Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 05:04 PM EDT

PDB ID	:	7UVM
Title	:	Crystal structure of human ClpP protease in complex with TR-27
Authors	:	Mabanglo, M.F.; Houry, W.A.
Deposited on	:	2022-05-02
Resolution	:	2.19 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 (i) 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 (i)) were used in the production of this report:

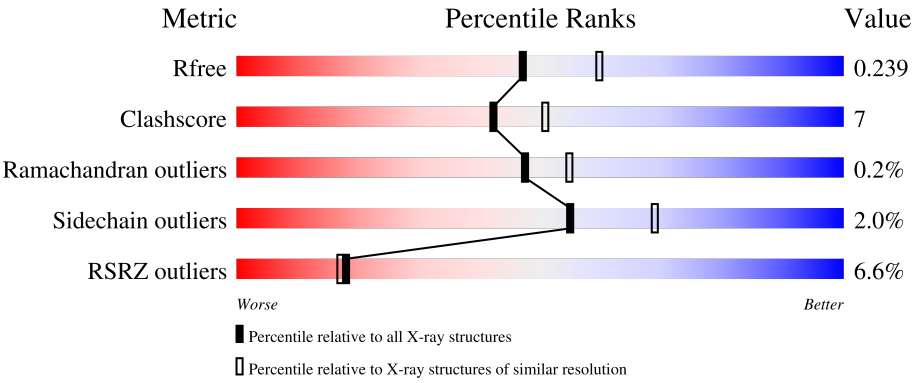
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.19 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	221	4% 66% 11% • 21%
1	B	221	3% 71% 6% • 22%
1	C	221	7% 65% 12% • 22%
1	D	221	4% 69% 9% • 21%
1	E	221	9% 67% 11% • 21%

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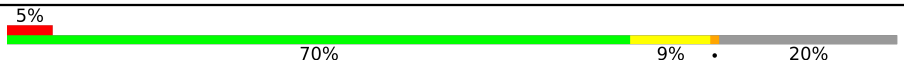
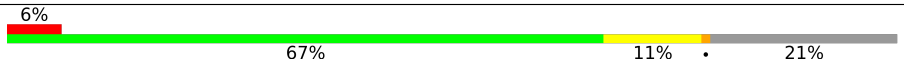
Mol	Chain	Length	Quality of chain
1	F	221	
1	G	221	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20131 atoms, of which 9967 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.

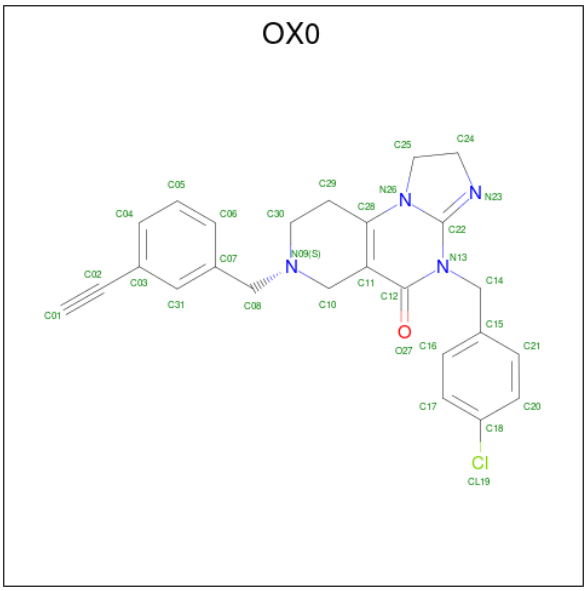
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	H	N	O	S	0	0	0
			2756	867	1398	232	246	13			
1	B	173	Total	C	H	N	O	S	0	0	0
			2732	861	1387	228	243	13			
1	C	173	Total	C	H	N	O	S	0	0	0
			2742	864	1389	231	245	13			
1	D	175	Total	C	H	N	O	S	0	0	0
			2771	872	1406	233	247	13			
1	E	175	Total	C	H	N	O	S	0	0	0
			2761	869	1403	230	246	13			
1	F	177	Total	C	H	N	O	S	0	1	0
			2806	882	1424	235	251	14			
1	G	174	Total	C	H	N	O	S	0	0	0
			2757	867	1399	232	246	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	cloning artifact	UNP Q16740
B	57	SER	-	cloning artifact	UNP Q16740
C	57	SER	-	cloning artifact	UNP Q16740
D	57	SER	-	cloning artifact	UNP Q16740
E	57	SER	-	cloning artifact	UNP Q16740
F	57	SER	-	cloning artifact	UNP Q16740
G	57	SER	-	cloning artifact	UNP Q16740

- Molecule 2 is (10R)-4-[(4-chlorophenyl)methyl]-7-[(3-ethynylphenyl)methyl]-2,4,6,7,8,9-hexahydroimidazo[1,2-a]pyrido[3,4-e]pyrimidin-5(1H)-one (three-letter code: OX0) (formula: $C_{25}H_{23}ClN_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	B	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	C	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	D	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	E	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	F	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		
2	G	1	Total	C	Cl	H	N	O	0	0
			54	25	1	23	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	62	Total	O	0	0
			62	62		
3	C	64	Total	O	0	0
			64	64		
3	D	70	Total	O	0	0
			70	70		
3	E	63	Total	O	0	0
			63	63		

