



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:21 AM UTC

PDB ID : 8ONN / pdb_00008onn
Title : Crystal structure of D-amino acid aminotransferase from Aminobacterium colombiense point mutant E113A complexed with 3-aminooxypropionic acid
Authors : Matyuta, I.O.; Boyko, K.M.; Minyaev, M.E.; Shilova, S.A.; Bezsudnova, E.Y.; Popov, V.O.
Deposited on : 2023-04-03
Resolution : 2.10 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:

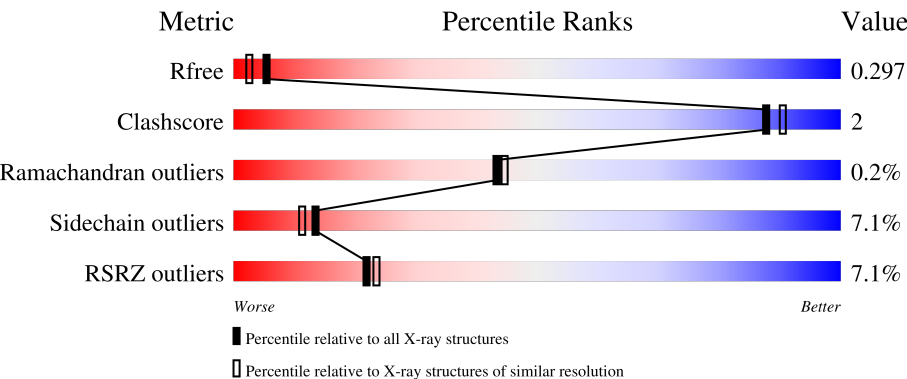
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	277	85% 13% .
1	B	277	16% 87% 10% ..
1	C	277	4% 87% 10% ..
1	D	277	4% 84% 14% ..

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Mol	Chain	Length	Quality of chain
1	E	277	10% 81% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10812 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.

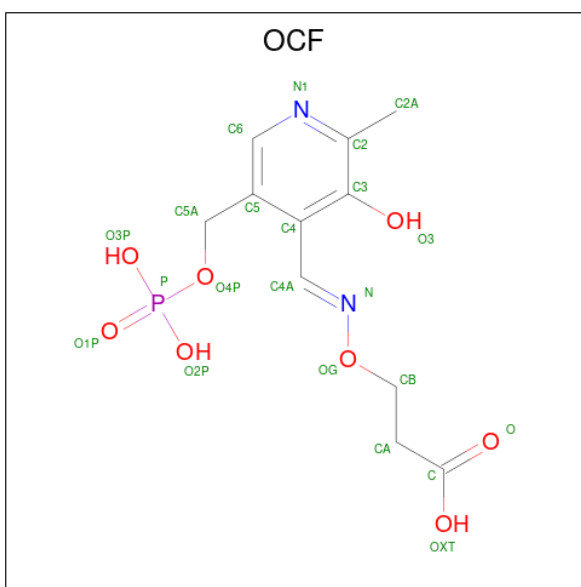
- Molecule 1 is a protein called Aminotransferase class IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	2	0
			2145	1370	364	400	11			
1	B	275	Total	C	N	O	S	0	0	0
			2079	1333	346	389	11			
1	C	275	Total	C	N	O	S	0	1	0
			2127	1360	361	395	11			
1	D	277	Total	C	N	O	S	0	2	0
			2150	1373	368	398	11			
1	E	268	Total	C	N	O	S	0	3	0
			2064	1329	339	385	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP D5EHC5
A	0	HIS	-	expression tag	UNP D5EHC5
A	113	ALA	GLU	engineered mutation	UNP D5EHC5
B	-1	GLY	-	expression tag	UNP D5EHC5
B	0	HIS	-	expression tag	UNP D5EHC5
B	113	ALA	GLU	engineered mutation	UNP D5EHC5
C	-1	GLY	-	expression tag	UNP D5EHC5
C	0	HIS	-	expression tag	UNP D5EHC5
C	113	ALA	GLU	engineered mutation	UNP D5EHC5
D	-1	GLY	-	expression tag	UNP D5EHC5
D	0	HIS	-	expression tag	UNP D5EHC5
D	113	ALA	GLU	engineered mutation	UNP D5EHC5
E	-1	GLY	-	expression tag	UNP D5EHC5
E	0	HIS	-	expression tag	UNP D5EHC5
E	113	ALA	GLU	engineered mutation	UNP D5EHC5

- Molecule 2 is 3-[(E)-[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylideneamino]oxypropanoic acid (CCD ID: OCF) (formula: C₁₁H₁₅N₂O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	D	1	Total	C	N	O	P	6	0
			22	11	2	8	1		

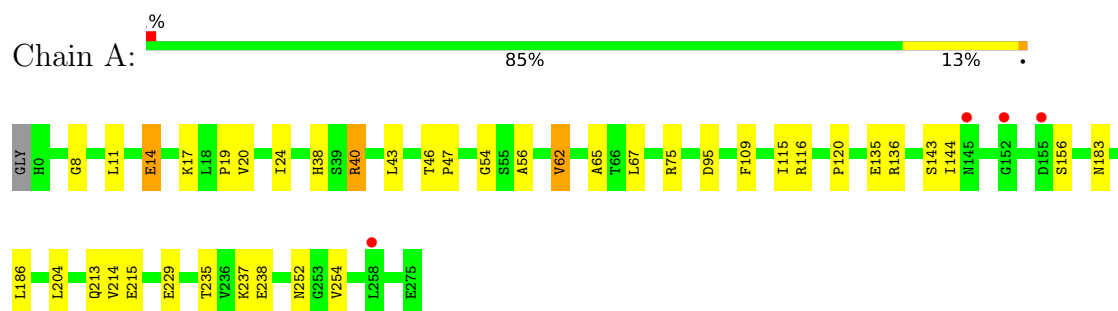
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	11	Total	O	0	0
			11	11		
3	C	44	Total	O	0	0
			44	44		
3	D	20	Total	O	0	0
			20	20		
3	E	31	Total	O	0	0
			31	31		

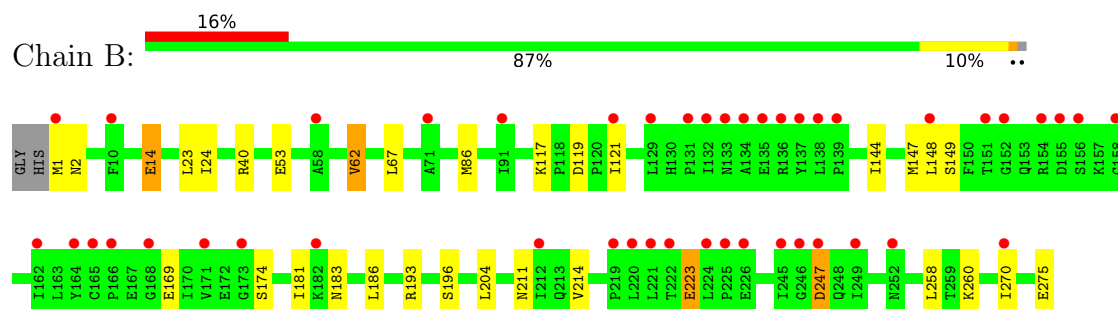
3 Residue-property plots

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.

