



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:16 AM UTC

PDB ID : 9JNF / pdb_00009jnf
Title : Crystal Structure of SME-1 E166A mutant in complex with Ertapenem
Authors : Dhankhar, K.; Hazra, S.
Deposited on : 2024-09-23
Resolution : 2.32 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

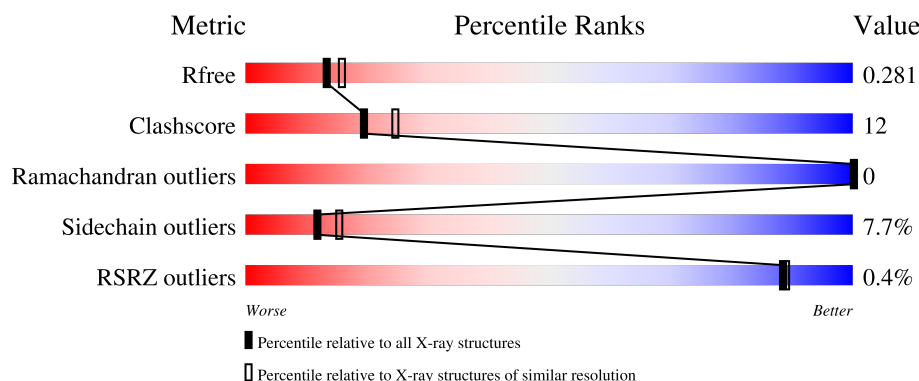
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	69% 24% . . .
1	B	275	70% 21% . . .

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	B	302	-	-	X	-
5	CL	B	304	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4301 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.

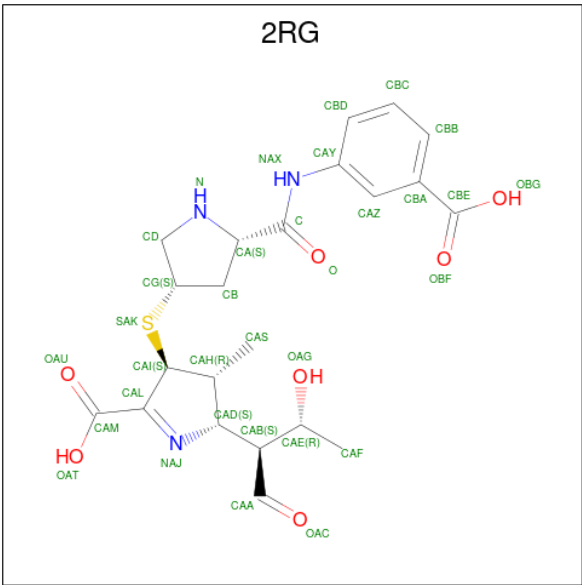
- Molecule 1 is a protein called beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	1	0
			2059	1289	364	399	7			
1	B	267	Total	C	N	O	S	0	0	0
			2053	1285	364	397	7			

There are 18 discrepancies between the modelled and reference sequences:

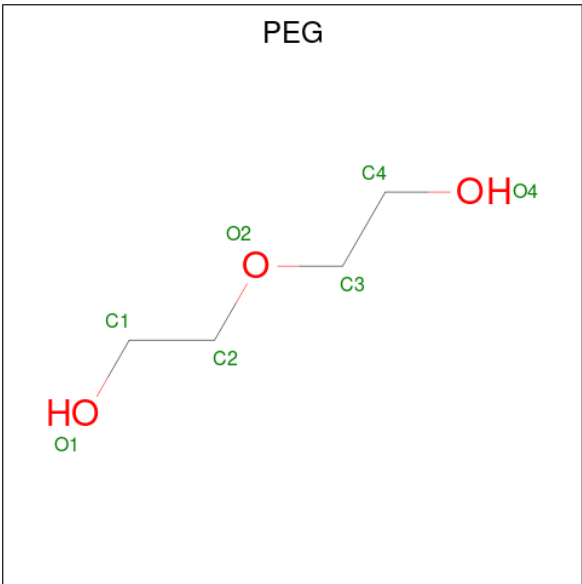
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q54488
A	0	GLY	-	expression tag	UNP Q54488
A	143	ALA	GLU	engineered mutation	UNP Q54488
A	268	HIS	-	expression tag	UNP Q54488
A	269	HIS	-	expression tag	UNP Q54488
A	270	HIS	-	expression tag	UNP Q54488
A	271	HIS	-	expression 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	143	ALA	GLU	engineered mutation	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,3R,4S)-4-((3S,5S)-5-[(3-carboxyphenyl)carbamoyl]pyrrolidin-3-yl)sulfany 1)-2-[(1S,2R)-1-formyl-2-hydroxypropyl]-3-methyl-3,4-dihydro-2H-pyrrole-5-carboxylic acid (CCD ID: 2RG) (formula: C₂₂H₂₇N₃O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	22	3	7	1		
2	B	1	Total	C	N	O	S	0	0
			33	22	3	7	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



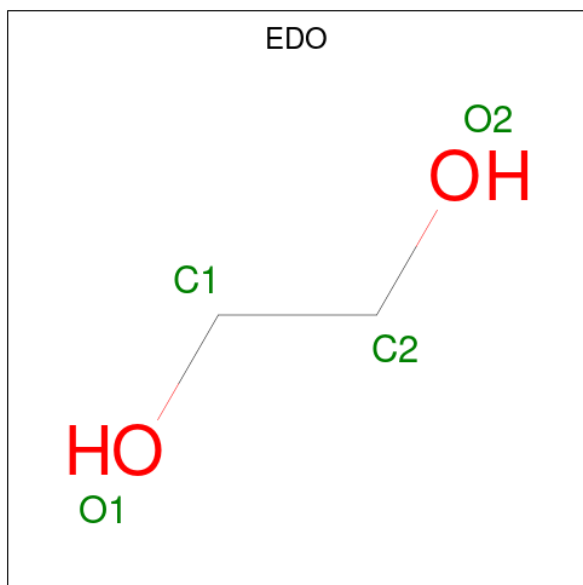
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

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

- Molecule 4 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
4	B	1	Total	C	O	0	0
			4	2	2		

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

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

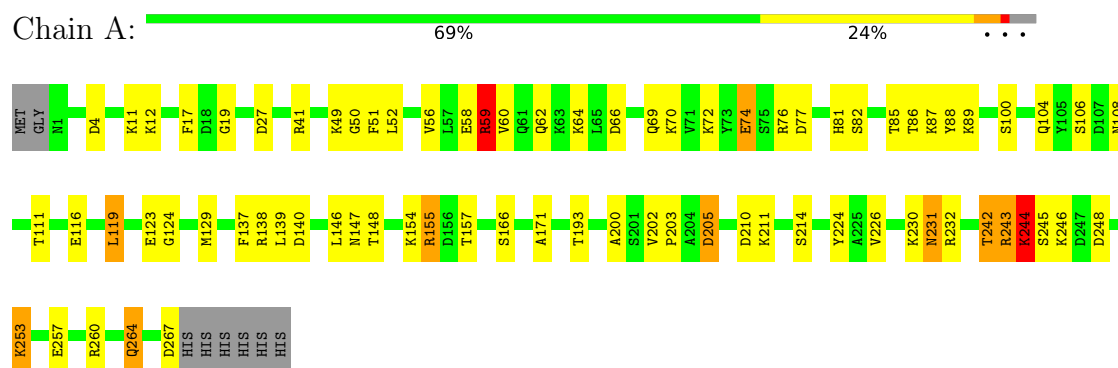
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		
6	B	50	Total	O	0	0
			50	50		