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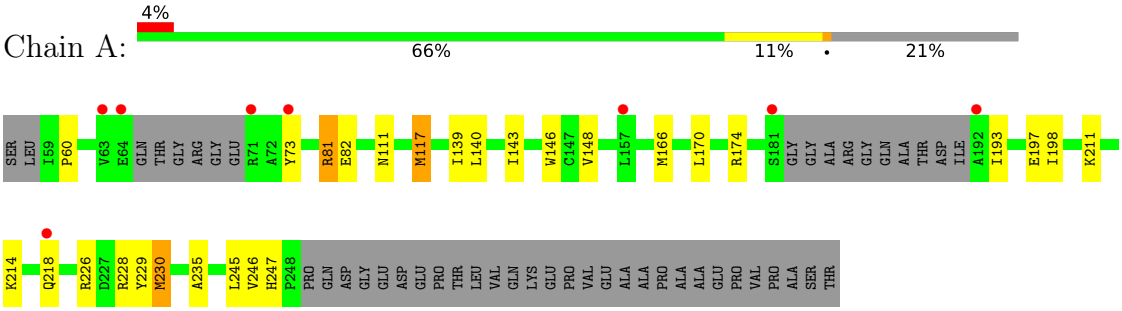
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	63	Total O 63 63	0	0
3	G	54	Total O 54 54	0	0

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.

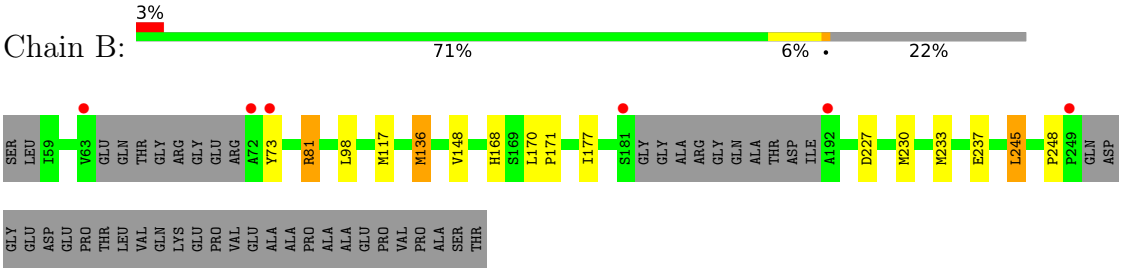
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain A:



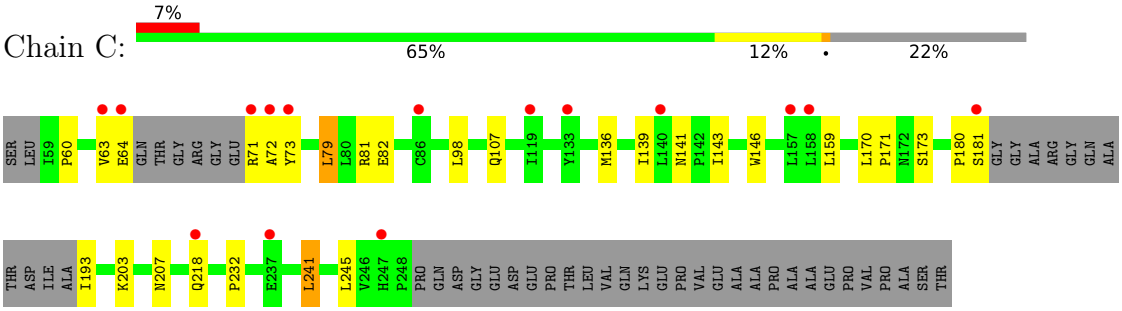
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain B:



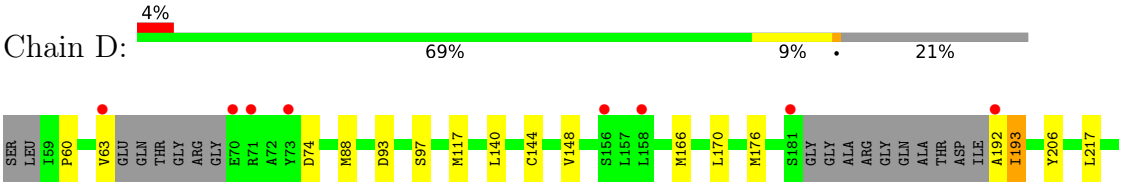
• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

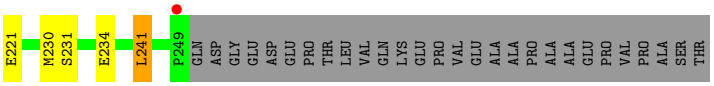
Chain C:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