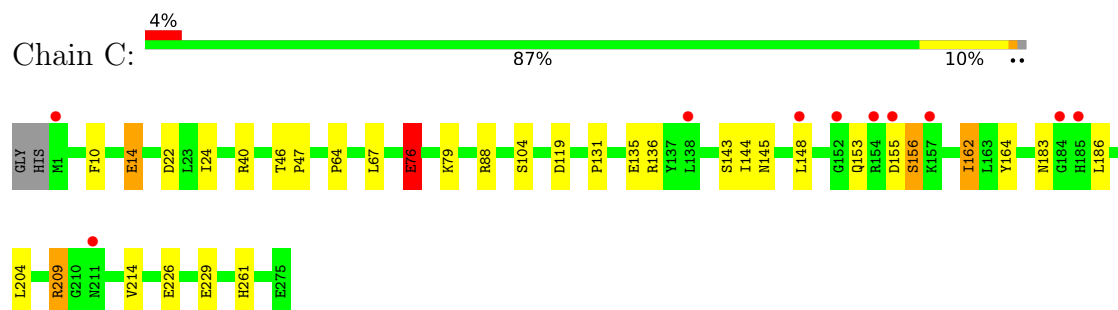
• Molecule 1: Aminotransferase class IV



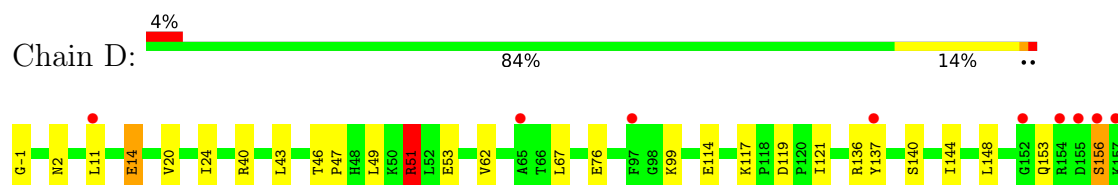
• Molecule 1: Aminotransferase class IV



• Molecule 1: Aminotransferase class IV

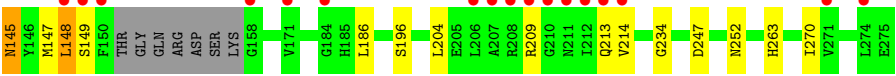
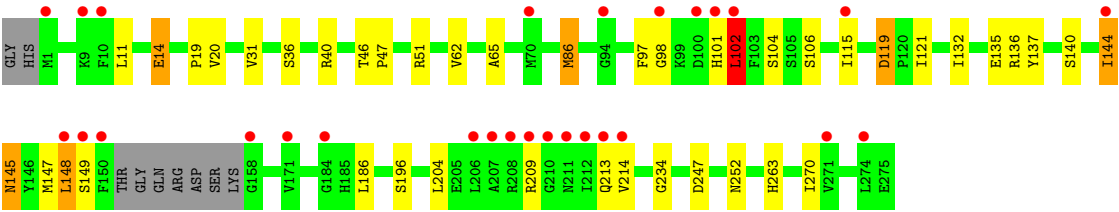
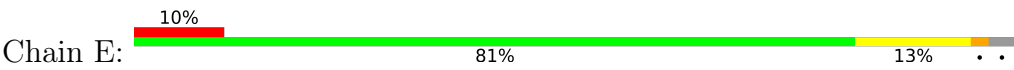


• Molecule 1: Aminotransferase class IV





● Molecule 1: Aminotransferase class IV



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.10Å 51.34Å 205.29Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	47.55 – 2.10 47.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.55-2.10) 97.8 (47.55-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.256 , 0.298 0.259 , 0.297	Depositor DCC
R_{free} test set	3975 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10812	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: OCF

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	1.47	14/2196 (0.6%)	1.59	8/2975 (0.3%)
1	B	1.30	0/2121	1.57	7/2881 (0.2%)
1	C	1.34	9/2173 (0.4%)	1.60	11/2946 (0.4%)
1	D	1.34	7/2200 (0.3%)	1.56	10/2979 (0.3%)
1	E	1.29	7/2116 (0.3%)	1.61	13/2871 (0.5%)
All	All	1.35	37/10806 (0.3%)	1.59	49/14652 (0.3%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ALA	C-O	8.97	1.34	1.24
1	C	64	PRO	C-O	-7.81	1.14	1.24
1	E	19	PRO	C-O	-7.11	1.15	1.23
1	E	31	VAL	C-O	6.92	1.31	1.23
1	A	95	ASP	C-O	6.77	1.32	1.24
1	E	234	GLY	C-O	6.35	1.30	1.23
1	C	143	SER	C-O	-6.32	1.15	1.23
1	D	255	PRO	C-O	-6.27	1.16	1.23
1	A	75	ARG	C-O	6.23	1.31	1.24
1	D	43	LEU	C-O	6.18	1.31	1.24
1	A	115	ILE	C-O	-6.08	1.17	1.24
1	E	145	ASN	C-O	-5.78	1.16	1.24
1	E	65	ALA	C-O	5.66	1.30	1.23
1	D	-1	GLY	N-CA	5.65	1.54	1.45
1	C	131	PRO	C-O	-5.58	1.17	1.23
1	A	8	GLY	C-O	5.56	1.31	1.24
1	E	136	ARG	C-O	-5.55	1.17	1.24
1	A	143	SER	C-O	-5.52	1.16	1.23
1	A	65	ALA	N-CA	5.48	1.52	1.45
1	D	178	PHE	C-O	5.47	1.30	1.24
1	C	22	ASP	C-O	5.46	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	LEU	C-O	5.45	1.30	1.24
1	A	116	ARG	C-O	5.42	1.31	1.23
1	C	88[A]	ARG	C-O	-5.38	1.19	1.24
1	C	88[B]	ARG	C-O	-5.38	1.19	1.24
1	D	2	ASN	C-O	-5.38	1.17	1.23
1	D	194	ALA	C-O	5.34	1.30	1.23
1	A	215	GLU	C-O	5.29	1.30	1.24
1	E	263	HIS	CE1-NE2	5.28	1.37	1.32
1	C	135	GLU	C-O	5.28	1.30	1.23
1	A	109	PHE	C-O	5.20	1.30	1.23
1	D	137	TYR	C-O	-5.13	1.17	1.23
1	A	238	GLU	C-O	5.12	1.30	1.24
1	C	261	HIS	CE1-NE2	5.09	1.37	1.32
1	A	38	HIS	CG-ND1	5.08	1.43	1.38
1	C	229	GLU	C-O	5.07	1.30	1.23
1	A	38	HIS	CD2-NE2	5.03	1.43	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ASP	CA-CB-CG	9.34	121.94	112.60
1	C	76	GLU	CB-CG-CD	8.95	127.81	112.60
1	B	247	ASP	CA-CB-CG	7.89	120.49	112.60
1	E	20	VAL	CA-C-N	7.69	130.92	120.38
1	E	20	VAL	C-N-CA	7.69	130.92	120.38
1	D	137	TYR	CA-C-O	-7.06	112.87	120.92
1	C	155	ASP	CA-C-N	7.01	132.10	122.77
1	C	155	ASP	C-N-CA	7.01	132.10	122.77
1	E	14	GLU	CB-CG-CD	6.88	124.31	112.60
1	C	14	GLU	CB-CG-CD	6.88	124.30	112.60
1	C	209	ARG	CB-CG-CD	6.80	126.94	111.30
1	E	247	ASP	CA-CB-CG	6.79	119.39	112.60
1	D	76	GLU	CB-CG-CD	6.62	123.85	112.60
1	A	14	GLU	CB-CG-CD	6.60	123.82	112.60
1	E	136	ARG	CA-C-O	-6.44	113.68	120.63
1	C	143	SER	CA-C-O	-6.37	114.73	121.99
1	A	40	ARG	CB-CG-CD	6.35	125.91	111.30
1	E	97	PHE	CA-C-N	6.29	126.64	120.98
1	E	97	PHE	C-N-CA	6.29	126.64	120.98
1	C	209	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	D	14	GLU	CB-CG-CD	6.22	123.18	112.60
1	B	2	ASN	CB-CA-C	6.22	120.14	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	GLU	CB-CG-CD	6.13	123.02	112.60
1	B	223	GLU	N-CA-CB	6.03	120.68	110.49
1	D	252	ASN	CA-CB-CG	5.91	118.51	112.60
1	D	53	GLU	CB-CG-CD	-5.88	102.60	112.60
1	D	62	VAL	N-CA-CB	5.84	116.89	110.53
1	C	145	ASN	CA-CB-CG	-5.64	106.96	112.60
1	E	98	GLY	O-C-N	5.62	126.61	122.62
1	C	145	ASN	CB-CA-C	5.61	119.86	110.88
1	D	51	ARG	CB-CG-CD	5.49	123.94	111.30
1	E	97	PHE	CB-CA-C	5.49	120.19	112.07
1	D	136	ARG	CG-CD-NE	-5.39	100.14	112.00
1	A	143	SER	CA-C-O	-5.37	115.76	121.94
1	A	54	GLY	CA-C-O	-5.36	114.98	120.66
1	A	19	PRO	CA-C-O	-5.34	115.26	121.34
1	B	53	GLU	CB-CG-CD	5.33	121.66	112.60
1	B	62	VAL	N-CA-CB	5.31	116.32	110.53
1	E	98	GLY	CA-C-O	-5.29	115.91	120.30
1	A	136	ARG	CG-CD-NE	-5.29	100.37	112.00
1	E	135	GLU	CA-C-N	5.27	127.60	120.38
1	E	135	GLU	C-N-CA	5.27	127.60	120.38
1	C	119	ASP	CB-CA-C	-5.24	100.97	109.56
1	A	235	THR	CA-CB-OG1	-5.23	101.75	109.60
1	D	114	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	185	HIS	N-CA-CB	5.07	118.65	110.85
1	E	137	TYR	N-CA-C	-5.05	107.15	113.72
1	A	62	VAL	N-CA-CB	5.01	115.99	110.53
1	B	275	GLU	CB-CA-C	5.00	119.60	110.10