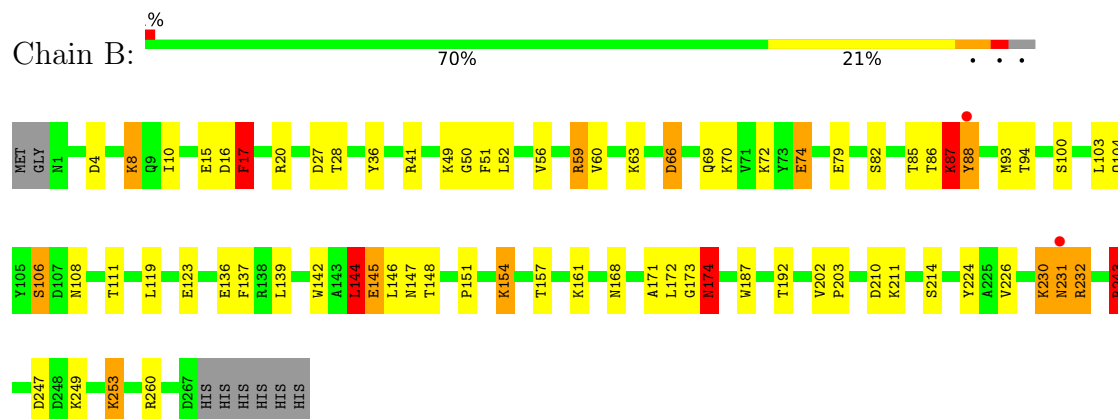
3 Residue-property plots

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



• Molecule 1: beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.11Å 50.67Å 130.34Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	23.95 – 2.32 23.95 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.95-2.32) 99.8 (23.95-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.183 , 0.280 0.184 , 0.281	Depositor DCC
R_{free} test set	1043 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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, EDO, 2RG, 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	0.79	0/2097	1.60	27/2828 (1.0%)
1	B	0.82	2/2088 (0.1%)	1.64	31/2816 (1.1%)
All	All	0.81	2/4185 (0.0%)	1.62	58/5644 (1.0%)

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	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	ARG	NE-CZ	5.54	1.39	1.33
1	B	151	PRO	CA-CB	5.07	1.60	1.53

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	CB-CA-C	-10.27	94.38	111.02
1	A	242	THR	OG1-CB-CG2	-9.05	91.20	109.30
1	A	253	LYS	N-CA-CB	-9.03	96.40	110.30
1	A	147	ASN	CB-CA-C	-8.85	96.68	111.02
1	B	253	LYS	N-CA-CB	-8.64	97.00	110.30
1	B	16	ASP	CA-CB-CG	8.27	120.87	112.60
1	B	17	PHE	N-CA-CB	8.23	122.41	110.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	GLU	CB-CG-CD	7.83	125.92	112.60
1	B	87	LYS	CB-CG-CD	7.79	129.23	111.30
1	B	243	ARG	CD-NE-CZ	7.16	134.42	124.40
1	B	27	ASP	CA-CB-CG	7.11	119.71	112.60
1	A	264	GLN	CB-CA-C	-6.99	96.11	110.38
1	B	88	TYR	CA-CB-CG	6.93	126.38	113.90
1	A	157	THR	CA-CB-OG1	-6.90	99.25	109.60
1	B	147	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	243	ARG	CA-CB-CG	-6.64	100.82	114.10
1	A	12	LYS	CG-CD-CE	-6.61	96.09	111.30
1	B	174	ASN	CB-CA-C	6.52	121.85	110.64
1	B	111	THR	CA-CB-OG1	-6.51	99.83	109.60
1	A	244	LYS	CG-CD-CE	6.47	126.17	111.30
1	A	81	HIS	CB-CA-C	6.28	120.27	111.86
1	A	264	GLN	N-CA-CB	6.25	119.92	110.30
1	A	74	GLU	N-CA-CB	6.24	120.75	110.39
1	B	144	LEU	N-CA-CB	6.14	119.54	110.33
1	A	248	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	232	ARG	CA-CB-CG	6.12	126.34	114.10
1	A	86	THR	CA-CB-OG1	-6.08	100.49	109.60
1	B	136	GLU	CB-CG-CD	5.95	122.72	112.60
1	B	136	GLU	N-CA-CB	5.91	119.45	110.42
1	B	230	LYS	CG-CD-CE	5.90	124.87	111.30
1	B	59	ARG	N-CA-CB	5.85	118.72	110.12
1	B	66	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	247	ASP	CB-CA-C	-5.82	98.55	109.72
1	B	4	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	59	ARG	CA-CB-CG	5.70	125.51	114.10
1	A	27	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	86	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	232	ARG	CA-CB-CG	5.62	125.35	114.10
1	A	77	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	192	THR	OG1-CB-CG2	5.46	120.22	109.30
1	A	230	LYS	CB-CA-C	5.44	118.94	110.67
1	B	249	LYS	CB-CG-CD	5.36	123.62	111.30
1	B	157	THR	CA-CB-OG1	-5.32	101.61	109.60
1	A	4	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	244	LYS	N-CA-CB	5.20	117.77	110.12
1	B	15	GLU	CA-C-N	5.19	127.19	120.44
1	B	15	GLU	C-N-CA	5.19	127.19	120.44
1	A	116	GLU	CG-CD-OE1	-5.18	106.48	118.40
1	A	111	THR	CA-CB-OG1	-5.16	101.86	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	148	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	243	ARG	CB-CG-CD	5.13	123.09	111.30
1	A	19	GLY	CA-C-N	-5.11	113.79	121.86
1	A	19	GLY	C-N-CA	-5.11	113.79	121.86
1	A	193	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	58	GLU	CB-CG-CD	5.02	121.13	112.60
1	B	8	LYS	CG-CD-CE	-5.01	99.77	111.30
1	B	88	TYR	N-CA-CB	5.00	117.89	110.49

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	155	ARG	Sidechain
1	B	20	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	2059	0	2049	40	0
1	B	2053	0	2043	57	0
2	A	33	0	24	4	0
2	B	33	0	24	5	0
3	A	7	0	10	0	0
3	B	7	0	10	4	0
4	B	4	0	6	3	0
5	B	1	0	0	2	0
6	A	54	0	0	3	0
6	B	50	0	0	5	0
All	All	4301	0	4166	97	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 12.

