



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2025 – 07:26 PM JST

PDB ID : 9KOO / pdb\_00009koo  
Title : Ligand binding domain of Pseudomonas Aeruginosa PAO1 chemoreceptor PctA in complex with MHF  
Authors : Songying, O.; Yanbo, Z.; Lei, Z.; Xinyu, Q.  
Deposited on : 2024-11-21  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

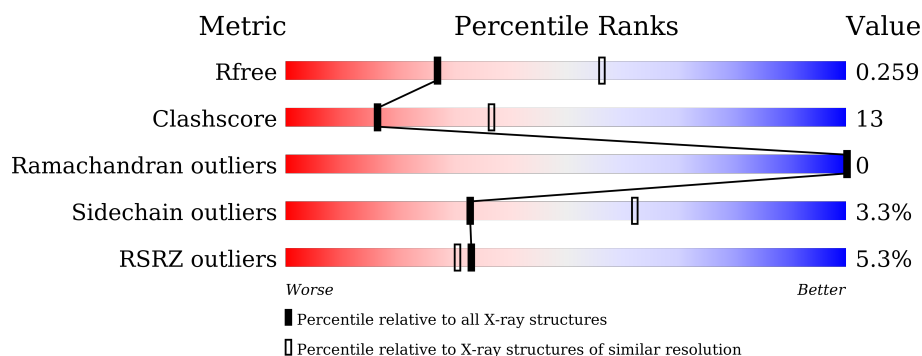
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 72%, yellow 72%, yellow 86%, grey 86%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>72%</span> <span>14%</span> <span>•</span> <span>14%</span> </div> </div>
1	B	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 54%, yellow 54%, yellow 82%, grey 82%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>8%</span> <span>54%</span> <span>28%</span> <span>•</span> <span>17%</span> </div> </div>

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	4XX	A	301	-	-	X	-
2	4XX	B	301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3788 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 Methyl-accepting chemotaxis protein PctA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1841	1170	306	360	5			
1	B	230	Total	C	N	O	S	0	0	0
			1753	1114	290	344	5			

There are 58 discrepancies between the modelled and reference sequences:

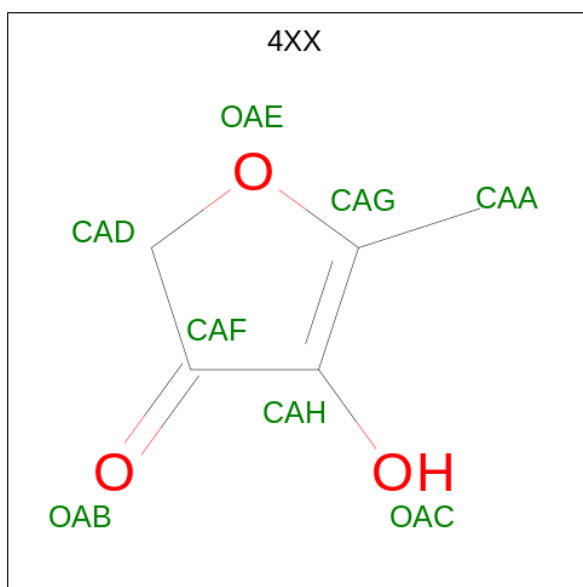
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP G3XD24
A	2	HIS	-	expression tag	UNP G3XD24
A	3	HIS	-	expression tag	UNP G3XD24
A	4	HIS	-	expression tag	UNP G3XD24
A	5	HIS	-	expression tag	UNP G3XD24
A	6	HIS	-	expression tag	UNP G3XD24
A	7	SER	-	expression tag	UNP G3XD24
A	8	SER	-	expression tag	UNP G3XD24
A	9	GLY	-	expression tag	UNP G3XD24
A	10	LEU	-	expression tag	UNP G3XD24
A	11	VAL	-	expression tag	UNP G3XD24
A	12	PRO	-	expression tag	UNP G3XD24
A	13	ARG	-	expression tag	UNP G3XD24
A	14	GLY	-	expression tag	UNP G3XD24
A	15	SER	-	expression tag	UNP G3XD24
A	16	HIS	-	expression tag	UNP G3XD24
A	17	MET	-	expression tag	UNP G3XD24
A	18	ALA	-	expression tag	UNP G3XD24
A	19	SER	-	expression tag	UNP G3XD24
A	20	MET	-	expression tag	UNP G3XD24
A	21	THR	-	expression tag	UNP G3XD24
A	22	GLY	-	expression tag	UNP G3XD24
A	23	GLY	-	expression tag	UNP G3XD24
A	24	GLN	-	expression tag	UNP G3XD24
A	25	GLN	-	expression tag	UNP G3XD24