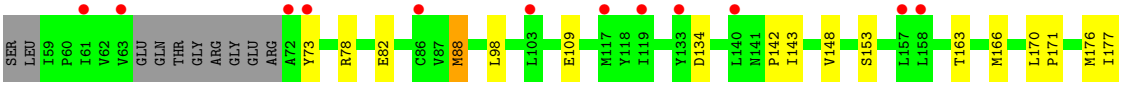
Chain D:

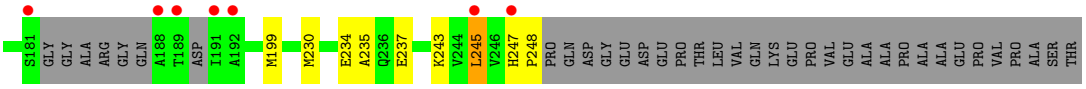




• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

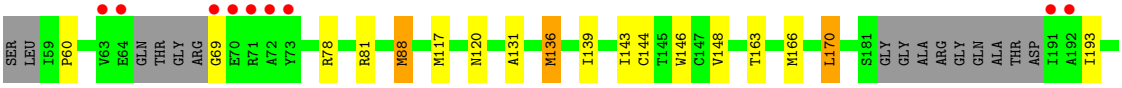
Chain E:

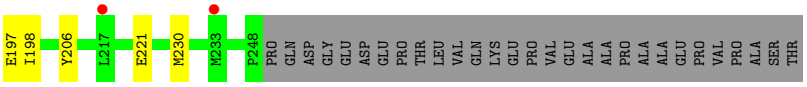




• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

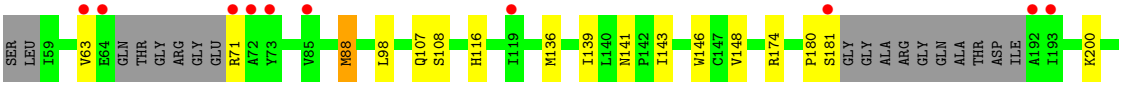
Chain F:

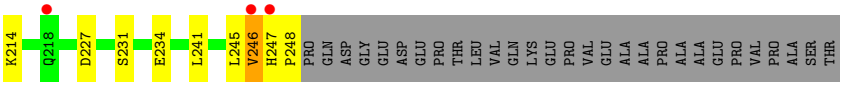




• Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.15Å 153.72Å 105.10Å 90.00° 117.76° 90.00°	Depositor
Resolution (Å)	29.40 – 2.19 29.40 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.40-2.19) 99.2 (29.40-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.197 , 0.237 0.199 , 0.239	Depositor DCC
R_{free} test set	2000 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20131	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: OX0

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	0.59	0/1382	0.76	2/1868 (0.1%)
1	B	0.67	1/1370 (0.1%)	0.77	2/1854 (0.1%)
1	C	0.63	0/1377	0.86	5/1861 (0.3%)
1	D	0.63	0/1390	0.80	4/1880 (0.2%)
1	E	0.65	0/1381	0.82	5/1867 (0.3%)
1	F	0.65	1/1409 (0.1%)	0.79	3/1904 (0.2%)
1	G	0.61	1/1382 (0.1%)	0.80	3/1868 (0.2%)
All	All	0.63	3/9691 (0.0%)	0.80	24/13102 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	136	MET	CG-SD	11.69	2.11	1.81
1	B	136	MET	CG-SD	8.87	2.04	1.81
1	G	136	MET	CG-SD	5.27	1.94	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	MET	CG-SD-CE	7.76	112.62	100.20
1	F	230	MET	CG-SD-CE	7.62	112.40	100.20
1	C	241	LEU	CB-CG-CD2	-7.20	98.75	111.00
1	C	170	LEU	CA-CB-CG	-7.01	99.18	115.30
1	F	170	LEU	CA-CB-CG	-6.64	100.03	115.30
1	E	199	MET	CG-SD-CE	6.29	110.27	100.20
1	D	176	MET	CG-SD-CE	-6.08	90.48	100.20
1	C	79	LEU	CB-CG-CD2	6.04	121.27	111.00
1	D	140	LEU	CB-CG-CD2	5.67	120.64	111.00
1	E	176	MET	CG-SD-CE	5.66	109.26	100.20
1	F	230	MET	CB-CG-SD	-5.51	95.87	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	88	MET	CB-CG-SD	5.50	128.91	112.40
1	G	227	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	227	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	C	136	MET	CB-CG-SD	-5.35	96.36	112.40
1	E	78	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	G	88	MET	CB-CG-SD	5.26	128.17	112.40
1	E	134	ASP	CB-CG-OD1	5.24	123.01	118.30
1	C	241	LEU	CA-CB-CG	5.20	127.26	115.30
1	G	241	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	A	166	MET	CG-SD-CE	5.12	108.40	100.20
1	E	134	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	D	241	LEU	CB-CG-CD1	-5.07	102.37	111.00
1	B	230	MET	CB-CG-SD	-5.02	97.33	112.40