There are no chirality outliers.

There are no planarity outliers.

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	2145	0	2168	6	0
1	B	2079	0	2055	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2127	0	2147	7	0
1	D	2150	0	2170	11	0
1	E	2064	0	2065	11	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
3	A	53	0	0	2	0
3	B	11	0	0	1	0
3	C	44	0	0	1	0
3	D	20	0	0	0	0
3	E	31	0	0	1	0
All	All	10812	0	10605	42	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 2.

All (42) 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:169:GLU:OE1	1:B:193:ARG:NH1	2.25	0.69
1:D:153:GLN:HA	1:D:156:SER:HB3	1.74	0.69
1:C:153:GLN:HA	1:C:156:SER:HB3	1.76	0.68
1:E:144:ILE:HB	1:E:147:MET:HE2	1.74	0.67
1:D:162:ILE:HD11	1:D:164:TYR:CE1	2.30	0.65
1:C:162:ILE:HD11	1:C:164:TYR:CE1	2.36	0.60
1:A:46:THR:HB	1:A:47:PRO:HD3	1.86	0.58
1:D:51:ARG:NH1	1:D:196:SER:O	2.39	0.55
1:A:204:LEU:HD22	1:A:214:VAL:HG11	1.88	0.55
1:C:46:THR:HB	1:C:47:PRO:HD3	1.89	0.53
1:E:86:MET:CE	3:E:305:HOH:O	2.57	0.53
1:C:204:LEU:HD22	1:C:214:VAL:HG11	1.93	0.50
1:A:252:ASN:HD21	1:A:254:VAL:HG22	1.77	0.50
1:E:132:ILE:HG21	1:E:144:ILE:HD13	1.94	0.50
1:B:204:LEU:HD22	1:B:214:VAL:HG11	1.94	0.49
1:E:204:LEU:HD22	1:E:214:VAL:HG11	1.95	0.49
1:E:132:ILE:HG21	1:E:144:ILE:CD1	2.44	0.47
1:E:119:ASP:OD2	1:E:119:ASP:N	2.48	0.46
1:B:119:ASP:OD1	1:B:121:ILE:HG22	2.15	0.46
1:D:46:THR:HB	1:D:47:PRO:HD3	1.98	0.46
1:B:149:SER:HB2	1:B:174:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:LEU:HD22	1:D:214:VAL:HG11	1.97	0.46
1:B:24:ILE:HD11	1:B:144:ILE:HG21	1.97	0.45
1:D:24:ILE:HD11	1:D:144:ILE:HG21	1.99	0.45
1:D:185:HIS:HE1	1:D:215:GLU:OE2	2.01	0.43
1:C:24:ILE:HD11	1:C:144:ILE:HG21	1.99	0.43
1:E:145:ASN:O	1:E:148:LEU:HG	2.18	0.43
1:D:185:HIS:CE1	1:D:215:GLU:OE2	2.72	0.43
1:A:135:GLU:HB2	3:A:445:HOH:O	2.19	0.42
1:D:250:ILE:O	1:D:252:ASN:O	2.36	0.42
1:E:36:SER:HB2	1:E:115:ILE:HD11	2.02	0.42
1:A:24:ILE:HD11	1:A:144:ILE:HG21	2.03	0.41
1:B:181:ILE:HD13	1:B:258:LEU:HD23	2.02	0.41
1:C:136:ARG:HD2	3:C:431:HOH:O	2.19	0.41
1:D:270:ILE:HD12	1:D:270:ILE:HA	1.90	0.41
1:E:46:THR:HB	1:E:47:PRO:HD3	2.02	0.41
1:E:140:SER:O	1:E:144:ILE:HG23	2.21	0.41
1:A:237:LYS:NZ	3:A:404:HOH:O	2.52	0.41
1:E:101:HIS:O	1:E:102:LEU:HB2	2.21	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.94	0.40
1:C:10:PHE:CE2	1:C:76:GLU:HG2	2.57	0.40
1:B:211:ASN:HB3	3:B:404:HOH:O	2.22	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	276/277 (100%)	269 (98%)	7 (2%)	0	100	100
1	B	273/277 (99%)	265 (97%)	7 (3%)	1 (0%)	30	28
1	C	274/277 (99%)	264 (96%)	10 (4%)	0	100	100
1	D	277/277 (100%)	269 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	267/277 (96%)	260 (97%)	5 (2%)	2 (1%)	18	15
All	All	1367/1385 (99%)	1327 (97%)	37 (3%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	GLU
1	E	102	LEU
1	E	149	SER