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP G3XD24
A	27	GLY	-	expression tag	UNP G3XD24
A	28	ARG	-	expression tag	UNP G3XD24
A	29	GLY	-	expression tag	UNP G3XD24
B	1	HIS	-	expression tag	UNP G3XD24
B	2	HIS	-	expression tag	UNP G3XD24
B	3	HIS	-	expression tag	UNP G3XD24
B	4	HIS	-	expression tag	UNP G3XD24
B	5	HIS	-	expression tag	UNP G3XD24
B	6	HIS	-	expression tag	UNP G3XD24
B	7	SER	-	expression tag	UNP G3XD24
B	8	SER	-	expression tag	UNP G3XD24
B	9	GLY	-	expression tag	UNP G3XD24
B	10	LEU	-	expression tag	UNP G3XD24
B	11	VAL	-	expression tag	UNP G3XD24
B	12	PRO	-	expression tag	UNP G3XD24
B	13	ARG	-	expression tag	UNP G3XD24
B	14	GLY	-	expression tag	UNP G3XD24
B	15	SER	-	expression tag	UNP G3XD24
B	16	HIS	-	expression tag	UNP G3XD24
B	17	MET	-	expression tag	UNP G3XD24
B	18	ALA	-	expression tag	UNP G3XD24
B	19	SER	-	expression tag	UNP G3XD24
B	20	MET	-	expression tag	UNP G3XD24
B	21	THR	-	expression tag	UNP G3XD24
B	22	GLY	-	expression tag	UNP G3XD24
B	23	GLY	-	expression tag	UNP G3XD24
B	24	GLN	-	expression tag	UNP G3XD24
B	25	GLN	-	expression tag	UNP G3XD24
B	26	MET	-	expression tag	UNP G3XD24
B	27	GLY	-	expression tag	UNP G3XD24
B	28	ARG	-	expression tag	UNP G3XD24
B	29	GLY	-	expression tag	UNP G3XD24

- Molecule 2 is 4-hydroxy-5-methylfuran-3(2H)-one (CCD ID: 4XX) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



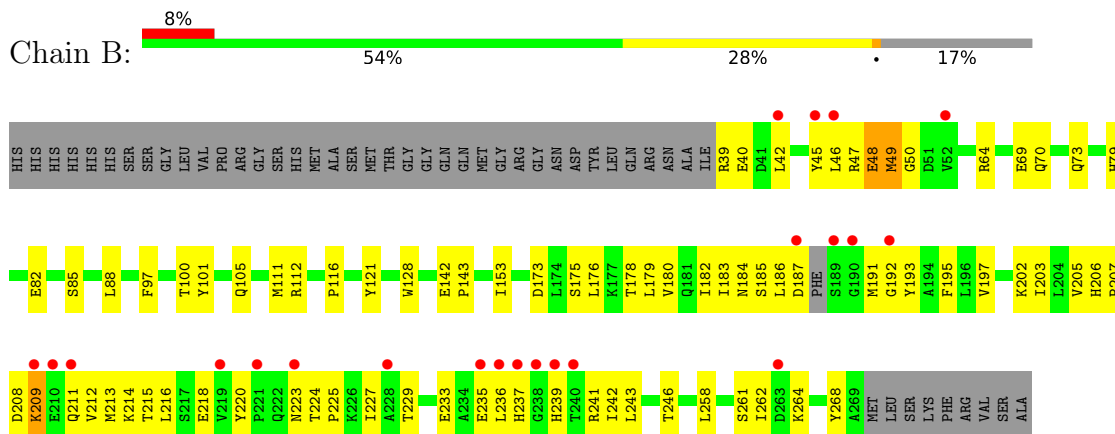
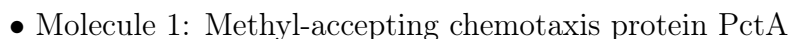
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	5	3		
2	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	78	Total	O	0	0
			78	78		



- Molecule 1: Methyl-accepting chemotaxis protein PctA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.97Å 76.17Å 117.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.24 – 2.70 36.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.24-2.70) 98.5 (36.24-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.207 , 0.260 0.205 , 0.259	Depositor DCC
$R_{free}$ test set	2000 reflections (7.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3788	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4XX

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	0.60	1/1881 (0.1%)	0.83	2/2564 (0.1%)
1	B	0.55	0/1790	0.86	1/2439 (0.0%)
All	All	0.57	1/3671 (0.0%)	0.84	3/5003 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	PRO	C-O	-5.24	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	PRO	N-CA-CB	-6.71	97.23	103.27
1	B	116	PRO	N-CA-CB	-6.58	97.46	103.25
1	A	151	GLU	CA-CB-CG	-5.47	103.16	114.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1841	0	1825	32	0
1	B	1753	0	1742	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	0	6	4	0
2	B	8	0	6	4	0
3	A	100	0	0	2	0
3	B	78	0	0	4	0
All	All	3788	0	3579	92	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 13.