All (97) 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:82:SER:H	4:B:303:EDO:H11	1.20	1.07
1:B:145:GLU:HG2	6:B:447:HOH:O	1.68	0.92
1:A:66:ASP:H	1:A:69:GLN:HE21	1.11	0.91
1:B:66:ASP:H	1:B:69:GLN:HE21	1.25	0.85
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.42	0.84
1:B:88:TYR:CD2	1:B:93:MET:HG2	2.13	0.84
1:A:66:ASP:O	1:A:69:GLN:HG2	1.78	0.84
1:B:66:ASP:O	1:B:69:GLN:HG2	1.79	0.82
1:B:214:SER:HB2	2:B:301:2RG:HAI	1.65	0.78
1:A:59:ARG:HG3	1:A:59:ARG:HH11	1.49	0.77
3:B:302:PEG:O4	3:B:302:PEG:H22	1.85	0.77
1:B:87:LYS:HG2	1:B:88:TYR:HD1	1.50	0.75
1:B:87:LYS:HD2	1:B:88:TYR:CE1	2.23	0.74
1:A:108:ASN:HD21	2:A:301:2RG:HAF	1.54	0.72
1:B:108:ASN:HD21	2:B:301:2RG:CAF	2.03	0.72
1:B:66:ASP:H	1:B:69:GLN:NE2	1.89	0.69
1:A:64:LYS:HD3	1:B:173:GLY:HA2	1.75	0.67
1:B:74:GLU:H	1:B:74:GLU:CD	2.03	0.67
1:A:108:ASN:HD21	2:A:301:2RG:CAF	2.07	0.67
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.11	0.66
1:B:108:ASN:HD21	2:B:301:2RG:HAF	1.60	0.65
1:B:154:LYS:N	1:B:154:LYS:HD2	2.10	0.65
1:B:82:SER:N	4:B:303:EDO:H11	2.03	0.65
1:B:82:SER:H	4:B:303:EDO:C1	2.05	0.64
1:B:145:GLU:HB3	6:B:447:HOH:O	1.98	0.64
1:B:211:LYS:NZ	5:B:304:CL:CL	2.62	0.63
1:A:264:GLN:HB2	6:A:410:HOH:O	1.99	0.62
1:A:257:GLU:OE2	1:A:260:ARG:HD2	2.00	0.60
1:B:87:LYS:HG2	1:B:88:TYR:CD1	2.35	0.60
1:A:62:GLN:HG2	1:B:28:THR:O	2.02	0.59
1:A:66:ASP:H	1:A:69:GLN:NE2	1.91	0.58
1:B:243:ARG:HG2	1:B:243:ARG:HH11	1.67	0.58
1:A:231:ASN:HA	6:A:436:HOH:O	2.03	0.58
1:B:139:LEU:HD11	1:B:146:LEU:HD22	1.86	0.58
1:A:139:LEU:HD11	1:A:146:LEU:HD22	1.86	0.56
1:B:142:TRP:CD2	3:B:302:PEG:H11	2.40	0.56
1:B:231:ASN:O	1:B:232:ARG:HB2	2.07	0.55
1:A:59:ARG:HG3	1:A:59:ARG:NH1	2.20	0.53
1:A:214:SER:HB2	2:A:301:2RG:HAI	1.88	0.53
1:B:145:GLU:CG	6:B:447:HOH:O	2.38	0.53
1:A:129:MET:HG3	1:A:137:PHE:CG	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HD2	1:A:154:LYS:HG2	1.91	0.52
1:A:59:ARG:HH12	1:B:174:ASN:ND2	2.08	0.52
1:B:72:LYS:HB3	1:B:74:GLU:OE2	2.10	0.52
1:B:145:GLU:CB	6:B:447:HOH:O	2.53	0.51
1:A:129:MET:HG3	1:A:137:PHE:CD1	2.46	0.51
1:B:79:GLU:HB3	1:B:144:LEU:HD23	1.93	0.51
1:A:171:ALA:CB	1:A:226:VAL:HG21	2.40	0.51
1:B:82:SER:HB3	1:B:85:THR:OG1	2.10	0.51
1:A:100:SER:O	1:A:104:GLN:HG3	2.11	0.50
1:B:49:LYS:HB2	1:B:211:LYS:HE3	1.93	0.50
1:A:171:ALA:HB1	1:A:226:VAL:HG21	1.93	0.49
1:B:50:GLY:HA3	1:B:224:TYR:OH	2.12	0.49
1:A:82:SER:HB3	1:A:85:THR:OG1	2.12	0.49
1:A:205:ASP:OD1	1:A:205:ASP:N	2.25	0.49
1:B:56:VAL:O	1:B:60:VAL:HG23	2.13	0.49
1:B:100:SER:O	1:B:104:GLN:HG3	2.12	0.48
1:B:108:ASN:HD21	2:B:301:2RG:HAFA	1.77	0.48
1:A:49:LYS:HB2	1:A:211:LYS:HE3	1.95	0.48
1:B:87:LYS:HD2	1:B:88:TYR:HE1	1.76	0.48
1:A:200:ALA:O	1:A:260:ARG:NH2	2.46	0.48
1:A:56:VAL:O	1:A:60:VAL:HG23	2.15	0.47
1:B:137:PHE:HB2	6:B:402:HOH:O	2.14	0.47
1:A:242:THR:C	1:A:243:ARG:HG3	2.40	0.46
1:B:10:ILE:HG21	1:B:36:TYR:CD2	2.50	0.46
1:A:51:PHE:O	1:A:52:LEU:C	2.58	0.46
1:B:17:PHE:CE2	1:B:243:ARG:HD2	2.51	0.45
1:B:106:SER:HB2	5:B:304:CL:CL	2.53	0.45
1:B:63:LYS:HB3	1:B:63:LYS:HE2	1.72	0.44
1:A:88:TYR:O	1:A:89:LYS:C	2.61	0.44
1:B:202:VAL:O	1:B:203:PRO:C	2.60	0.43
1:A:76:ARG:O	1:A:89:LYS:NZ	2.48	0.43
1:A:244:LYS:HA	1:A:244:LYS:HD3	1.43	0.43
1:A:66:ASP:N	1:A:69:GLN:HE21	1.95	0.43
1:B:69:GLN:O	1:B:94:THR:HA	2.19	0.43
1:B:243:ARG:HG2	1:B:243:ARG:NH1	2.30	0.43
1:B:103:LEU:C	1:B:103:LEU:HD23	2.42	0.43
1:B:87:LYS:HD2	1:B:88:TYR:CD1	2.54	0.42
1:B:142:TRP:CE2	3:B:302:PEG:H11	2.53	0.42
1:A:50:GLY:HA3	1:A:224:TYR:OH	2.19	0.42
1:B:51:PHE:O	1:B:52:LEU:C	2.59	0.42
1:B:17:PHE:CD2	1:B:243:ARG:HD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:302:PEG:O4	3:B:302:PEG:C2	2.64	0.42
1:B:100:SER:HB3	1:B:187:TRP:CE2	2.55	0.42
1:A:59:ARG:HH12	1:B:174:ASN:CG	2.27	0.42
1:A:140:ASP:OD2	1:A:155:ARG:HA	2.19	0.42
1:A:146:LEU:C	1:A:146:LEU:HD12	2.45	0.41
1:B:168:ASN:ND2	1:B:172:LEU:HD12	2.36	0.41
1:A:245:SER:O	1:A:246:LYS:C	2.62	0.41
1:B:161:LYS:HB2	1:B:161:LYS:HE3	1.95	0.41
1:A:202:VAL:O	1:A:203:PRO:C	2.63	0.41
2:B:301:2RG:HAH	2:B:301:2RG:HG	1.86	0.41
2:A:301:2RG:HN	2:A:301:2RG:HAZ	1.84	0.41
1:A:119:LEU:O	1:A:124:GLY:HA3	2.21	0.41
1:B:79:GLU:HB3	1:B:144:LEU:CD2	2.50	0.40
1:A:166:SER:N	6:A:408:HOH:O	2.53	0.40
1:B:171:ALA:CB	1:B:226:VAL:HG21	2.51	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	266/275 (97%)	257 (97%)	9 (3%)	0	100	100
1	B	265/275 (96%)	252 (95%)	13 (5%)	0	100	100
All	All	531/550 (96%)	509 (96%)	22 (4%)	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%)	199 (93%)	16 (7%)	13	16
1	B	214/223 (96%)	197 (92%)	17 (8%)	11	15
All	All	429/446 (96%)	396 (92%)	33 (8%)	12	15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	17	PHE
1	A	59	ARG
1	A	70	LYS
1	A	72	LYS
1	A	74	GLU
1	A	87	LYS
1	A	106	SER
1	A	119	LEU
1	A	123	GLU
1	A	205	ASP
1	A	210	ASP
1	A	231	ASN
1	A	244	LYS
1	A	253	LYS
1	A	267	ASP
1	B	8	LYS
1	B	17	PHE
1	B	41	ARG
1	B	70	LYS
1	B	74	GLU
1	B	87	LYS
1	B	106	SER
1	B	119	LEU
1	B	144	LEU
1	B	145	GLU
1	B	154	LYS
1	B	174	ASN
1	B	210	ASP
1	B	230	LYS
1	B	231	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	243	ARG
1	B	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	69	GLN
1	A	81	HIS
1	A	168	ASN
1	B	69	GLN
1	B	81	HIS
1	B	108	ASN
1	B	135	ASN
1	B	168	ASN
1	B	174	ASN
1	B	231	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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	0.60	0	5,5,5	0.54	0
4	EDO	B	303	-	3,3,3	0.88	0	2,2,2	1.36	0
2	2RG	A	301	1	32,35,35	1.84	3 (9%)	27,50,50	2.21	7 (25%)
3	PEG	A	302	-	6,6,6	0.24	0	5,5,5	0.22	0
2	2RG	B	301	1	32,35,35	2.15	4 (12%)	27,50,50	1.86	7 (25%)