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	1358	1398	1398	20	0
1	B	1345	1387	1386	19	0
1	C	1353	1389	1393	31	0
1	D	1365	1406	1405	19	0
1	E	1358	1403	1401	25	0
1	F	1382	1424	1423	22	0
1	G	1358	1399	1398	16	0
2	A	31	23	0	1	0
2	B	31	23	0	1	0
2	C	31	23	0	1	0
2	D	31	23	0	0	0
2	E	31	23	0	1	0
2	F	31	23	0	0	0
2	G	31	23	0	0	0
3	A	52	0	0	0	0
3	B	62	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	64	0	0	2	0
3	D	70	0	0	2	0
3	E	63	0	0	2	0
3	F	63	0	0	1	0
3	G	54	0	0	0	0
All	All	10164	9967	9804	134	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 7.

All (134) 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:136:MET:CG	1:B:136:MET:SD	2.04	1.46
1:F:136:MET:CG	1:F:136:MET:SD	2.11	1.39
1:E:163:THR:OG1	1:E:166:MET:HE3	1.33	1.24
1:E:148:VAL:HG12	1:E:170:LEU:HD12	1.23	1.08
1:E:163:THR:OG1	1:E:166:MET:CE	2.02	1.08
1:B:148:VAL:HG12	1:B:170:LEU:HD12	1.41	1.02
1:C:203:LYS:NZ	1:C:207:ASN:HD21	1.59	0.99
1:C:203:LYS:NZ	1:C:207:ASN:ND2	2.16	0.93
1:A:146:TRP:HZ3	1:A:245:LEU:HD21	1.36	0.89
1:C:203:LYS:HZ2	1:C:207:ASN:CG	1.75	0.89
1:G:245:LEU:O	1:G:246:VAL:HG23	1.72	0.89
1:C:203:LYS:HZ3	1:C:207:ASN:HD21	1.20	0.88
1:E:148:VAL:CG1	1:E:170:LEU:HD12	2.09	0.82
1:C:203:LYS:HZ3	1:C:207:ASN:ND2	1.77	0.80
1:C:159:LEU:HD21	1:C:241:LEU:HD21	1.61	0.80
1:B:81:ARG:HH21	1:C:63:VAL:CG2	1.95	0.80
1:C:64:GLU:O	1:C:71:ARG:N	2.14	0.79
1:B:73:TYR:OH	1:B:81:ARG:NE	2.16	0.77
1:D:148:VAL:HG12	1:D:170:LEU:HD12	1.70	0.73
1:F:197:GLU:OE1	1:G:174:ARG:NH1	2.21	0.73
1:E:234:GLU:O	1:E:237:GLU:HG3	1.87	0.73
1:E:143:ILE:H	1:E:163:THR:HG23	1.53	0.73
1:E:109:GLU:OE2	3:E:401:HOH:O	2.08	0.72
1:C:218:GLN:OE1	3:C:401:HOH:O	2.07	0.72
1:E:143:ILE:H	1:E:163:THR:CG2	2.03	0.71
1:D:217:LEU:HB2	3:D:416:HOH:O	1.88	0.71
1:F:136:MET:SD	1:F:136:MET:CB	2.81	0.68
1:F:163:THR:HG21	1:F:166:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:LEU:HD12	1:E:245:LEU:O	1.95	0.67
1:B:168:HIS:ND1	1:B:245:LEU:HD11	2.10	0.67
1:C:180:PRO:O	1:C:181:SER:HB2	1.94	0.66
1:C:203:LYS:NZ	1:C:207:ASN:CG	2.45	0.65
1:F:148:VAL:HG12	1:F:170:LEU:HD12	1.78	0.64
1:A:148:VAL:CG1	1:A:170:LEU:HD23	2.28	0.64
1:F:144[B]:CYS:SG	1:F:146:TRP:NE1	2.72	0.63
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.81	0.62
1:C:203:LYS:O	1:C:203:LYS:HD3	2.00	0.62
1:C:73:TYR:OH	1:D:63:VAL:HG13	1.99	0.62
1:A:228:ARG:O	1:A:229:TYR:HB2	2.00	0.62
1:F:163:THR:HG21	1:F:166:MET:HE2	1.82	0.62
1:A:146:TRP:CZ3	1:A:245:LEU:HD21	2.28	0.61
1:A:148:VAL:HG12	1:A:170:LEU:HD23	1.82	0.61
1:E:243:LYS:NZ	3:E:402:HOH:O	2.33	0.61
1:A:60:PRO:HD2	1:G:98:LEU:HD11	1.82	0.60
1:B:148:VAL:CG1	1:B:170:LEU:HD12	2.25	0.60
1:D:234:GLU:OE2	3:D:401:HOH:O	2.17	0.59
1:B:136:MET:SD	1:B:136:MET:CB	2.88	0.58
1:D:231:SER:OG	1:D:234:GLU:HG2	2.03	0.58
1:E:142:PRO:HA	1:E:163:THR:HG21	1.85	0.58
1:E:163:THR:HG1	1:E:166:MET:HE3	1.61	0.56
1:A:226:ARG:CZ	1:A:228:ARG:HD2	2.35	0.56
1:B:81:ARG:NH2	1:C:63:VAL:HG21	2.21	0.56
1:F:163:THR:CG2	1:F:166:MET:HE2	2.36	0.55
1:F:148:VAL:HG12	1:F:170:LEU:CD1	2.37	0.55
1:F:148:VAL:CG1	1:F:170:LEU:HD12	2.37	0.55
1:G:247:HIS:HB2	1:G:248:PRO:HD2	1.90	0.54
1:B:233:MET:O	1:B:237:GLU:HG3	2.08	0.53
1:B:81:ARG:HH21	1:C:63:VAL:HG21	1.69	0.53
1:B:81:ARG:NH2	1:C:63:VAL:CG2	2.70	0.53
1:D:241:LEU:HD12	1:D:241:LEU:C	2.30	0.53
1:E:163:THR:HG1	1:E:166:MET:CE	2.20	0.52
1:G:116:HIS:HD2	1:G:146:TRP:HE1	1.58	0.52
1:C:171:PRO:HG3	1:C:245:LEU:O	2.09	0.52
1:E:98:LEU:HD11	1:F:60:PRO:HD2	1.92	0.52
1:F:136:MET:HG2	1:F:143:ILE:CD1	2.40	0.52
1:F:69:GLY:O	3:F:401:HOH:O	2.19	0.51