All (92) 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:88:LEU:HD22	1:B:100:THR:HG22	1.45	0.98
1:B:208:ASP:HB3	1:B:211:GLN:HG2	1.46	0.94
1:A:210:GLU:O	1:A:214:LYS:HE2	1.87	0.75
1:A:126:ARG:HE	2:A:301:4XX:H4	1.51	0.75
1:A:46:LEU:HD21	1:A:262:ILE:HG13	1.69	0.74
1:A:138:LEU:CD1	1:A:252:PRO:HG2	2.20	0.71
1:A:188:PHE:O	1:A:191:MET:HB2	1.90	0.71
1:B:143:PRO:HG2	1:B:213:MET:SD	2.31	0.70
1:B:121:TYR:OH	2:B:301:4XX:H4	1.92	0.69
1:B:197:VAL:HG23	1:B:203:ILE:HD13	1.74	0.69
1:A:138:LEU:HD11	1:A:252:PRO:HG2	1.76	0.66
1:A:128:TRP:HE1	2:A:301:4XX:H5	1.61	0.65
1:B:212:VAL:HG12	1:B:213:MET:HG2	1.78	0.65
1:A:180:VAL:HG23	1:A:205:VAL:HG13	1.80	0.64
1:B:180:VAL:HG22	1:B:205:VAL:CG1	2.27	0.64
1:B:187:ASP:OD1	1:B:187:ASP:N	2.20	0.62
1:B:128:TRP:HE1	2:B:301:4XX:H5	1.65	0.62
1:A:186:LEU:H	1:A:186:LEU:HD23	1.66	0.61
1:B:128:TRP:NE1	2:B:301:4XX:H5	2.14	0.61
1:B:143:PRO:HA	1:B:153:ILE:O	2.01	0.60
1:B:206:HIS:ND1	1:B:207:PRO:HD2	2.16	0.60
1:B:39:ARG:HG2	1:B:39:ARG:O	2.00	0.60
1:B:82:GLU:OE1	1:B:82:GLU:N	2.35	0.59
1:B:202:LYS:HD2	1:B:213:MET:HA	1.86	0.57
1:B:264:LYS:HE2	1:B:268:TYR:CE2	2.41	0.56
1:A:128:TRP:HE1	2:A:301:4XX:CAD	2.18	0.56
1:B:241:ARG:HA	1:B:262:ILE:O	2.06	0.56
1:A:129:TYR:O	1:A:133:VAL:HG23	2.05	0.56
1:B:195:PHE:CE1	1:B:203:ILE:HD12	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:PHE:HB3	1:B:173:ASP:O	2.07	0.55
1:B:236:LEU:O	1:B:237:HIS:HB2	2.06	0.55
1:A:101:TYR:HB3	1:A:111:MET:HG3	1.89	0.55
1:B:180:VAL:HG22	1:B:205:VAL:HG13	1.87	0.54
1:A:195:PHE:HB2	1:A:205:VAL:O	2.07	0.54
1:B:233:GLU:OE2	1:B:264:LYS:NZ	2.39	0.54
1:A:75:LEU:CD2	1:A:84:VAL:HG22	2.38	0.53
1:A:111:MET:HE1	1:A:115:SER:HB3	1.91	0.53
1:B:82:GLU:H	1:B:82:GLU:CD	2.17	0.52
1:B:242:ILE:O	1:B:243:LEU:HD22	2.10	0.52
1:B:49:MET:HA	1:B:49:MET:CE	2.39	0.51
1:B:215:THR:HG22	1:B:218:GLU:CD	2.35	0.51
1:B:208:ASP:HB3	1:B:211:GLN:CG	2.29	0.51
1:B:183:ILE:HG13	1:B:184:ASN:ND2	2.26	0.51
1:A:112:ARG:HA	1:A:113:PRO:C	2.36	0.50
1:B:101:TYR:HB3	1:B:111:MET:HG3	1.93	0.50
1:A:138:LEU:HD12	1:A:252:PRO:HG2	1.93	0.50
1:B:49:MET:HA	1:B:49:MET:HE3	1.94	0.50
1:A:92:ALA:HB2	1:B:69:GLU:HG2	1.94	0.50
1:B:235:GLU:HA	1:B:239:HIS:O	2.12	0.50
1:B:197:VAL:CG2	1:B:203:ILE:HD13	2.42	0.49
1:B:180:VAL:HG11	1:B:207:PRO:HA	1.95	0.49
1:B:246:THR:OG1	3:B:401:HOH:O	2.20	0.49
1:A:208:ASP:HA	3:A:428:HOH:O	2.13	0.48
1:A:138:LEU:HD12	1:A:138:LEU:O	2.14	0.47
1:B:182:ILE:O	1:B:185:SER:HB3	2.14	0.47
1:B:142:GLU:HB3	1:B:143:PRO:HD2	1.95	0.47
1:A:82:GLU:H	1:A:82:GLU:CD	2.23	0.47
1:A:250:GLY:O	1:A:251:LEU:HD23	2.15	0.47
1:B:175:SER:HB3	1:B:178:THR:OG1	2.15	0.46
1:B:206:HIS:CE1	1:B:211:GLN:HG3	2.51	0.46
1:B:178:THR:O	1:B:182:ILE:HG12	2.16	0.46
1:A:126:ARG:HE	2:A:301:4XX:CAD	2.22	0.46
1:B:209:LYS:HB3	1:B:209:LYS:HE2	1.51	0.46
1:A:138:LEU:O	1:A:252:PRO:HB2	2.16	0.45
1:B:79:HIS:ND1	3:B:403:HOH:O	2.32	0.45
1:B:264:LYS:HE2	1:B:268:TYR:HE2	1.80	0.45
1:B:220:TYR:HE1	1:B:236:LEU:HB2	1.82	0.45