5.3.2 Protein sidechains [i](#)

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	236/240 (98%)	223 (94%)	13 (6%)	19	18
1	B	218/240 (91%)	202 (93%)	16 (7%)	13	10
1	C	230/240 (96%)	217 (94%)	13 (6%)	18	17
1	D	233/240 (97%)	214 (92%)	19 (8%)	10	8
1	E	222/240 (92%)	202 (91%)	20 (9%)	9	6
All	All	1139/1200 (95%)	1058 (93%)	81 (7%)	13	11

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	14	GLU
1	A	17	LYS
1	A	20	VAL
1	A	40	ARG
1	A	62	VAL
1	A	67	LEU
1	A	120	PRO
1	A	156	SER

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	186	LEU
1	A	213	GLN
1	A	229	GLU
1	B	1	MET
1	B	14	GLU
1	B	23	LEU
1	B	40	ARG
1	B	62	VAL
1	B	67	LEU
1	B	86	MET
1	B	117	LYS
1	B	147	MET
1	B	148	LEU
1	B	183	ASN
1	B	186	LEU
1	B	196	SER
1	B	247	ASP
1	B	260	LYS
1	B	270	ILE
1	C	14	GLU
1	C	40	ARG
1	C	67	LEU
1	C	76	GLU
1	C	79	LYS
1	C	104	SER
1	C	148	LEU
1	C	156	SER
1	C	162	ILE
1	C	183	ASN
1	C	186	LEU
1	C	209	ARG
1	C	226	GLU
1	D	11	LEU
1	D	14	GLU
1	D	20	VAL
1	D	40	ARG
1	D	51	ARG
1	D	67	LEU
1	D	99	LYS
1	D	117	LYS
1	D	119	ASP

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Mol	Chain	Res	Type
1	D	121	ILE
1	D	140	SER
1	D	148	LEU
1	D	156	SER
1	D	162	ILE
1	D	186	LEU
1	D	209	ARG
1	D	213	GLN
1	D	226	GLU
1	D	252	ASN
1	E	11	LEU
1	E	14	GLU
1	E	40	ARG
1	E	51	ARG
1	E	62	VAL
1	E	86	MET
1	E	102	LEU
1	E	104	SER
1	E	106	SER
1	E	119	ASP
1	E	121	ILE
1	E	144	ILE
1	E	148	LEU
1	E	186	LEU
1	E	196	SER
1	E	209[A]	ARG
1	E	209[B]	ARG
1	E	213	GLN
1	E	252	ASN
1	E	270	ILE

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	0	HIS
1	A	2	ASN
1	A	38	HIS
1	B	2	ASN
1	B	38	HIS
1	B	183	ASN
1	C	2	ASN
1	D	38	HIS

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Mol	Chain	Res	Type
1	D	101	HIS
1	D	185	HIS
1	E	26	GLN

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](#)

4 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	OCF	D	301	-	22,22,22	1.69	3 (13%)	28,30,30	1.62	5 (17%)
2	OCF	C	301	-	22,22,22	0.86	0	28,30,30	1.72	8 (28%)
2	OCF	A	301	-	22,22,22	1.19	2 (9%)	28,30,30	1.72	6 (21%)
2	OCF	B	301	-	22,22,22	0.86	0	28,30,30	1.13	3 (10%)

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	OCF	D	301	-	-	4/14/14/14	0/1/1/1
2	OCF	C	301	-	-	5/14/14/14	0/1/1/1
2	OCF	A	301	-	-	3/14/14/14	0/1/1/1
2	OCF	B	301	-	-	5/14/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	OCF	OXT-C	-4.76	1.15	1.30
2	A	301	OCF	C3-C2	-3.17	1.37	1.41
2	D	301	OCF	CA-CB	3.14	1.60	1.51
2	D	301	OCF	O3-C3	-2.68	1.30	1.36
2	A	301	OCF	O3-C3	-2.13	1.32	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OCF	CB-CA-C	-5.74	105.23	113.11
2	D	301	OCF	O4P-C5A-C5	3.90	116.67	109.36
2	C	301	OCF	O3P-P-O2P	3.75	121.85	107.80
2	C	301	OCF	O3P-P-O4P	-3.66	97.12	106.67
2	C	301	OCF	CB-CA-C	3.44	117.83	113.11
2	C	301	OCF	O4P-C5A-C5	3.26	115.47	109.36
2	A	301	OCF	O2P-P-O4P	-3.15	98.45	106.67
2	D	301	OCF	O3P-P-O2P	3.14	119.56	107.80
2	D	301	OCF	CB-CA-C	3.01	117.23	113.11
2	D	301	OCF	OG-N-C4A	2.65	114.80	110.83
2	B	301	OCF	O4P-C5A-C5	2.65	114.33	109.36
2	D	301	OCF	C3-C2-N1	-2.50	117.80	120.96
2	A	301	OCF	O-C-CA	-2.50	115.17	123.09
2	B	301	OCF	CB-CA-C	2.39	116.39	113.11
2	A	301	OCF	O3P-P-O1P	2.36	120.03	110.83
2	A	301	OCF	C6-N1-C2	2.26	123.30	119.20
2	C	301	OCF	OG-N-C4A	2.25	114.19	110.83
2	C	301	OCF	OG-CB-CA	2.23	115.73	109.14
2	A	301	OCF	C3-C2-N1	-2.20	118.19	120.96
2	B	301	OCF	C4-C3-C2	-2.14	118.94	120.14
2	C	301	OCF	C3-C4-C4A	-2.10	116.61	120.40
2	C	301	OCF	C5-C4-C4A	2.04	124.62	121.47

There are no chirality outliers.