1:F:136:MET:HG2	1:F:143:ILE:HD13	1.92	0.51
1:G:146:TRP:HZ3	1:G:245:LEU:HD11	1.75	0.50
1:E:163:THR:OG1	1:E:166:MET:HE2	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ILE:HD11	1:A:143:ILE:HD11	1.94	0.50
1:D:230:MET:HB3	1:D:234:GLU:HG3	1.93	0.50
1:A:193:ILE:HD12	1:A:197:GLU:HG3	1.94	0.49
1:A:81:ARG:HG2	3:B:460:HOH:O	2.12	0.49
1:C:81:ARG:NH2	3:C:402:HOH:O	2.12	0.49
1:D:63:VAL:O	1:D:63:VAL:HG23	2.13	0.49
1:F:197:GLU:OE2	1:G:174:ARG:HD3	2.13	0.49
1:D:148:VAL:CG1	1:D:170:LEU:HD12	2.39	0.48
1:C:146:TRP:CZ3	1:C:245:LEU:HD11	2.49	0.48
1:E:247:HIS:HB2	1:E:248:PRO:CD	2.43	0.48
1:A:174:ARG:NH2	1:G:200:LYS:HE2	2.29	0.48
1:A:226:ARG:NH2	1:A:228:ARG:HD2	2.30	0.47
1:D:93:ASP:CB	1:E:88:MET:HE3	2.45	0.47
1:G:231:SER:OG	1:G:234:GLU:HG3	2.14	0.47
1:C:107:GLN:HG3	1:C:141:ASN:OD1	2.14	0.47
1:C:98:LEU:HD11	1:D:60:PRO:HD2	1.97	0.47
1:F:163:THR:CG2	1:F:166:MET:CE	2.93	0.46
1:G:180:PRO:O	1:G:181:SER:HB3	2.14	0.46
1:E:230:MET:CE	1:E:235:ALA:HA	2.45	0.46
1:D:93:ASP:HB2	1:E:88:MET:HE3	1.97	0.46
1:A:246:VAL:HG13	1:A:247:HIS:ND1	2.31	0.46
1:B:168:HIS:HB3	1:B:245:LEU:HD12	1.98	0.46
1:G:146:TRP:CZ3	1:G:245:LEU:HD11	2.50	0.46
1:F:193:ILE:HG22	1:F:198:ILE:HG13	1.98	0.46
1:A:111:ASN:ND2	1:A:111:ASN:H	2.14	0.45
1:E:143:ILE:H	1:E:163:THR:HG21	1.81	0.45
1:D:93:ASP:CB	1:E:88:MET:CE	2.95	0.45
1:C:146:TRP:HZ3	1:C:245:LEU:HD11	1.81	0.44
1:C:139:ILE:HD11	1:C:143:ILE:HD11	2.00	0.44
1:B:148:VAL:HG11	2:B:301:OX0:C02	2.48	0.43
1:F:88:MET:HG3	1:F:120:ASN:HB3	2.00	0.43
1:C:72:ALA:O	1:C:73:TYR:CD1	2.71	0.43
1:D:93:ASP:HB2	1:E:88:MET:CE	2.47	0.43
1:F:206:TYR:CE2	1:F:221:GLU:HG2	2.52	0.43
1:G:107:GLN:HG3	1:G:141:ASN:OD1	2.18	0.43
1:B:171:PRO:HD3	1:B:245:LEU:O	2.17	0.43
1:C:146:TRP:HZ3	1:C:245:LEU:CD1	2.32	0.43
1:G:63:VAL:HA	1:G:71:ARG:O	2.19	0.43
1:E:82:GLU:OE1	2:E:301:OX0:N23	2.51	0.43
1:A:193:ILE:HG13	1:A:198:ILE:HG13	1.99	0.43
1:D:117:MET:HE3	1:D:117:MET:HB3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD23	1:B:248:PRO:HG2	2.01	0.42
1:E:177:ILE:HD13	1:E:177:ILE:HG21	1.82	0.42
1:F:193:ILE:CG2	1:F:198:ILE:HG13	2.48	0.42
1:C:193:ILE:O	1:C:193:ILE:HG23	2.19	0.42
1:D:206:TYR:CE2	1:D:221:GLU:HG2	2.54	0.42
1:C:173:SER:O	1:C:232:PRO:HD3	2.18	0.42
1:C:203:LYS:HD3	1:C:203:LYS:C	2.40	0.42
1:D:192:ALA:O	1:D:193:ILE:O	2.38	0.42
1:A:117:MET:HE2	1:A:117:MET:HB2	1.95	0.42
1:B:177:ILE:HD13	1:B:177:ILE:HG21	1.80	0.42
1:A:82:GLU:CG	2:A:301:OX0:N23	2.83	0.41
1:A:211:LYS:O	1:A:214:LYS:HE3	2.20	0.41
1:C:82:GLU:OE1	2:C:301:OX0:N23	2.52	0.41
1:B:168:HIS:ND1	1:B:245:LEU:CD1	2.81	0.41
1:D:144:CYS:SG	1:D:166:MET:CE	3.09	0.41
1:B:73:TYR:OH	1:B:81:ARG:CD	2.68	0.41
1:F:131:ALA:HB1	1:G:148:VAL:HG22	2.02	0.41
1:F:139:ILE:HD11	1:F:143:ILE:HD11	2.03	0.41
1:E:247:HIS:HB2	1:E:248:PRO:HD2	2.03	0.41
1:B:98:LEU:HD11	1:C:60:PRO:HD2	2.03	0.40
1:C:79:LEU:O	1:C:82:GLU:HB2	2.22	0.40
1:D:144:CYS:SG	1:D:166:MET:HE3	2.61	0.40
1:A:230:MET:HG3	1:A:235:ALA:HB2	2.02	0.40
1:G:247:HIS:HB2	1:G:248:PRO:CD	2.51	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	168/221 (76%)	161 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	167/221 (76%)	163 (98%)	4 (2%)	0	100 100
1	C	167/221 (76%)	163 (98%)	4 (2%)	0	100 100
1	D	169/221 (76%)	165 (98%)	3 (2%)	1 (1%)	25 26
1	E	167/221 (76%)	162 (97%)	5 (3%)	0	100 100
1	F	172/221 (78%)	169 (98%)	3 (2%)	0	100 100
1	G	168/221 (76%)	161 (96%)	6 (4%)	1 (1%)	25 26
All	All	1178/1547 (76%)	1144 (97%)	32 (3%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	193	ILE
1	G	246	VAL