1:B:211:GLN:HA	1:B:211:GLN:OE1	2.18	0.44
1:A:180:VAL:CG2	1:A:205:VAL:HG13	2.45	0.43
1:A:90:GLN:NE2	1:B:70:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HD11	2:B:301:4XX:OAC	2.19	0.43
1:B:176:LEU:O	1:B:179:LEU:N	2.48	0.43
1:B:216:LEU:HD11	1:B:227:ILE:HD11	1.99	0.43
1:A:196:LEU:CD2	1:A:248:ILE:HD11	2.49	0.43
1:B:195:PHE:HE1	1:B:203:ILE:HD12	1.83	0.43
1:B:47:ARG:CG	1:B:48:GLU:N	2.80	0.43
1:B:85:SER:HB2	1:B:112:ARG:NH2	2.33	0.43
1:B:69:GLU:HG3	1:B:73:GLN:NE2	2.35	0.42
1:B:85:SER:HB2	1:B:112:ARG:HH21	1.84	0.42
1:A:85:SER:OG	1:A:112:ARG:NH1	2.53	0.42
1:B:203:ILE:HG12	1:B:214:LYS:O	2.20	0.42
1:B:105:GLN:NE2	3:B:405:HOH:O	2.39	0.42
1:B:50:GLY:HA2	1:B:258:LEU:CD2	2.50	0.42
1:A:191:MET:HB3	1:A:262:ILE:HG23	2.02	0.41
1:A:77:ARG:HH11	1:A:77:ARG:HB2	1.85	0.41
1:B:193:TYR:CD1	1:B:193:TYR:C	2.98	0.41
1:B:224:THR:HA	1:B:225:PRO:HD3	1.86	0.41
1:B:192:GLY:HA3	1:B:261:SER:O	2.21	0.40
1:A:158:THR:HA	1:A:159:PRO:HD3	1.94	0.40
1:B:45:TYR:O	1:B:46:LEU:C	2.62	0.40
1:A:236:LEU:O	3:A:401:HOH:O	2.22	0.40
1:B:64:ARG:NH2	3:B:404:HOH:O	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/278 (86%)	230 (97%)	8 (3%)	0	100	100
1	B	226/278 (81%)	217 (96%)	9 (4%)	0	100	100
All	All	464/556 (84%)	447 (96%)	17 (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	199/229 (87%)	195 (98%)	4 (2%)	50	78
1	B	190/229 (83%)	181 (95%)	9 (5%)	22	49
All	All	389/458 (85%)	376 (97%)	13 (3%)	33	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	68	VAL
1	A	98	SER
1	A	112	ARG
1	B	40	GLU
1	B	42	LEU
1	B	48	GLU
1	B	49	MET
1	B	186	LEU
1	B	191	MET
1	B	209	LYS
1	B	223	ASN
1	B	229	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	181	GLN
1	B	90	GLN
1	B	105	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	4XX	A	301	-	6,8,8	3.54	4 (66%)	7,11,11	5.23	6 (85%)
2	4XX	B	301	-	6,8,8	3.91	4 (66%)	7,11,11	5.85	7 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4XX	A	301	-	-	-	0/1/1/1
2	4XX	B	301	-	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	4XX	OAE-CAD	7.34	1.57	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	4XX	OAE-CAD	6.51	1.56	1.44
2	B	301	4XX	CAH-CAG	4.00	1.45	1.35
2	A	301	4XX	CAH-CAG	3.53	1.44	1.35
2	A	301	4XX	OAB-CAF	-3.14	1.16	1.23
2	B	301	4XX	OAB-CAF	-2.86	1.17	1.23
2	B	301	4XX	CAH-CAF	-2.71	1.41	1.46
2	A	301	4XX	CAH-CAF	-2.31	1.42	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	4XX	CAA-CAG-CAH	-9.72	117.54	133.13
2	B	301	4XX	OAE-CAG-CAH	-8.91	102.52	113.34
2	B	301	4XX	CAA-CAG-CAH	-8.39	119.68	133.13
2	A	301	4XX	OAE-CAG-CAH	-6.23	105.78	113.34
2	B	301	4XX	CAF-CAH-CAG	-5.25	104.14	109.36
2	A	301	4XX	OAE-CAG-CAA	5.19	120.44	113.61
2	B	301	4XX	OAC-CAH-CAG	-4.40	115.61	128.43
2	B	301	4XX	OAB-CAF-CAH	3.82	129.16	125.46
2	B	301	4XX	OAE-CAG-CAA	3.77	118.58	113.61
2	B	301	4XX	OAC-CAH-CAF	-3.71	115.99	122.61
2	A	301	4XX	OAC-CAH-CAG	-3.67	117.73	128.43
2	A	301	4XX	CAF-CAH-CAG	-3.20	106.18	109.36
2	A	301	4XX	OAB-CAF-CAH	2.54	127.92	125.46