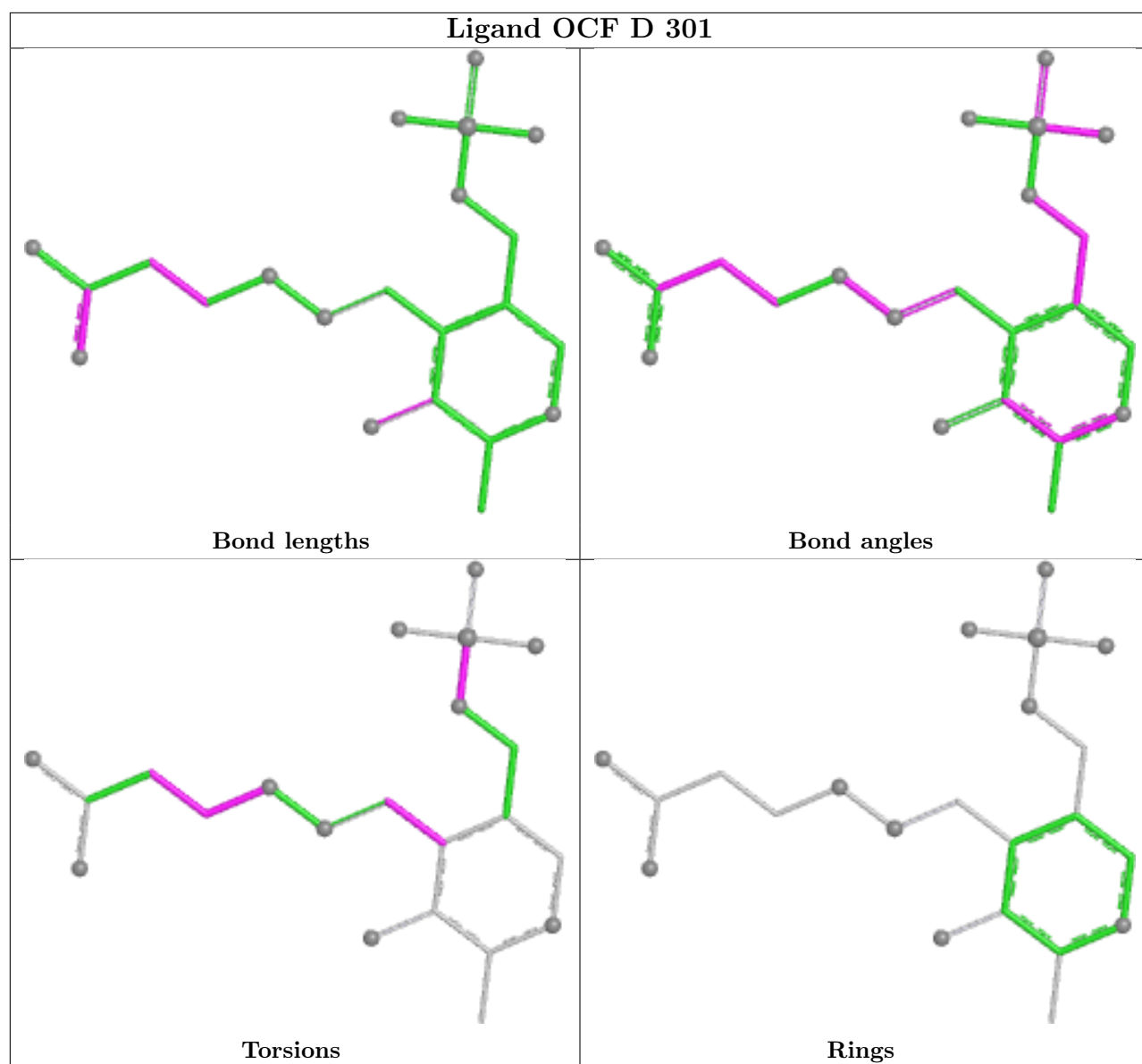
All (17) torsion outliers are listed below:

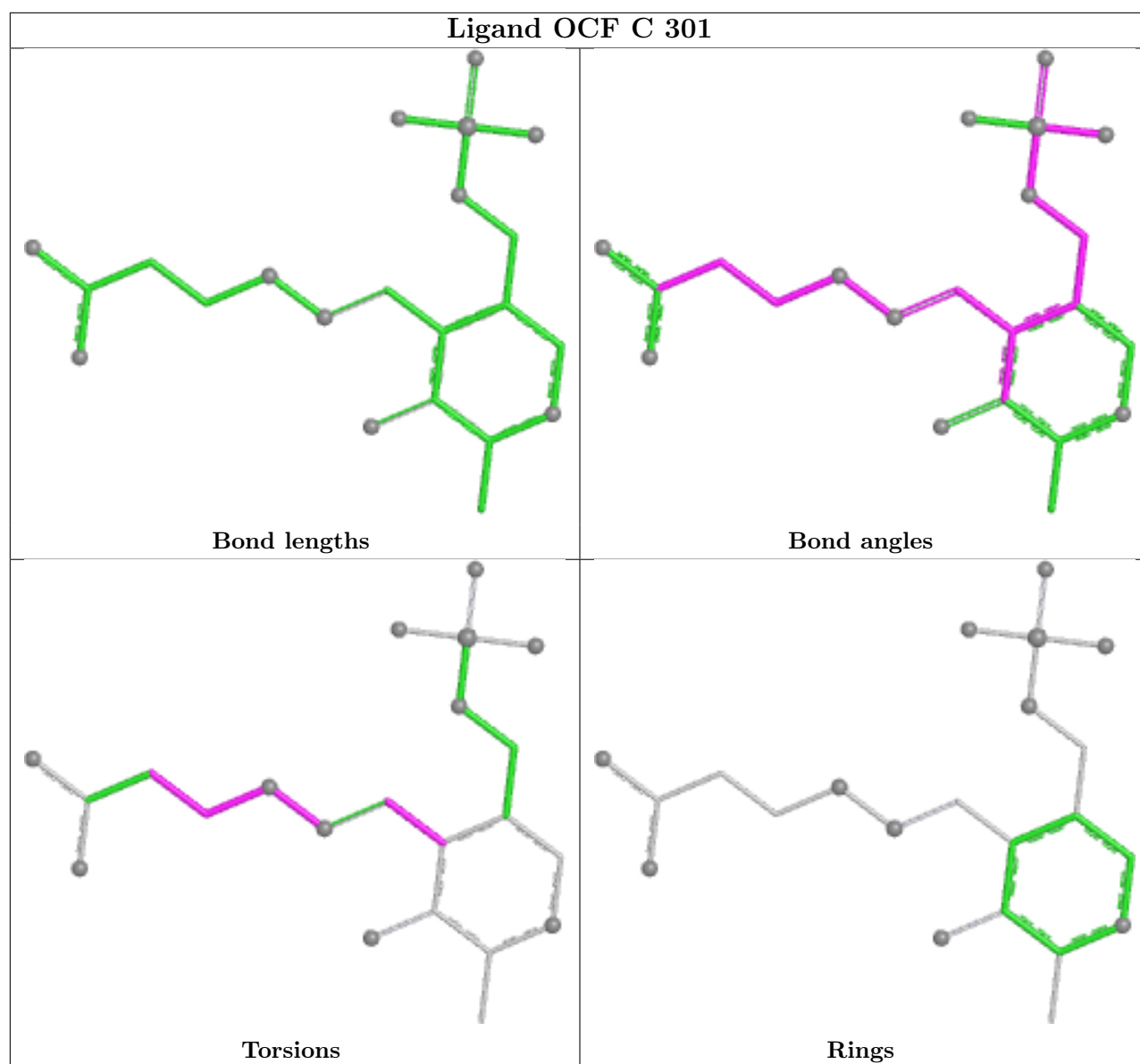
Mol	Chain	Res	Type	Atoms
2	A	301	OCF	C4A-N-OG-CB
2	A	301	OCF	CA-CB-OG-N
2	B	301	OCF	C3-C4-C4A-N
2	B	301	OCF	C4-C4A-N-OG
2	B	301	OCF	C-CA-CB-OG
2	C	301	OCF	C3-C4-C4A-N
2	C	301	OCF	C4A-N-OG-CB
2	C	301	OCF	C-CA-CB-OG
2	D	301	OCF	C3-C4-C4A-N
2	D	301	OCF	C-CA-CB-OG
2	C	301	OCF	CA-CB-OG-N
2	D	301	OCF	CA-CB-OG-N
2	B	301	OCF	OXT-C-CA-CB
2	B	301	OCF	O-C-CA-CB
2	A	301	OCF	C3-C4-C4A-N
2	C	301	OCF	C5-C4-C4A-N
2	D	301	OCF	C5A-O4P-P-O1P