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	151/185 (82%)	147 (97%)	4 (3%)	46 58
1	B	150/185 (81%)	147 (98%)	3 (2%)	55 69
1	C	151/185 (82%)	151 (100%)	0	100 100
1	D	152/185 (82%)	150 (99%)	2 (1%)	69 81
1	E	151/185 (82%)	146 (97%)	5 (3%)	38 49
1	F	154/185 (83%)	150 (97%)	4 (3%)	46 58
1	G	151/185 (82%)	148 (98%)	3 (2%)	55 69
All	All	1060/1295 (82%)	1039 (98%)	21 (2%)	55 69

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	TYR

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Mol	Chain	Res	Type
1	A	81	ARG
1	A	117	MET
1	A	218	GLN
1	B	81	ARG
1	B	117	MET
1	B	245	LEU
1	D	74	ASP
1	D	97	SER
1	E	73	TYR
1	E	88	MET
1	E	153	SER
1	E	171	PRO
1	E	245	LEU
1	F	78	ARG
1	F	81	ARG
1	F	88	MET
1	F	117	MET
1	G	88	MET
1	G	108	SER
1	G	214	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	218	GLN
1	B	218	GLN
1	C	178	HIS
1	D	179	GLN
1	E	236	GLN
1	F	218	GLN
1	G	116	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	OX0	E	301	-	35,35,35	6.88	16 (45%)	43,50,50	2.33	13 (30%)
2	OX0	C	301	-	35,35,35	6.99	17 (48%)	43,50,50	2.38	16 (37%)
2	OX0	F	301	-	35,35,35	6.83	16 (45%)	43,50,50	2.20	15 (34%)
2	OX0	D	301	-	35,35,35	6.72	15 (42%)	43,50,50	2.20	13 (30%)
2	OX0	G	301	-	35,35,35	6.91	18 (51%)	43,50,50	2.31	14 (32%)
2	OX0	A	301	-	35,35,35	7.06	18 (51%)	43,50,50	2.37	12 (27%)
2	OX0	B	301	-	35,35,35	6.89	19 (54%)	43,50,50	2.02	14 (32%)