There are no chirality outliers.

There are no torsion outliers.

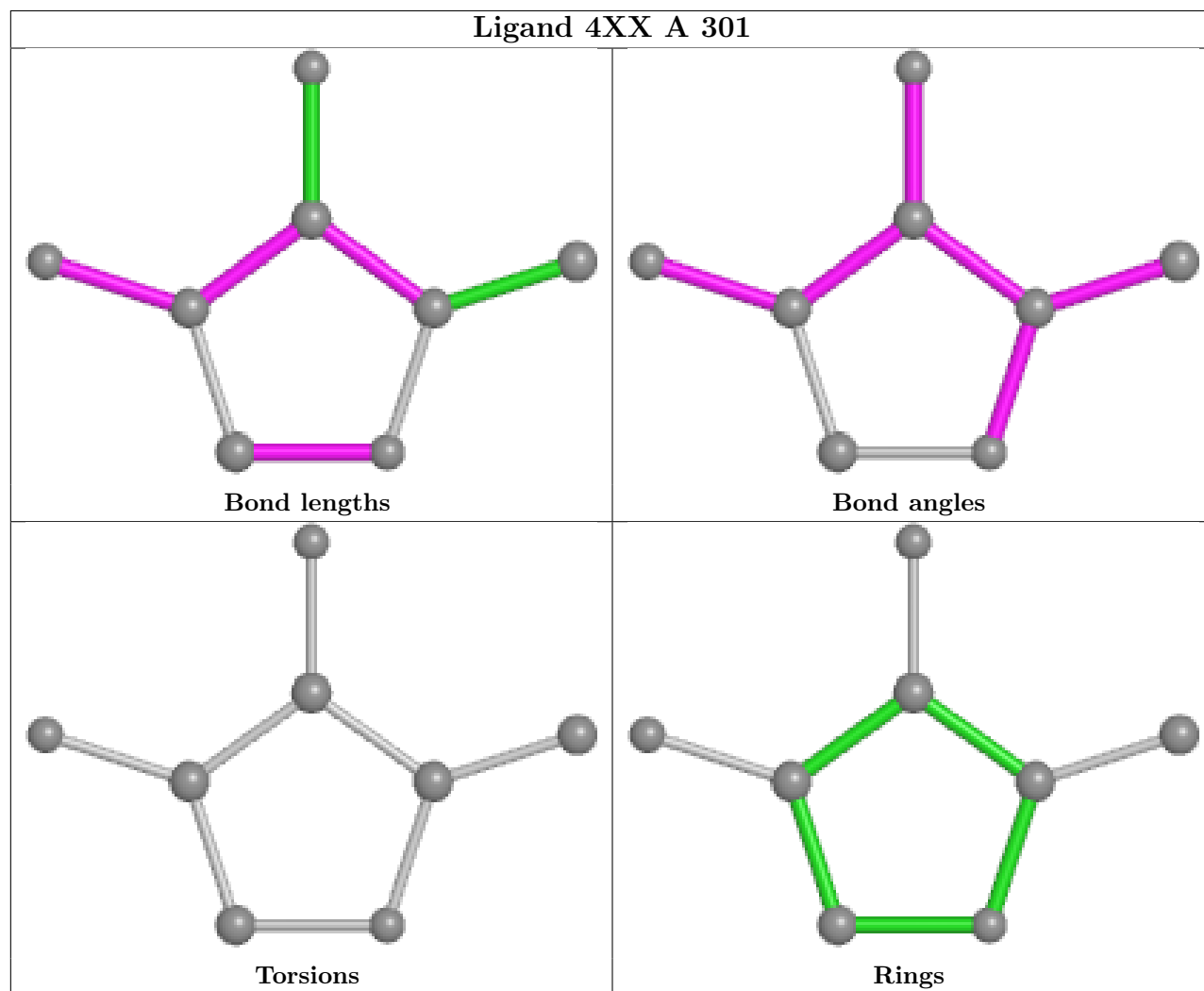
There are no ring outliers.