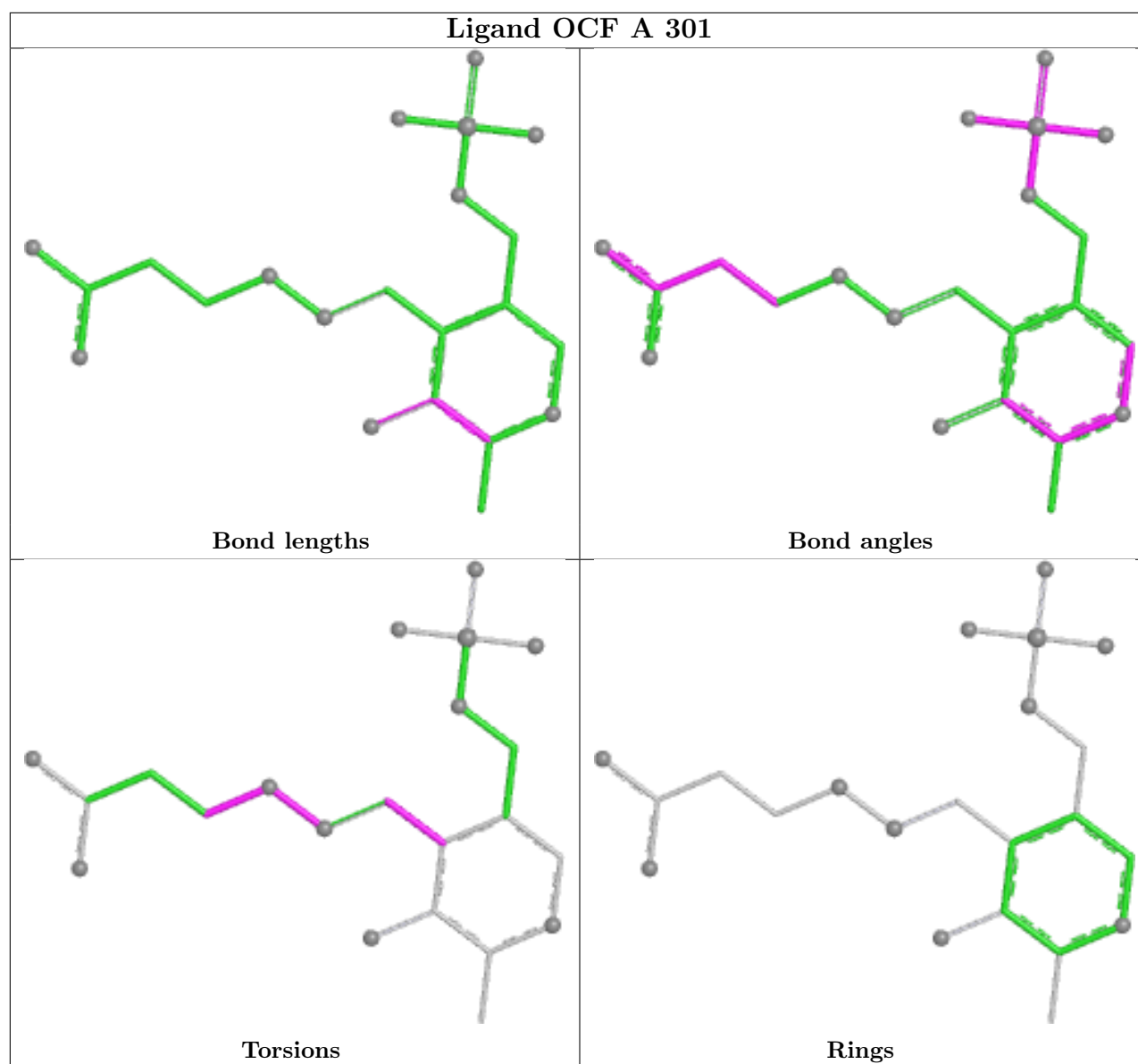
There are no ring outliers.