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	OX0	E	301	-	-	1/10/25/25	0/5/5/5
2	OX0	C	301	-	-	0/10/25/25	0/5/5/5
2	OX0	F	301	-	-	1/10/25/25	0/5/5/5
2	OX0	D	301	-	-	0/10/25/25	0/5/5/5
2	OX0	G	301	-	-	1/10/25/25	0/5/5/5
2	OX0	A	301	-	-	0/10/25/25	0/5/5/5
2	OX0	B	301	-	-	2/10/25/25	0/5/5/5

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	OX0	C22-N23	33.98	1.55	1.28
2	A	301	OX0	C22-N23	33.89	1.55	1.28
2	E	301	OX0	C22-N23	33.17	1.54	1.28
2	B	301	OX0	C22-N23	33.16	1.54	1.28
2	G	301	OX0	C22-N23	33.05	1.54	1.28
2	F	301	OX0	C22-N23	32.84	1.54	1.28
2	D	301	OX0	C22-N23	32.46	1.54	1.28
2	E	301	OX0	C10-N09	12.46	1.58	1.46
2	A	301	OX0	C10-N09	12.05	1.57	1.46
2	G	301	OX0	C10-N09	11.92	1.57	1.46
2	B	301	OX0	C10-N09	11.71	1.57	1.46
2	C	301	OX0	C10-N09	11.65	1.57	1.46
2	D	301	OX0	C10-N09	10.15	1.56	1.46
2	F	301	OX0	C10-N09	10.06	1.55	1.46
2	E	301	OX0	C08-N09	-9.43	1.29	1.47
2	A	301	OX0	C08-N09	-9.38	1.29	1.47
2	C	301	OX0	C08-N09	-9.17	1.29	1.47
2	F	301	OX0	C08-N09	-8.77	1.30	1.47
2	F	301	OX0	C25-N26	-8.70	1.34	1.47
2	G	301	OX0	C08-N09	-8.55	1.31	1.47
2	G	301	OX0	C29-C28	-8.53	1.37	1.49
2	D	301	OX0	C25-N26	-8.49	1.34	1.47
2	B	301	OX0	C08-N09	-8.32	1.31	1.47
2	B	301	OX0	C25-N26	-8.27	1.35	1.47
2	F	301	OX0	C30-N09	-8.25	1.24	1.46
2	A	301	OX0	C25-N26	-8.13	1.35	1.47
2	C	301	OX0	C25-N26	-8.05	1.35	1.47
2	A	301	OX0	C30-N09	-8.03	1.24	1.46
2	G	301	OX0	C25-N26	-8.02	1.35	1.47
2	E	301	OX0	C25-N26	-7.86	1.35	1.47
2	D	301	OX0	C29-C28	-7.76	1.38	1.49
2	F	301	OX0	C29-C28	-7.76	1.38	1.49
2	G	301	OX0	C30-N09	-7.75	1.25	1.46
2	A	301	OX0	C29-C28	-7.74	1.38	1.49
2	C	301	OX0	C30-N09	-7.71	1.25	1.46
2	B	301	OX0	C30-N09	-7.69	1.25	1.46
2	B	301	OX0	C29-C28	-7.59	1.38	1.49
2	D	301	OX0	C30-N09	-7.58	1.26	1.46
2	D	301	OX0	C08-N09	-7.52	1.33	1.47
2	C	301	OX0	C29-C28	-7.51	1.38	1.49
2	E	301	OX0	C30-N09	-7.29	1.26	1.46
2	E	301	OX0	C29-C28	-7.17	1.39	1.49
2	D	301	OX0	C30-C29	4.88	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	OX0	C30-C29	4.73	1.64	1.52
2	B	301	OX0	C10-C11	-4.70	1.44	1.51
2	D	301	OX0	C10-C11	-4.69	1.44	1.51
2	E	301	OX0	C30-C29	4.59	1.64	1.52
2	D	301	OX0	C28-C11	4.53	1.48	1.36
2	C	301	OX0	C30-C29	4.51	1.64	1.52
2	A	301	OX0	C22-N13	4.49	1.47	1.37
2	G	301	OX0	C10-C11	-4.49	1.44	1.51
2	A	301	OX0	C30-C29	4.31	1.63	1.52
2	B	301	OX0	C30-C29	4.22	1.63	1.52
2	A	301	OX0	C28-C11	4.21	1.47	1.36
2	D	301	OX0	C03-C02	4.21	1.54	1.44
2	G	301	OX0	C30-C29	4.21	1.63	1.52
2	B	301	OX0	C03-C02	4.20	1.54	1.44
2	C	301	OX0	C22-N13	4.16	1.46	1.37
2	F	301	OX0	C03-C02	4.15	1.54	1.44
2	F	301	OX0	C24-N23	4.15	1.54	1.47
2	A	301	OX0	C03-C02	4.14	1.54	1.44
2	E	301	OX0	C03-C02	4.13	1.54	1.44
2	G	301	OX0	C03-C02	4.09	1.53	1.44