2 monomers are involved in 8 short contacts:

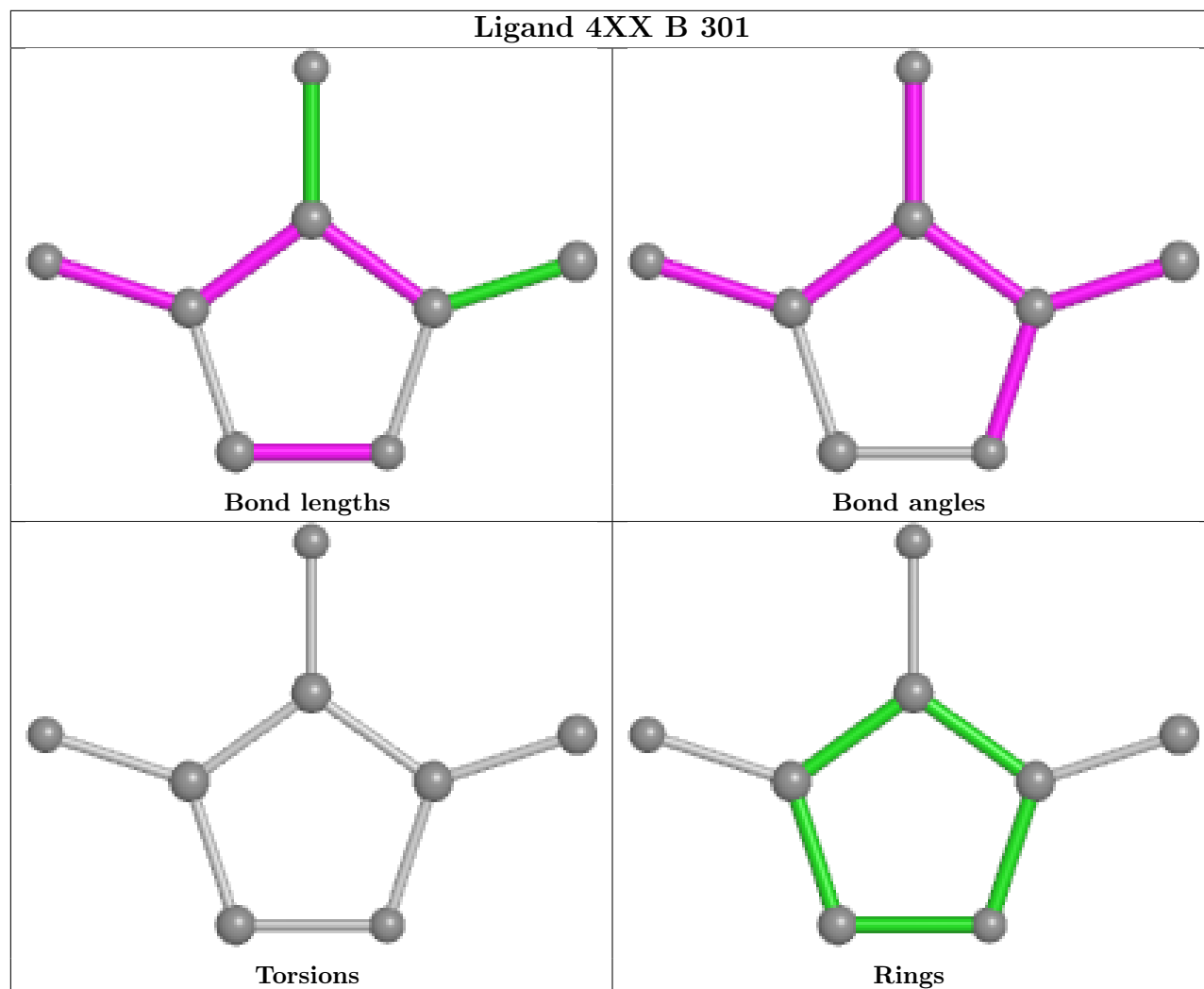
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	4XX	4	0
2	B	301	4XX	4	0