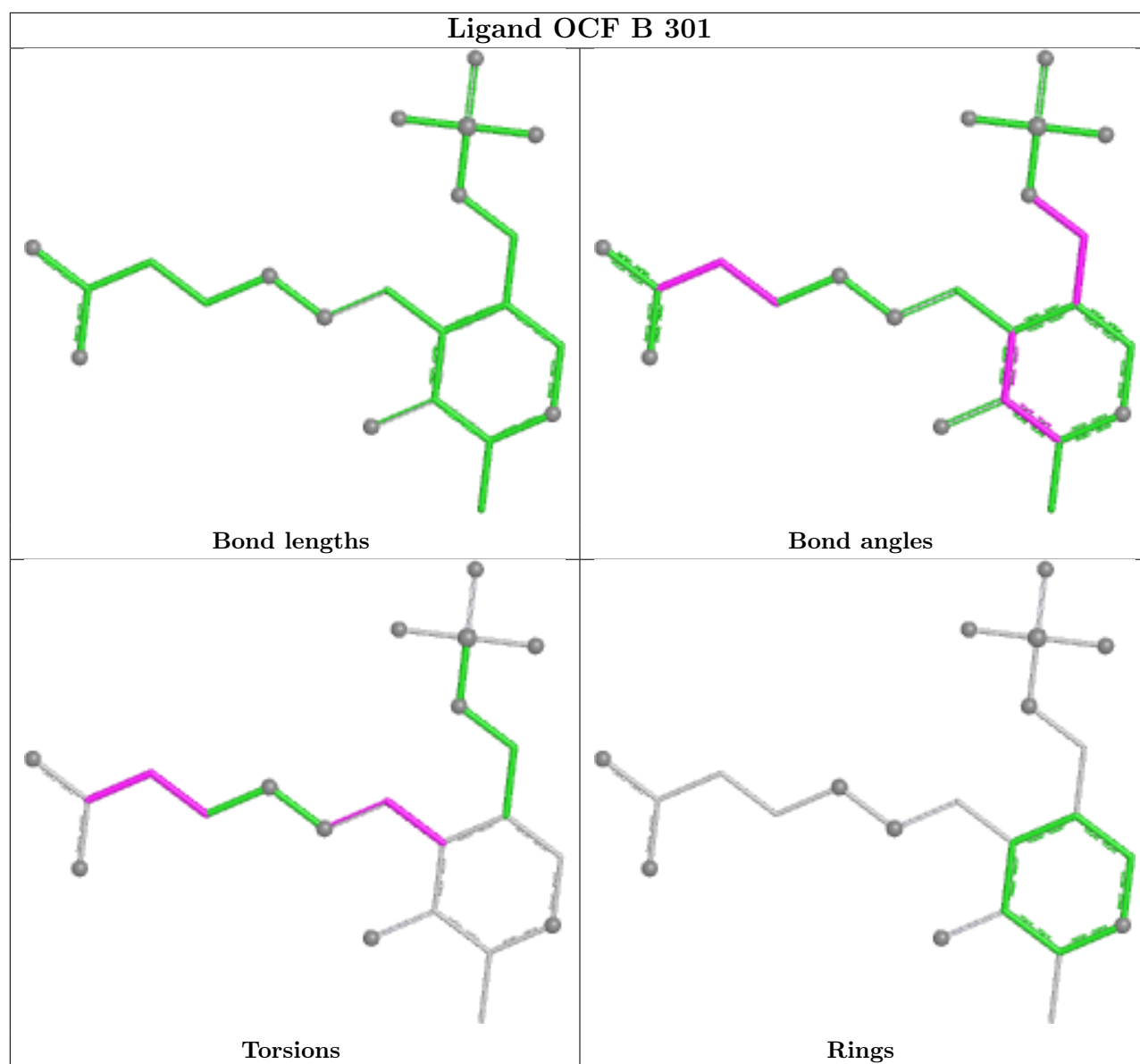
No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/277 (99%)	0.32	4 (1%) 73 75	18, 30, 46, 76	2 (0%)
1	B	275/277 (99%)	1.23	45 (16%) 4 4	29, 48, 77, 92	0
1	C	275/277 (99%)	0.63	10 (3%) 46 48	15, 38, 57, 78	1 (0%)
1	D	277/277 (100%)	0.68	11 (3%) 42 44	20, 40, 55, 76	2 (0%)
1	E	268/277 (96%)	0.96	28 (10%) 11 12	24, 41, 62, 87	3 (1%)
All	All	1371/1385 (98%)	0.76	98 (7%) 22 23	15, 39, 63, 92	8 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	ASP	5.4
1	B	221	LEU	5.1
1	E	150	PHE	5.0
1	E	101	HIS	4.8
1	B	137	TYR	4.7
1	B	138	LEU	4.6
1	E	102	LEU	3.7
1	D	137	TYR	3.7
1	E	148	LEU	3.6
1	A	155	ASP	3.5
1	B	168	GLY	3.5
1	C	152	GLY	3.5
1	B	154	ARG	3.5
1	B	249	ILE	3.5
1	E	271	VAL	3.5
1	B	10	PHE	3.4
1	B	1	MET	3.3
1	E	209[A]	ARG	3.3
1	B	148	LEU	3.3
1	C	155	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	158	GLY	3.3
1	B	220	LEU	3.2
1	E	10	PHE	3.2
1	E	149	SER	3.2
1	B	139	PRO	3.2
1	C	138	LEU	3.2
1	D	154[A]	ARG	3.2
1	B	135	GLU	3.1
1	B	252	ASN	3.0
1	E	213	GLN	3.0
1	C	157	LYS	3.0
1	C	154	ARG	2.9
1	E	207	ALA	2.9
1	C	185	HIS	2.9
1	D	249	ILE	2.9
1	A	152	GLY	2.9
1	E	210	GLY	2.8
1	B	134	ALA	2.8
1	B	270	ILE	2.8
1	E	212	ILE	2.8
1	E	208	ARG	2.8
1	B	247	ASP	2.8
1	B	152	GLY	2.8
1	D	156	SER	2.7
1	B	164	TYR	2.7
1	B	171	VAL	2.7
1	E	211	ASN	2.7
1	B	131	PRO	2.6
1	D	157	LYS	2.6
1	B	136	ARG	2.6
1	E	1	MET	2.6
1	B	151	THR	2.6
1	B	222	THR	2.6
1	B	245	ILE	2.5
1	B	133	ASN	2.5
1	B	182	LYS	2.5
1	B	162	ILE	2.5
1	B	212	ILE	2.4
1	B	246	GLY	2.4
1	D	155	ASP	2.4
1	B	71	ALA	2.4
1	E	274	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	152	GLY	2.4
1	E	94	GLY	2.4
1	B	219	PRO	2.4
1	D	11	LEU	2.3
1	E	98	GLY	2.3
1	C	1	MET	2.3
1	B	156	SER	2.3
1	B	224	LEU	2.3
1	D	97	PHE	2.3
1	E	184	GLY	2.3
1	B	226	GLU	2.3
1	B	225	PRO	2.3
1	E	115	ILE	2.2
1	E	171	VAL	2.2
1	B	58	ALA	2.2
1	E	206	LEU	2.2
1	E	214	VAL	2.2
1	A	258	LEU	2.2
1	C	211	ASN	2.2
1	C	184	GLY	2.2
1	B	132	ILE	2.1
1	D	270	ILE	2.1
1	E	144	ILE	2.1
1	B	129	LEU	2.1
1	E	9	LYS	2.1
1	E	70	MET	2.1
1	E	100	ASP	2.1
1	B	91	ILE	2.1
1	B	165	CYS	2.1
1	A	145[A]	ASN	2.1
1	B	121	ILE	2.1
1	B	173	GLY	2.1
1	B	166	PRO	2.1
1	D	65	ALA	2.1
1	C	148	LEU	2.0
1	B	158	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

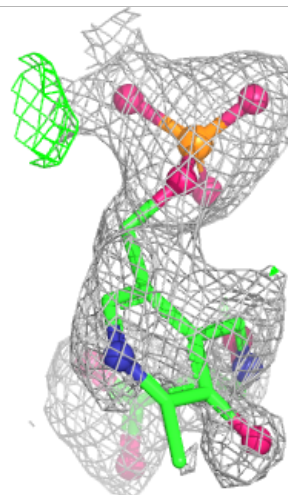
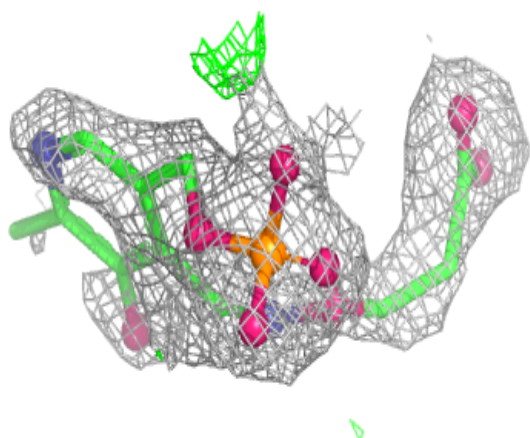
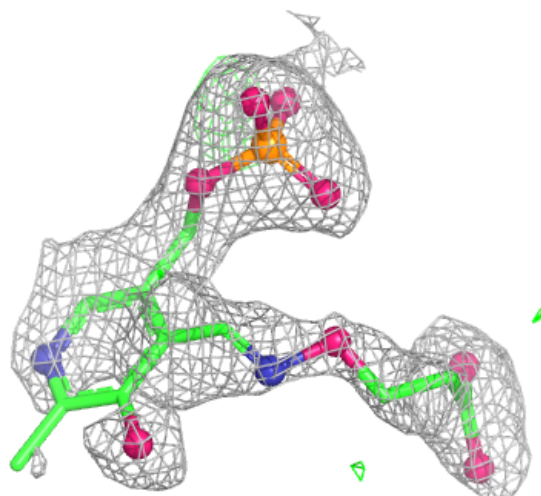
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OCF	B	301	22/22	0.91	0.12	26,33,36,36	22
2	OCF	D	301	22/22	0.95	0.08	0,30,32,34	6
2	OCF	C	301	22/22	0.96	0.08	29,37,50,51	0
2	OCF	A	301	22/22	0.96	0.09	20,27,43,50	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.