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	-	-	3/4/4/4	-
4	EDO	B	303	-	-	1/1/1/1	-
2	2RG	A	301	1	-	9/26/55/55	0/3/3/3
3	PEG	A	302	-	-	3/4/4/4	-
2	2RG	B	301	1	-	7/26/55/55	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	2RG	CAM-CAL	-10.16	1.30	1.48
2	A	301	2RG	CAM-CAL	-8.60	1.33	1.48
2	B	301	2RG	CAI-CAH	-3.12	1.53	1.55
2	B	301	2RG	OAT-CAM	-3.09	1.22	1.30
2	B	301	2RG	CAI-SAK	-2.91	1.77	1.84
2	A	301	2RG	OAU-CAM	2.45	1.28	1.22
2	A	301	2RG	CAL-NAJ	2.18	1.30	1.28

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	2RG	C-CA-N	6.68	124.43	111.02
2	B	301	2RG	CAZ-CAY-NAX	-5.40	102.59	120.13
2	A	301	2RG	OAU-CAM-CAL	-4.66	114.86	121.13
2	B	301	2RG	CBD-CAY-NAX	4.66	136.06	120.41
2	A	301	2RG	OAT-CAM-CAL	3.89	123.18	115.73
2	A	301	2RG	CB-CA-N	-3.52	99.42	106.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2RG	OAU-CAM-CAL	-3.34	116.64	121.13
2	A	301	2RG	CAY-NAX-C	2.57	133.24	127.37
2	A	301	2RG	OAC-CAA-CAB	-2.44	119.45	125.27
2	B	301	2RG	OAG-CAE-CAF	-2.24	102.99	109.68
2	B	301	2RG	CAY-NAX-C	-2.11	122.56	127.37
2	A	301	2RG	CB-CA-C	-2.09	108.13	111.38
2	B	301	2RG	OAC-CAA-CAB	-2.07	120.34	125.27
2	B	301	2RG	CBB-CBA-CBE	2.04	124.40	120.37

There are no chirality outliers.

All (23) torsion outliers are listed below:

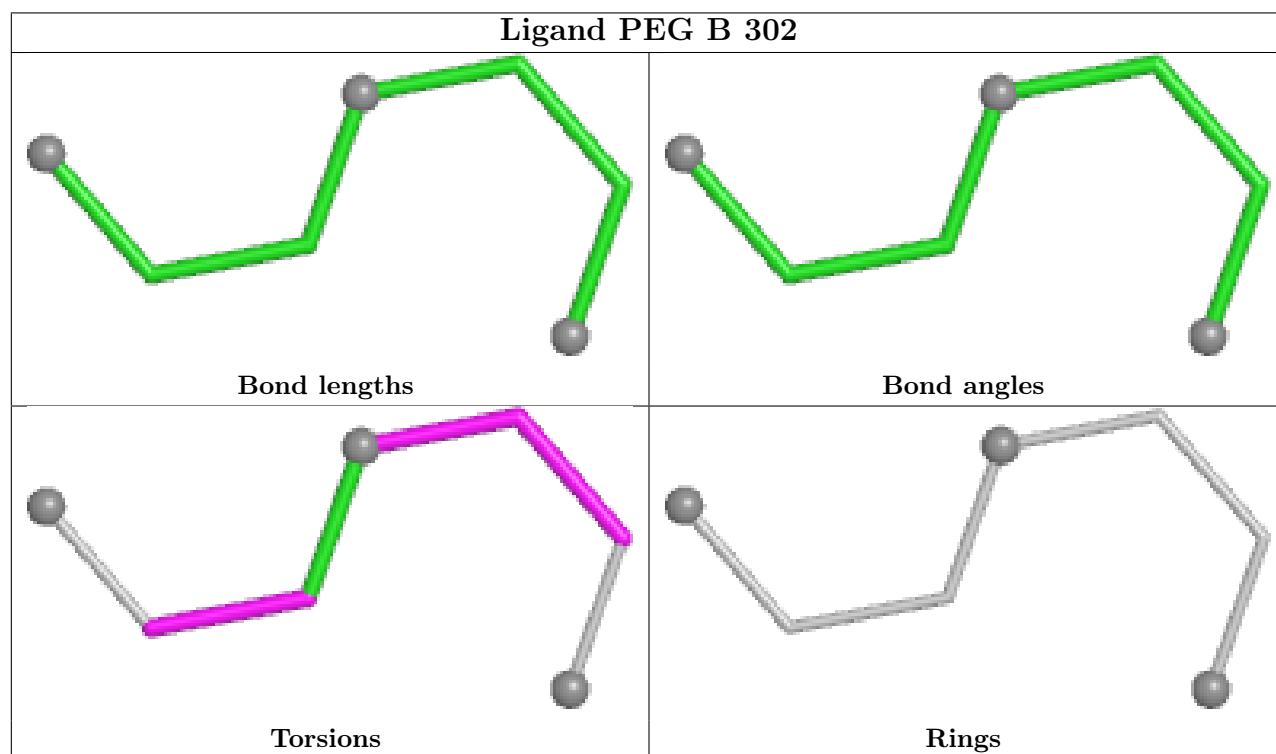
Mol	Chain	Res	Type	Atoms
2	A	301	2RG	O-C-CA-N
2	A	301	2RG	NAX-C-CA-N
2	A	301	2RG	NAX-C-CA-CB
2	A	301	2RG	CA-C-NAX-CAY
2	A	301	2RG	CAA-CAB-CAE-CAF
2	A	301	2RG	CAA-CAB-CAE-OAG
2	A	301	2RG	CAD-CAB-CAE-CAF
2	B	301	2RG	CA-C-NAX-CAY
2	B	301	2RG	CAA-CAB-CAE-CAF
2	B	301	2RG	CAA-CAB-CAE-OAG
2	B	301	2RG	CAD-CAB-CAE-CAF
2	B	301	2RG	CAH-CAI-SAK-CG
2	A	301	2RG	O-C-NAX-CAY
3	B	302	PEG	C4-C3-O2-C2
2	B	301	2RG	O-C-NAX-CAY
3	A	302	PEG	O1-C1-C2-O2
4	B	303	EDO	O1-C1-C2-O2
2	A	301	2RG	CAD-CAB-CAE-OAG
2	B	301	2RG	CAD-CAB-CAE-OAG
3	B	302	PEG	O2-C3-C4-O4
3	A	302	PEG	C1-C2-O2-C3
3	B	302	PEG	O1-C1-C2-O2
3	A	302	PEG	C4-C3-O2-C2

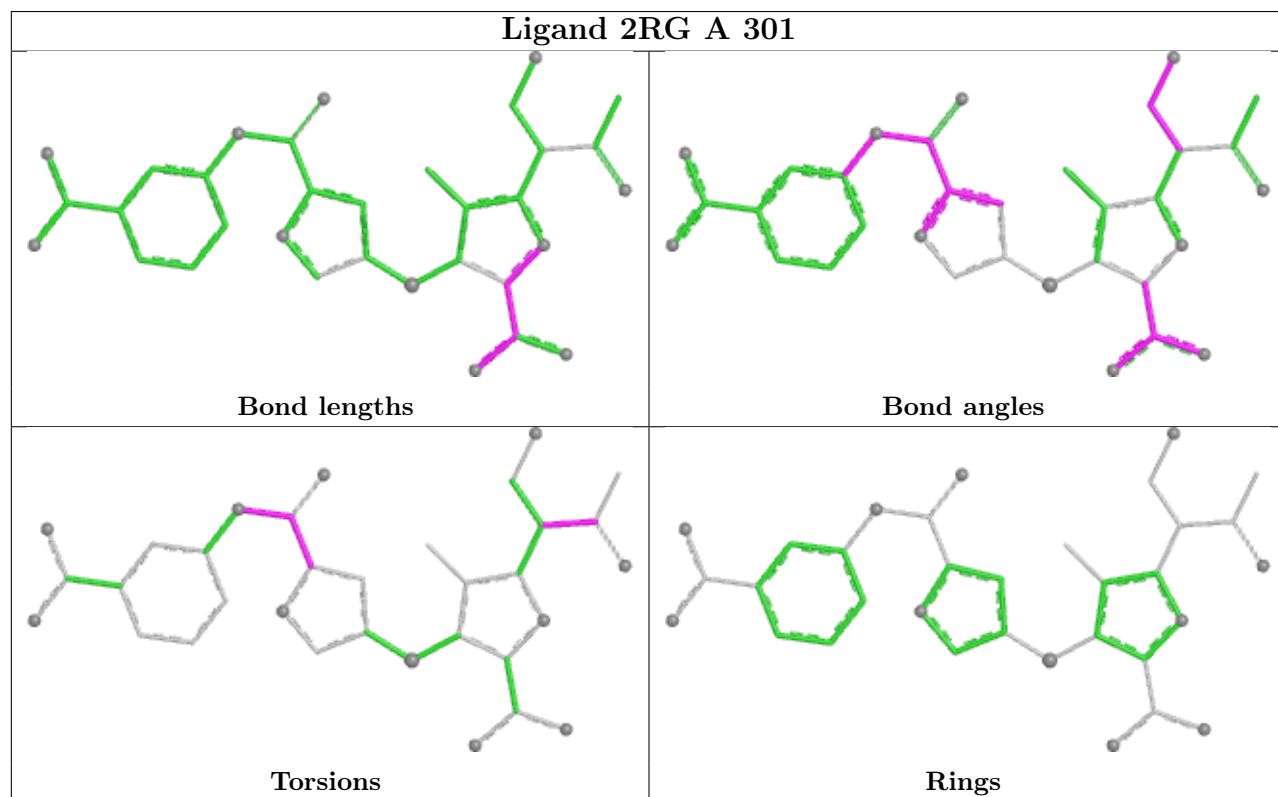
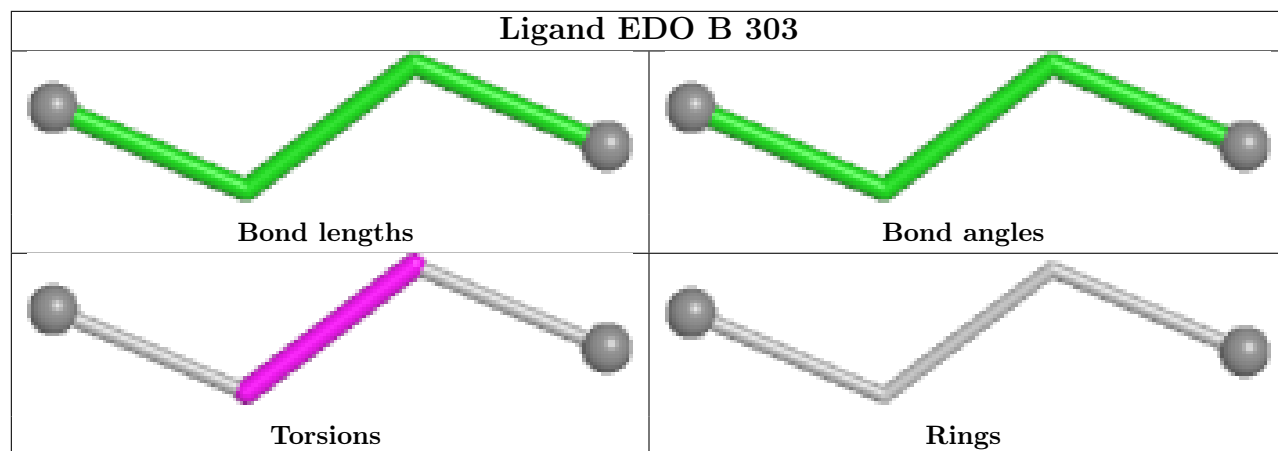
There are no ring outliers.