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	240/278 (86%)	-0.29	3 (1%) 74 74	8, 19, 45, 57	0
1	B	230/278 (82%)	0.38	22 (9%) 15 14	10, 31, 73, 94	0
All	All	470/556 (84%)	0.04	25 (5%) 33 31	8, 23, 68, 94	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	LEU	3.9
1	B	238	GLY	3.7
1	B	189	SER	3.6
1	B	52	VAL	3.6
1	B	190	GLY	3.2
1	B	45	TYR	3.1
1	B	223	ASN	2.9
1	B	237	HIS	2.9
1	B	239	HIS	2.6
1	B	228	ALA	2.6
1	B	235	GLU	2.5
1	B	210	GLU	2.5
1	B	221	PRO	2.5
1	A	164	GLY	2.5
1	B	192	GLY	2.5
1	A	165	ASN	2.5
1	B	42	LEU	2.4
1	B	219	VAL	2.4
1	B	187	ASP	2.3
1	B	209	LYS	2.2
1	B	263	ASP	2.2
1	B	240	THR	2.1
1	B	211	GLN	2.1
1	B	46	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	189	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

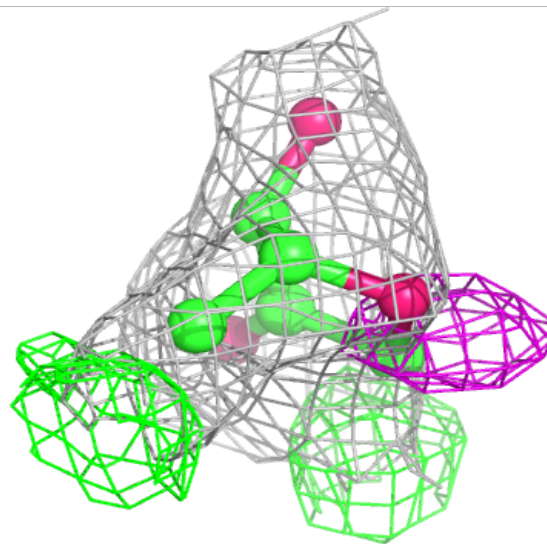
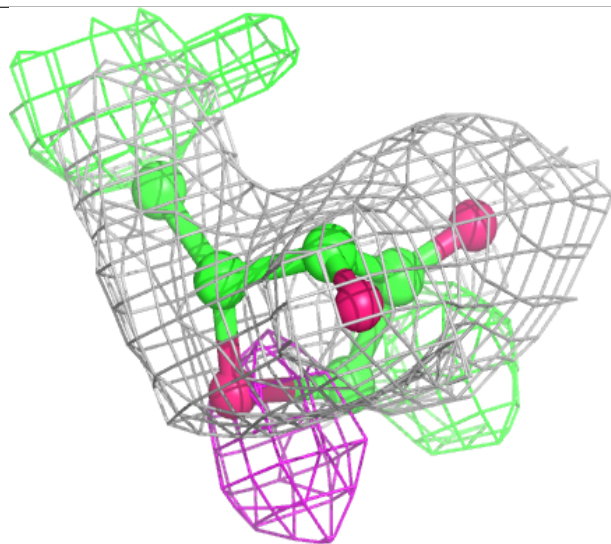
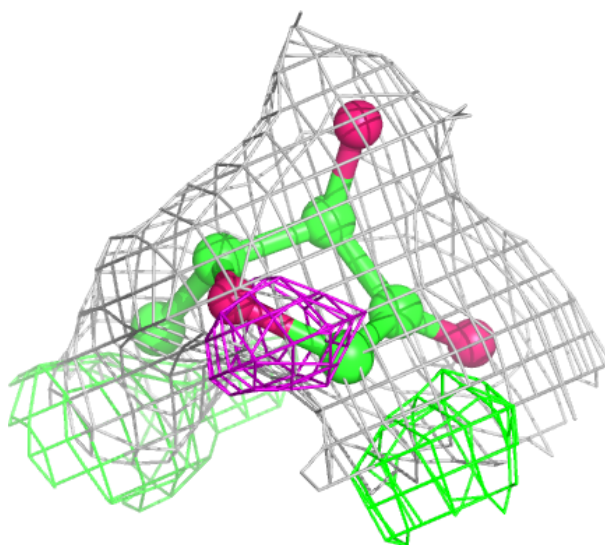
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	4XX	B	301	8/8	0.79	0.16	22,25,32,33	0
2	4XX	A	301	8/8	0.82	0.15	10,16,20,23	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.