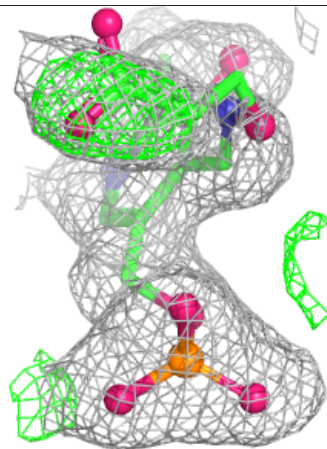
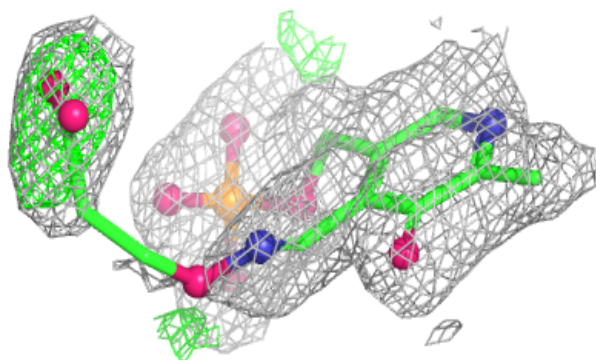
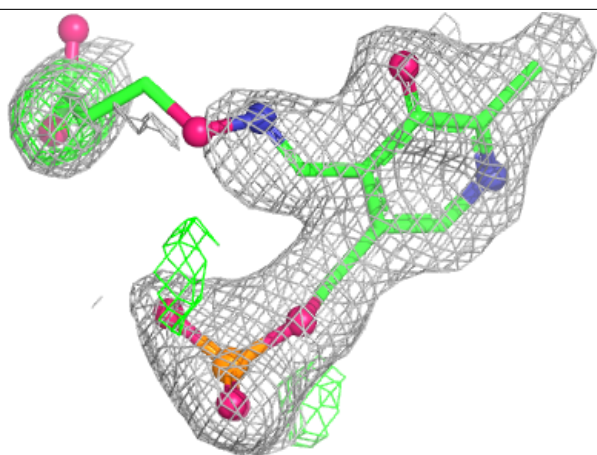
Electron density around OCF B 301:

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



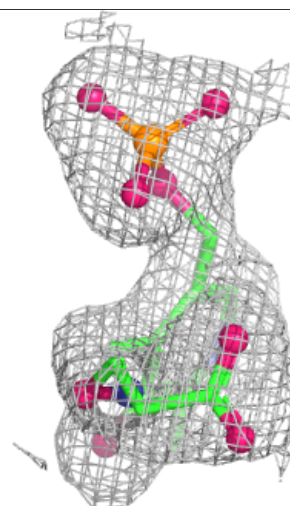
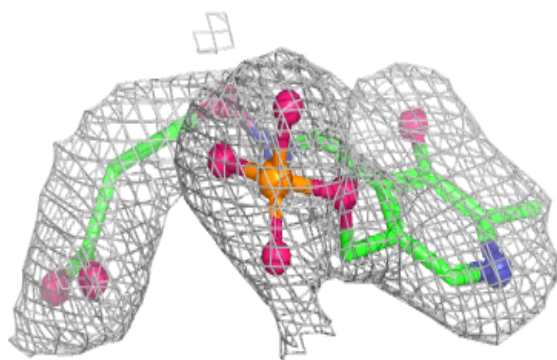
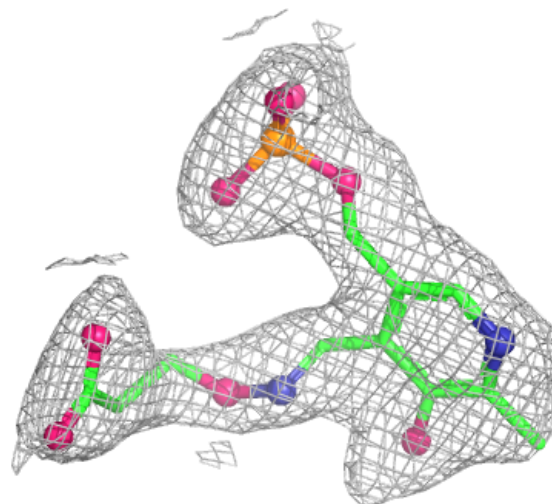
Electron density around OCF D 301:

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



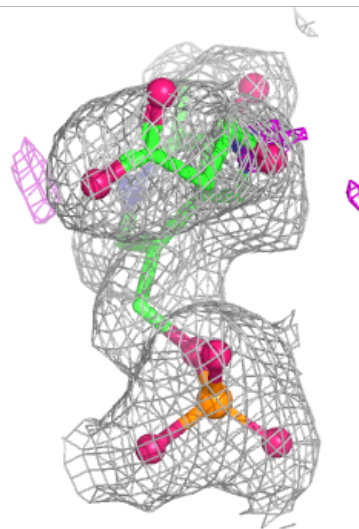
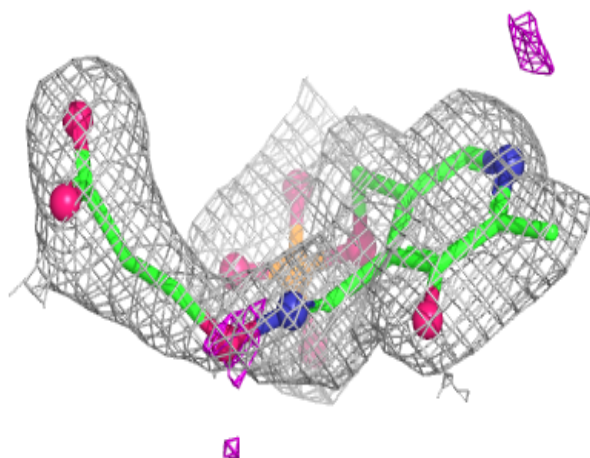
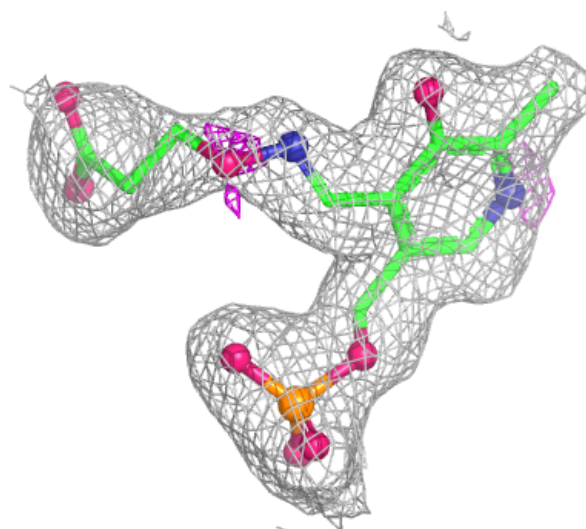
Electron density around OCF C 301:

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



Electron density around OCF 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 [i](#)

There are no such residues in this entry.