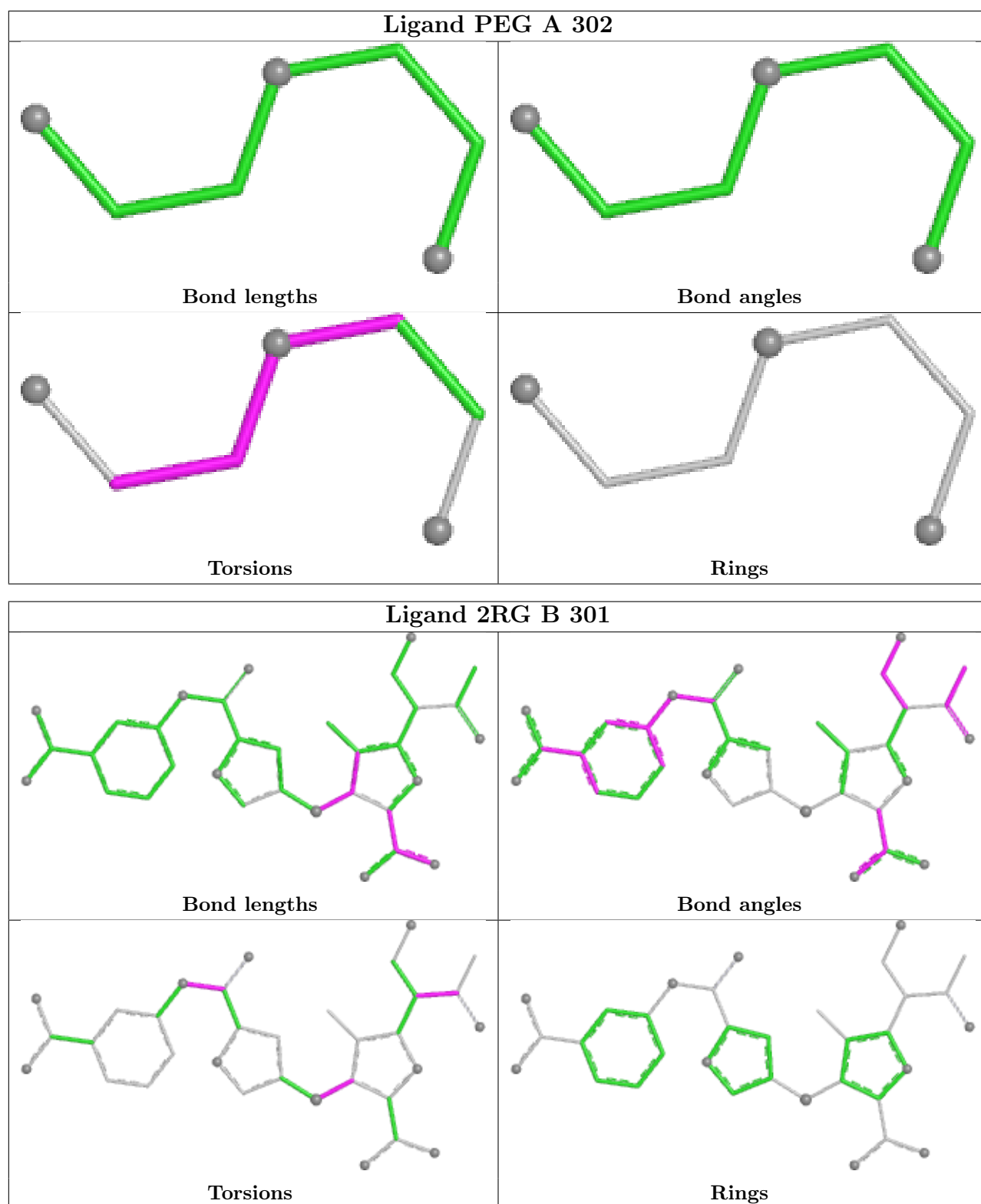
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	PEG	4	0
4	B	303	EDO	3	0
2	A	301	2RG	4	0
2	B	301	2RG	5	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.32	0	100 100	9, 17, 30, 50	1 (0%)
1	B	267/275 (97%)	-0.32	2 (0%)	84 85	9, 17, 32, 43	0
All	All	534/550 (97%)	-0.32	2 (0%)	88 89	9, 17, 31, 50	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	TYR	2.7
1	B	231	ASN	2.1

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.

