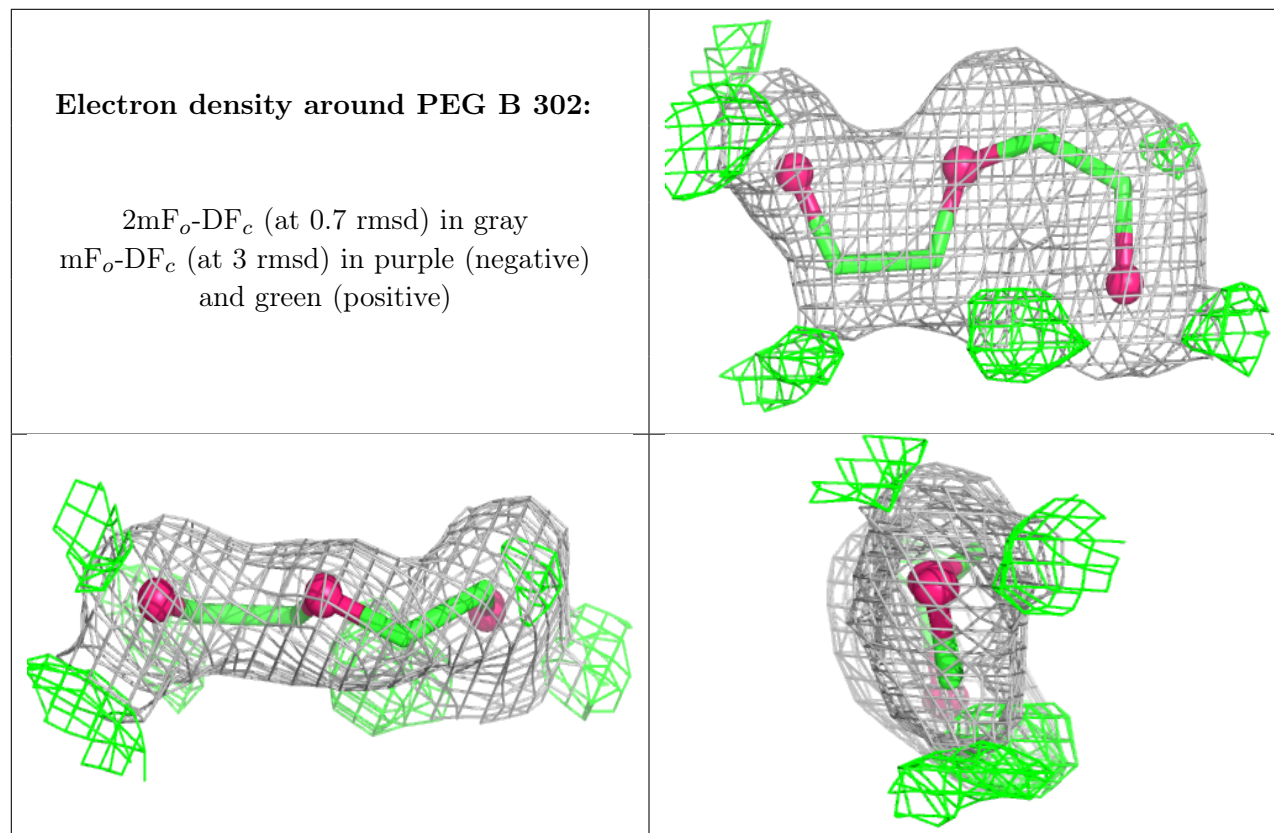
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	302	7/7	0.87	0.10	22,26,28,31	0
2	DGK	B	301	37/37	0.95	0.06	17,22,36,38	0
2	DGK	A	301	37/37	0.96	0.06	17,20,33,34	0
4	CL	B	303	1/1	0.98	0.16	42,42,42,42	0
4	CL	A	303	1/1	0.98	0.07	37,37,37,37	0
4	CL	A	304	1/1	0.98	0.20	38,38,38,38	0
4	CL	A	305	1/1	0.98	0.18	41,41,41,41	0