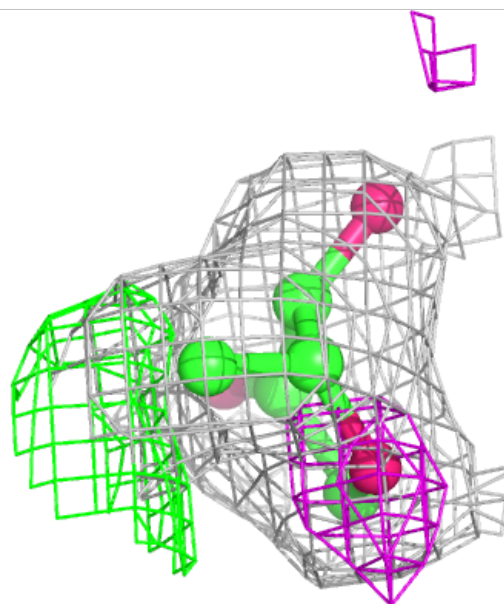
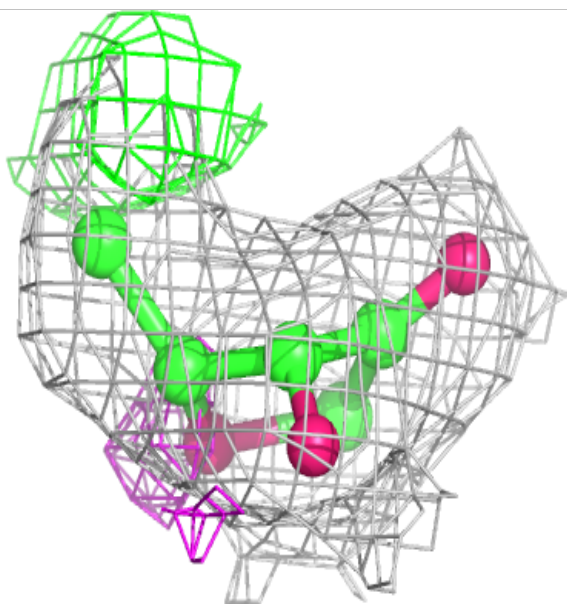
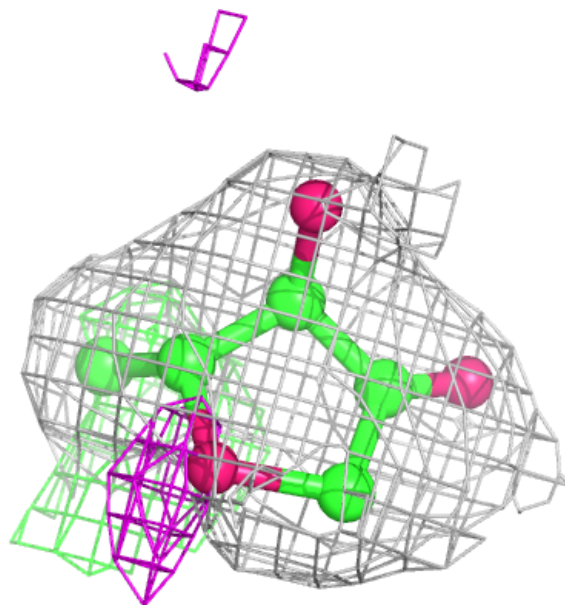
**Electron density around 4XX B 301:**

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



**Electron density around 4XX 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.