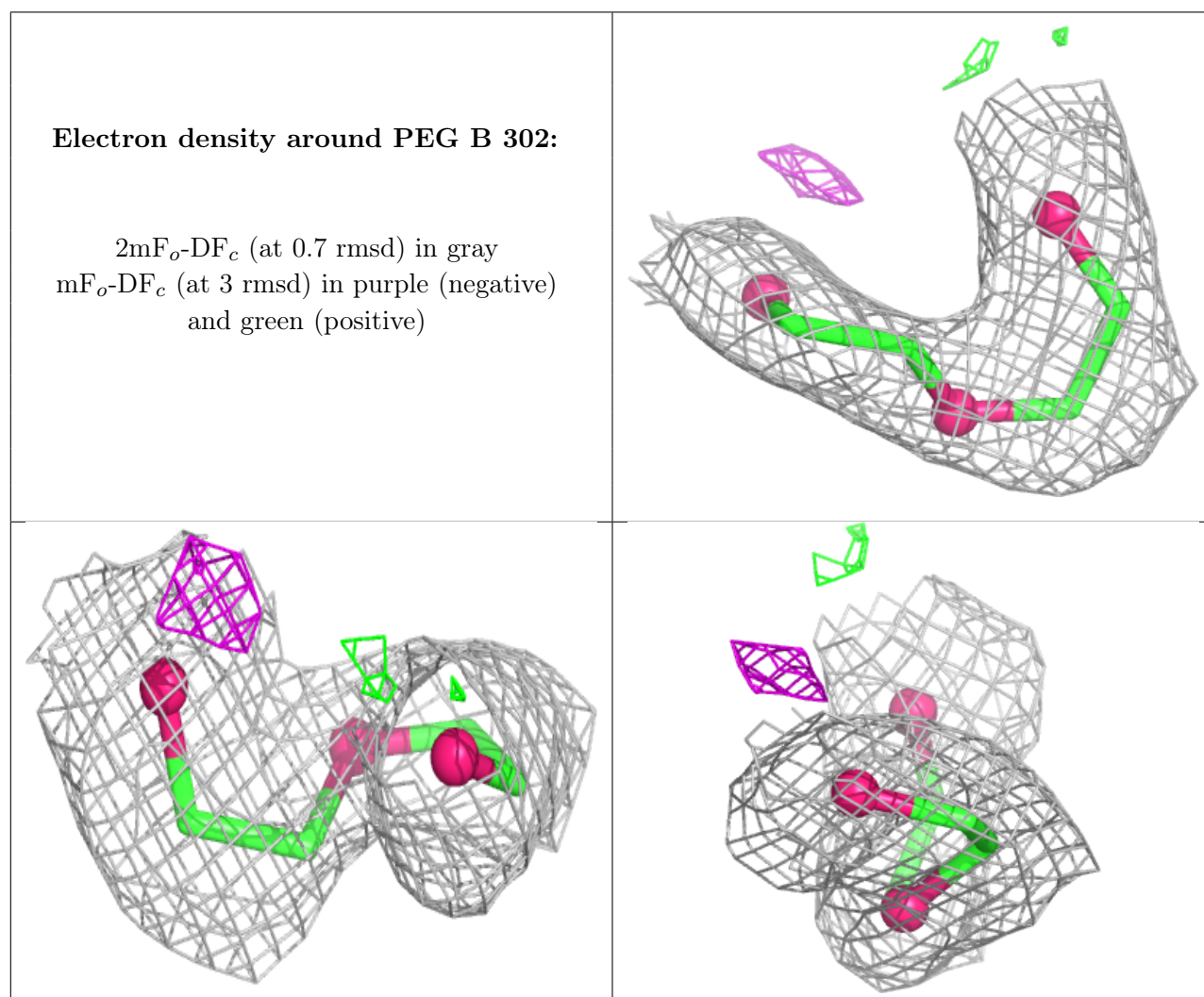
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	B	302	7/7	0.84	0.12	27,28,29,30	0
3	PEG	A	302	7/7	0.89	0.10	26,27,27,29	0
4	EDO	B	303	4/4	0.90	0.11	26,27,27,27	0

Continued on next page...

Continued from previous page...

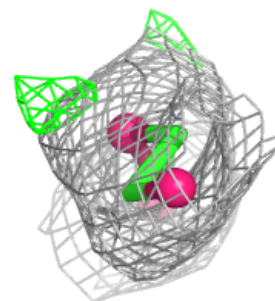
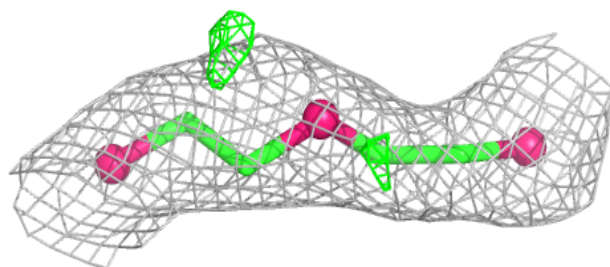
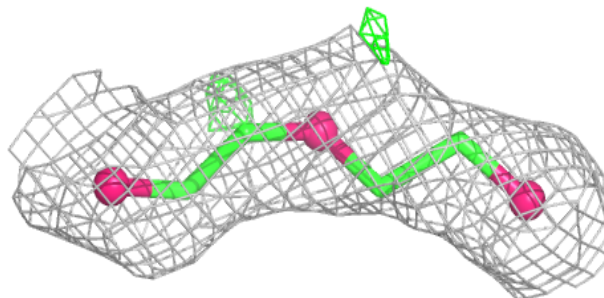
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2RG	A	301	33/33	0.91	0.10	16,23,43,45	0
2	2RG	B	301	33/33	0.93	0.09	16,23,50,51	0
5	CL	B	304	1/1	0.98	0.15	37,37,37,37	0

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.

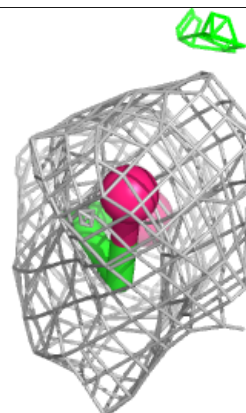
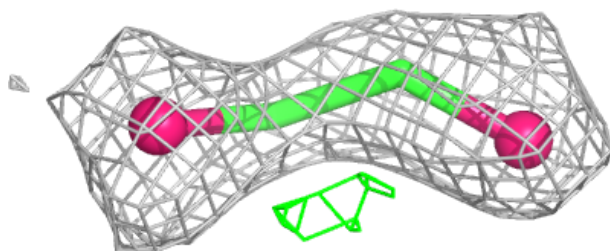
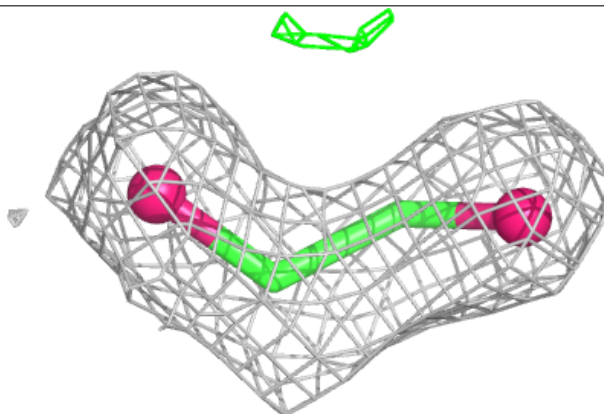


Electron density around PEG A 302:

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

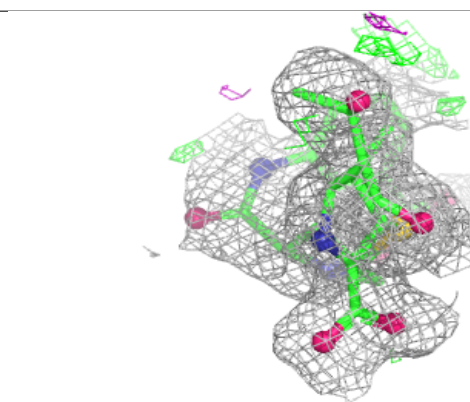
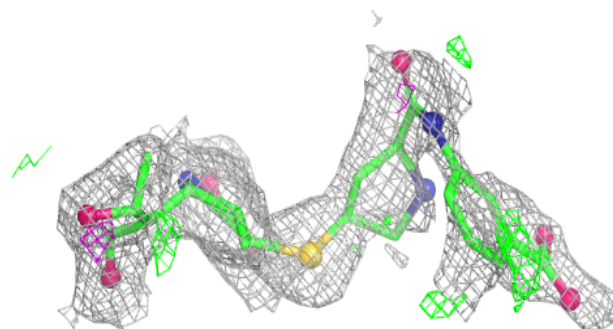
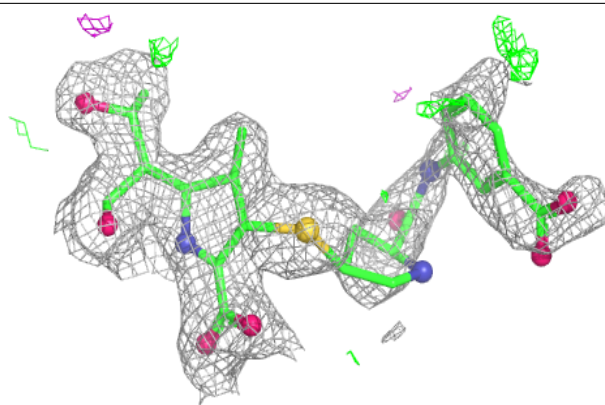
**Electron density around EDO B 303:**

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

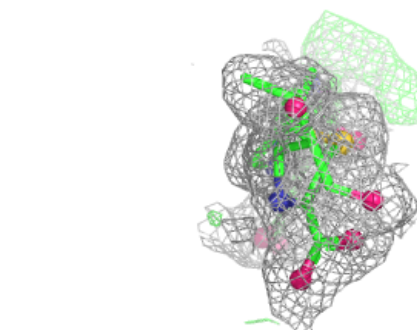
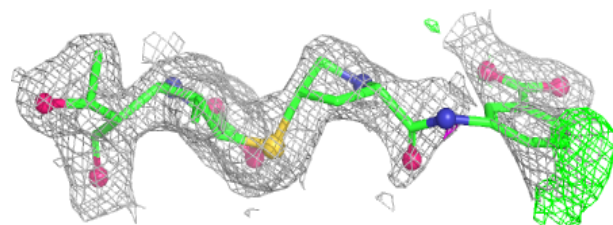
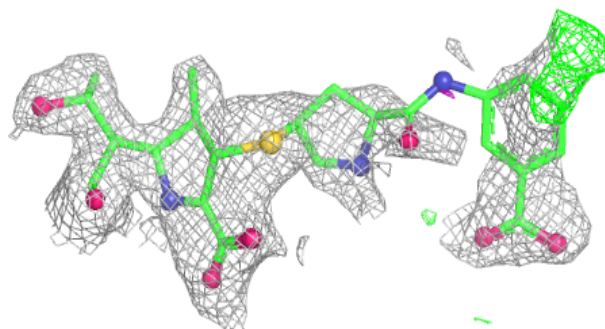


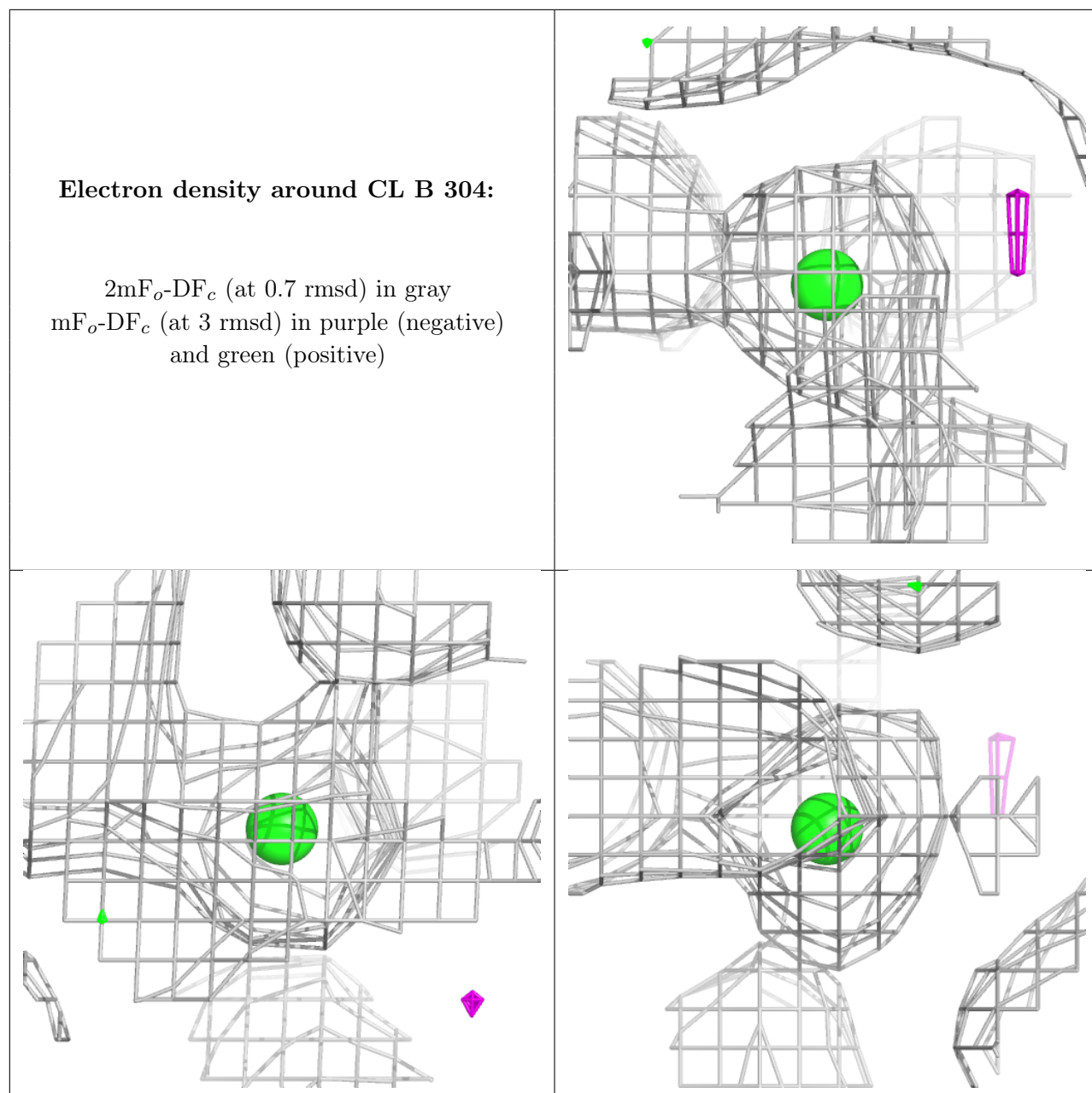
Electron density around 2RG A 301:

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

**Electron density around 2RG 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 ⓘ

There are no such residues in this entry.