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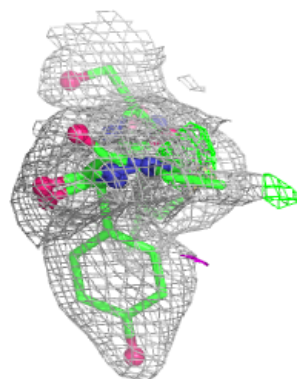
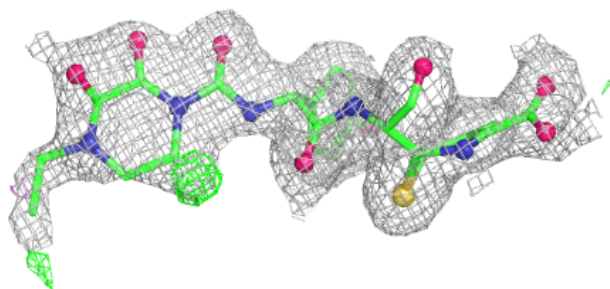
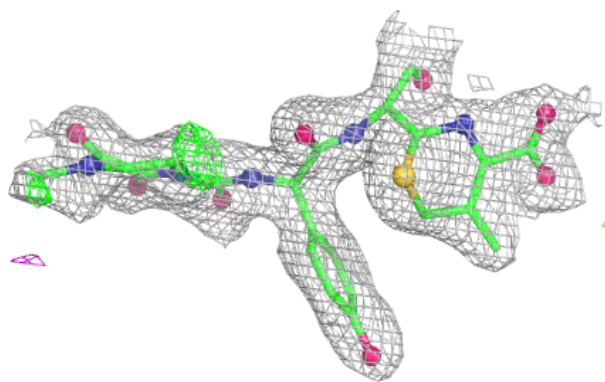
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	A	302	1/1	0.99	0.20	40,40,40,40	0
4	CL	A	306	1/1	0.99	0.13	34,34,34,34	0

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.

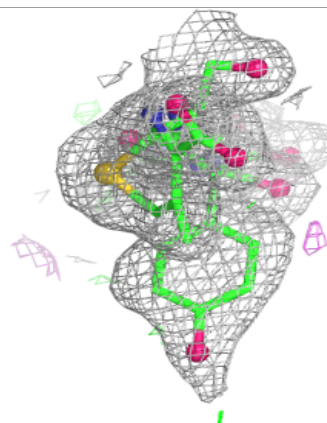
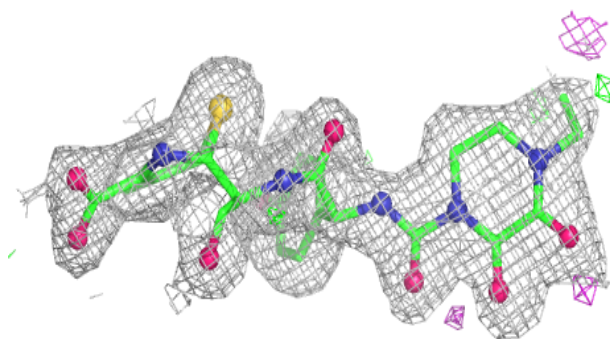
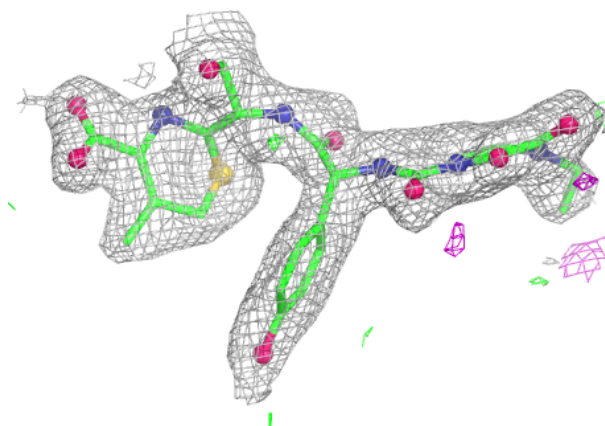


Electron density around DGK B 301:

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

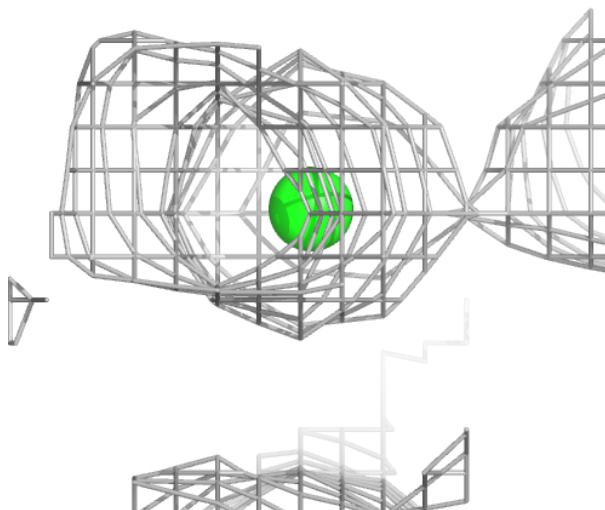
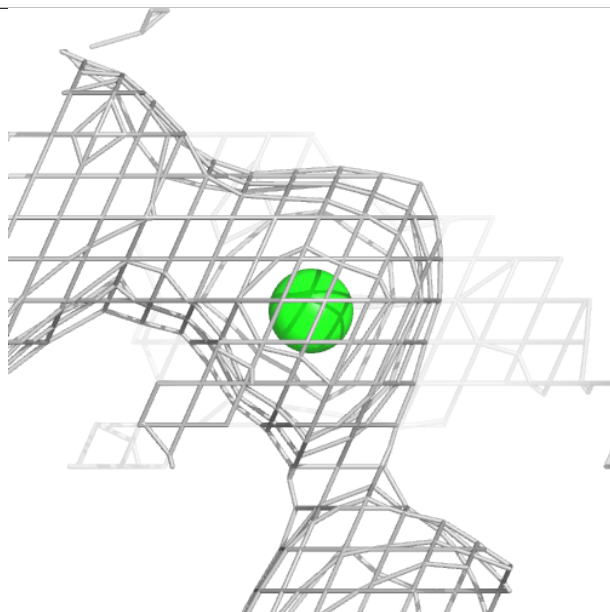
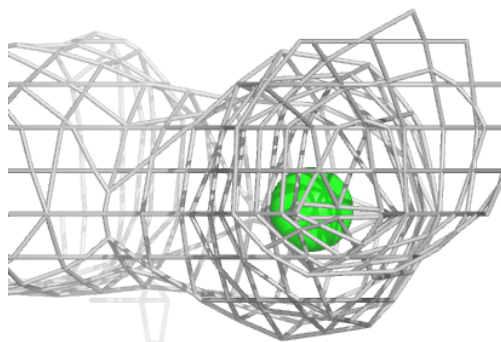
**Electron density around DGK A 301:**

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



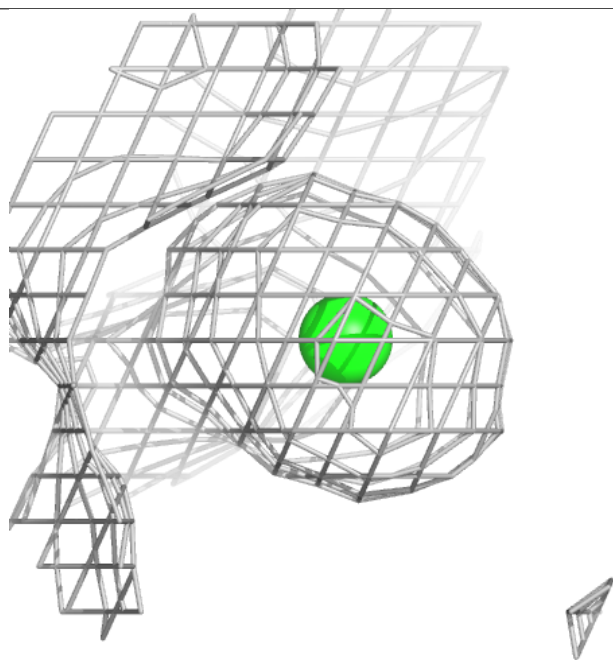
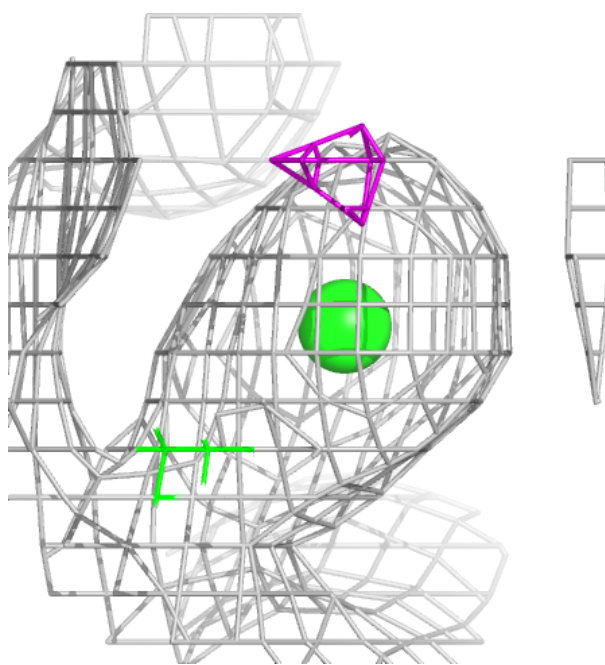
Electron density around CL B 303:

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



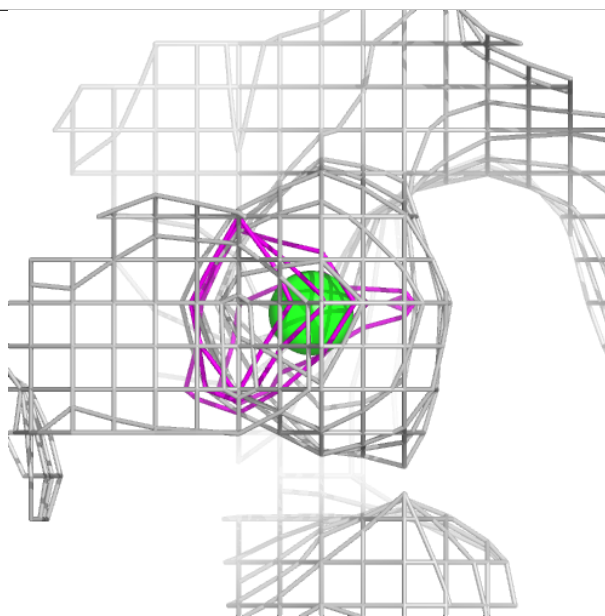
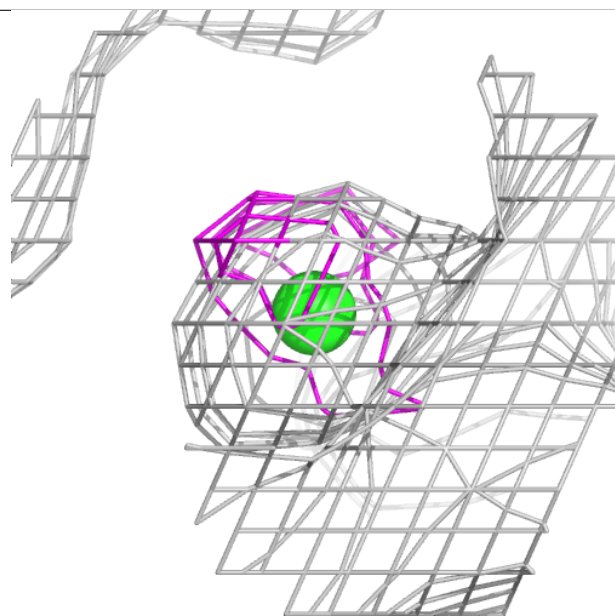
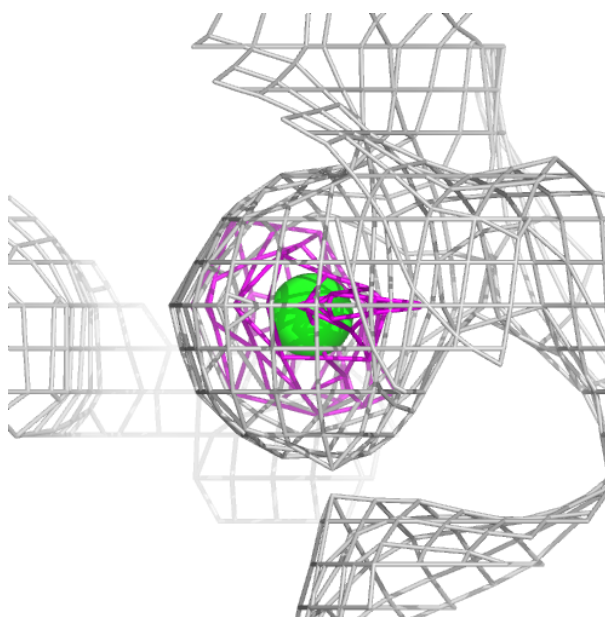
Electron density around CL A 303:

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



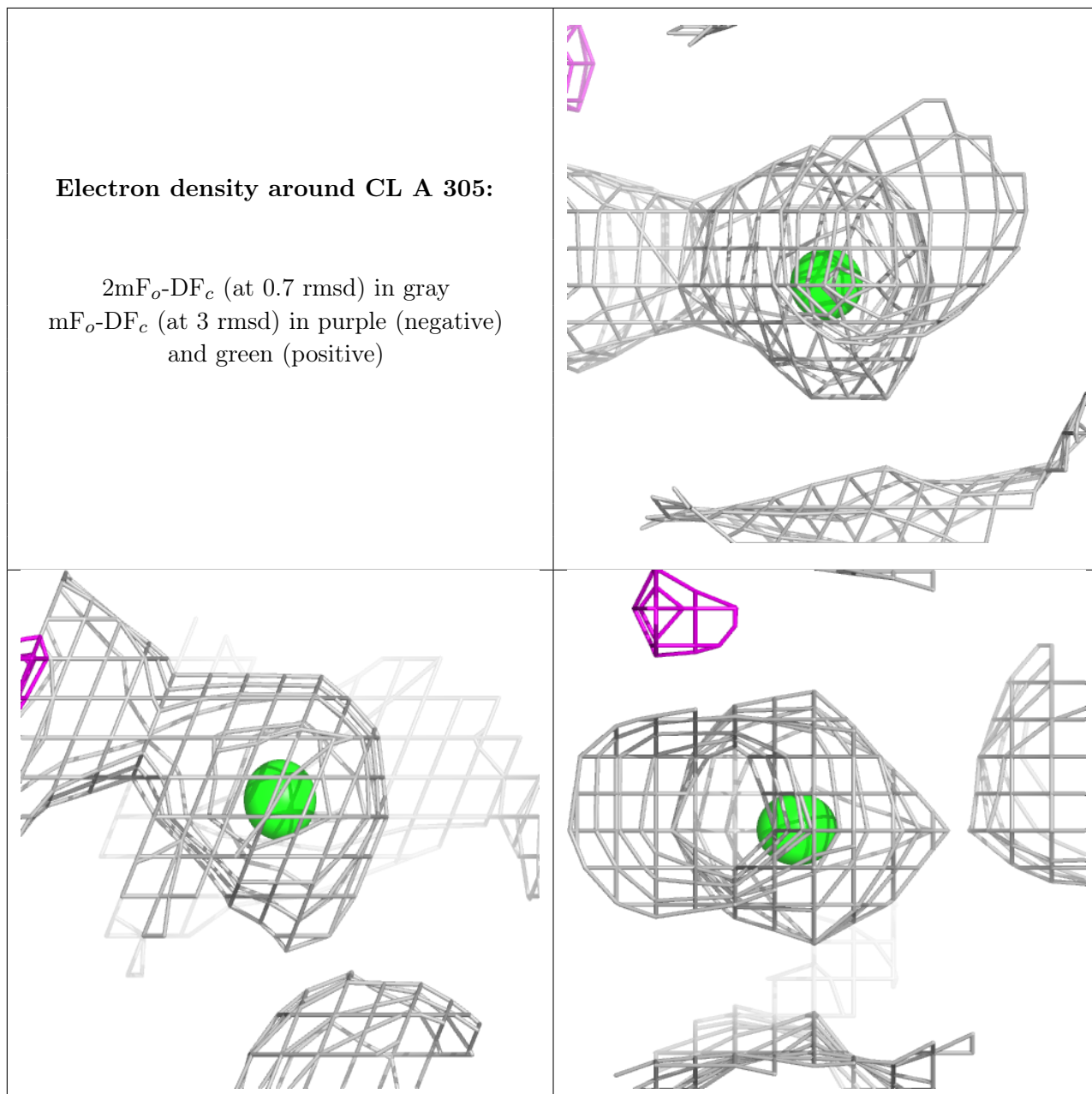
Electron density around CL A 304:

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



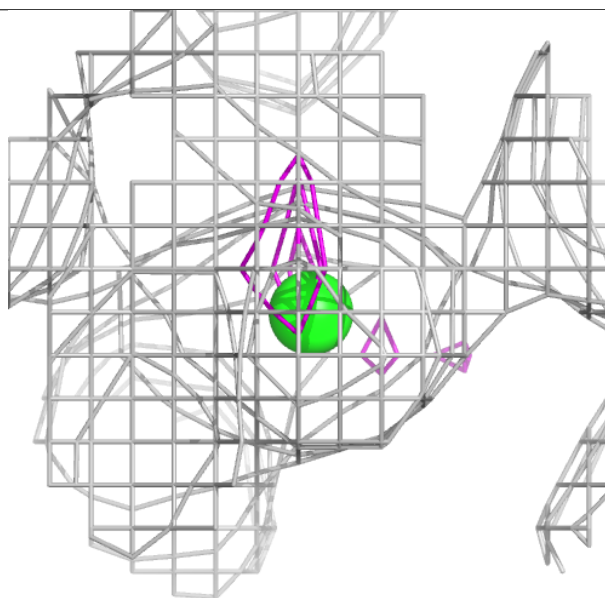
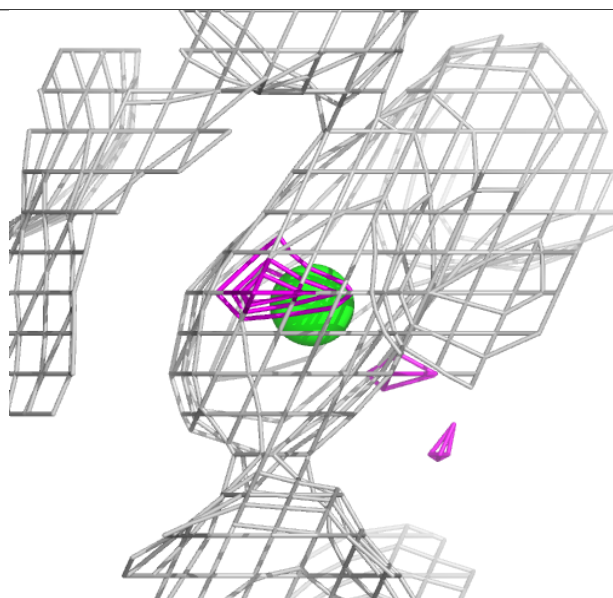
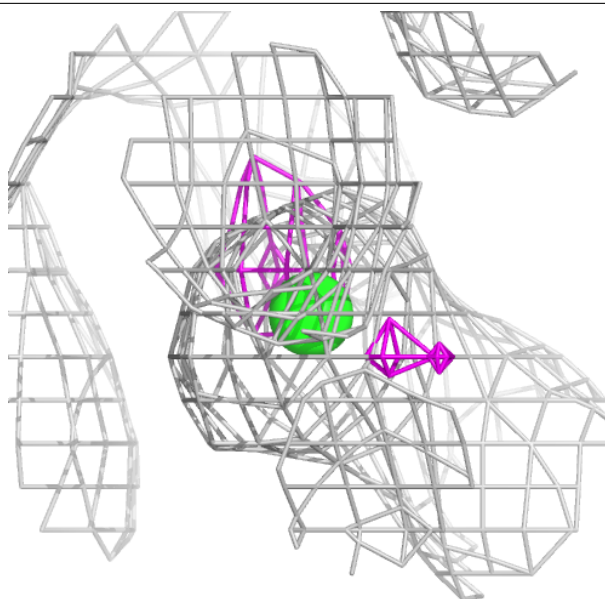
Electron density around CL A 305:

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



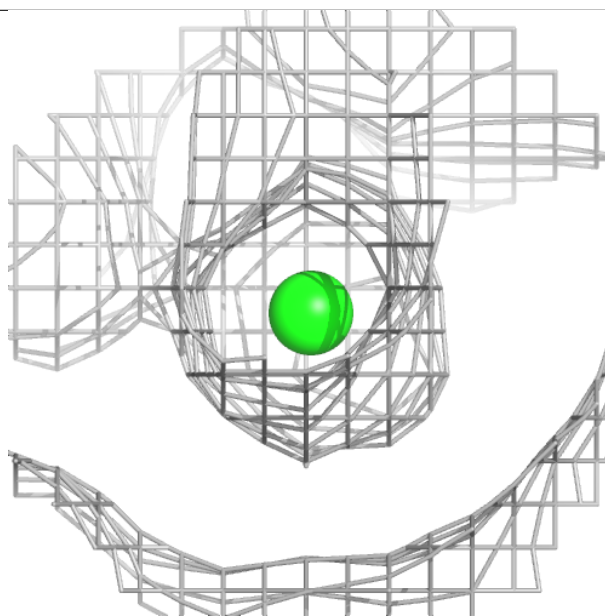
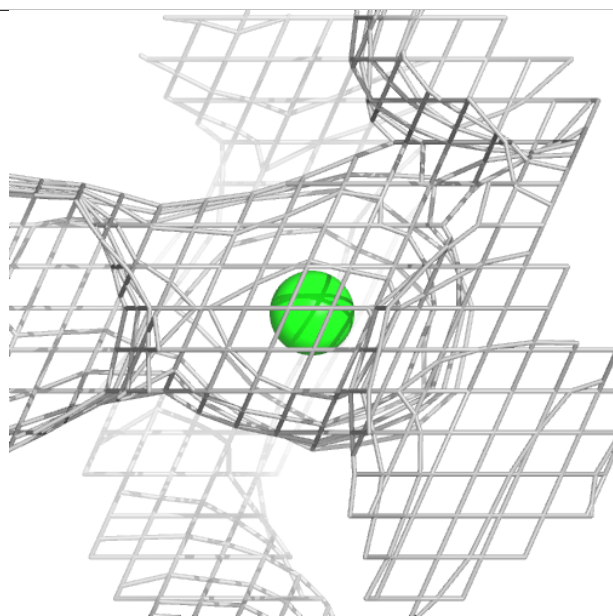
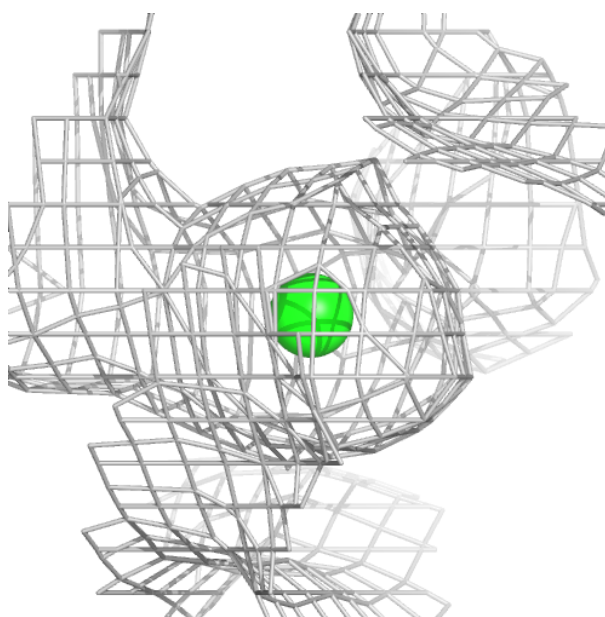
Electron density around CL A 302:

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



Electron density around CL A 306:

$2mF_o-DF_c$ (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.