2	F	301	OX0	C28-C11	4.08	1.46	1.36
2	A	301	OX0	C28-N26	4.04	1.47	1.39
2	F	301	OX0	C10-C11	-4.04	1.45	1.51
2	G	301	OX0	C28-C11	4.04	1.46	1.36
2	G	301	OX0	C22-N13	4.03	1.46	1.37
2	D	301	OX0	C12-N13	4.02	1.47	1.40
2	B	301	OX0	C22-N13	4.00	1.46	1.37
2	F	301	OX0	C22-N13	3.98	1.46	1.37
2	F	301	OX0	C12-C11	3.97	1.53	1.44
2	C	301	OX0	C03-C02	3.97	1.53	1.44
2	A	301	OX0	C10-C11	-3.95	1.45	1.51
2	B	301	OX0	C28-C11	3.95	1.46	1.36
2	G	301	OX0	C28-N26	3.91	1.47	1.39
2	D	301	OX0	C22-N13	3.82	1.45	1.37
2	D	301	OX0	C24-N23	3.80	1.54	1.47
2	E	301	OX0	C28-C11	3.78	1.46	1.36
2	A	301	OX0	C12-C11	3.76	1.53	1.44
2	C	301	OX0	C10-C11	-3.76	1.45	1.51
2	E	301	OX0	C22-N13	3.74	1.45	1.37
2	E	301	OX0	C24-N23	3.68	1.54	1.47
2	B	301	OX0	C12-C11	3.66	1.53	1.44
2	C	301	OX0	C24-N23	3.64	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	OX0	C28-N26	3.64	1.46	1.39
2	E	301	OX0	C10-C11	-3.62	1.45	1.51
2	C	301	OX0	C28-C11	3.57	1.45	1.36
2	E	301	OX0	C28-N26	3.54	1.46	1.39
2	A	301	OX0	C24-N23	3.33	1.53	1.47
2	D	301	OX0	C12-C11	3.31	1.52	1.44
2	D	301	OX0	C28-N26	3.31	1.46	1.39
2	A	301	OX0	C12-N13	3.25	1.46	1.40
2	B	301	OX0	C24-N23	3.23	1.53	1.47
2	B	301	OX0	C28-N26	3.21	1.46	1.39
2	B	301	OX0	C12-N13	3.18	1.46	1.40
2	C	301	OX0	C28-N26	3.17	1.46	1.39
2	G	301	OX0	C24-N23	3.17	1.53	1.47
2	C	301	OX0	C12-C11	3.05	1.51	1.44
2	E	301	OX0	C12-C11	2.95	1.51	1.44
2	G	301	OX0	C12-C11	2.90	1.51	1.44
2	C	301	OX0	C12-N13	2.77	1.45	1.40
2	G	301	OX0	C12-N13	2.69	1.45	1.40
2	F	301	OX0	C12-N13	2.64	1.45	1.40
2	F	301	OX0	C31-C03	2.62	1.44	1.39
2	G	301	OX0	C06-C07	2.32	1.43	1.38
2	E	301	OX0	C12-N13	2.29	1.44	1.40
2	B	301	OX0	C14-N13	-2.21	1.43	1.47
2	G	301	OX0	C14-N13	-2.20	1.43	1.47
2	A	301	OX0	C22-N26	2.15	1.42	1.37
2	E	301	OX0	C06-C07	2.10	1.43	1.38
2	C	301	OX0	C06-C07	2.10	1.43	1.38
2	C	301	OX0	C18-CL19	2.09	1.79	1.74
2	A	301	OX0	C14-C15	2.05	1.55	1.51
2	B	301	OX0	C18-CL19	2.04	1.79	1.74
2	A	301	OX0	C18-CL19	2.04	1.78	1.74
2	B	301	OX0	C06-C07	2.03	1.43	1.38
2	B	301	OX0	C17-C18	2.02	1.41	1.38
2	G	301	OX0	C18-CL19	2.00	1.78	1.74

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	OX0	C24-C25-N26	8.70	106.99	101.24
2	E	301	OX0	C24-C25-N26	8.30	106.73	101.24
2	G	301	OX0	C29-C30-N09	7.68	118.20	111.23
2	G	301	OX0	C24-C25-N26	7.04	105.90	101.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	OX0	C24-C25-N26	6.71	105.68	101.24
2	C	301	OX0	C29-C30-N09	6.59	117.22	111.23
2	B	301	OX0	C29-C30-N09	6.23	116.89	111.23
2	A	301	OX0	C29-C30-N09	5.90	116.59	111.23
2	C	301	OX0	C14-N13-C12	5.58	126.06	117.80
2	E	301	OX0	C29-C30-N09	5.46	116.19	111.23
2	F	301	OX0	C14-N13-C12	5.41	125.81	117.80
2	D	301	OX0	C14-N13-C12	5.32	125.68	117.80
2	E	301	OX0	C29-C28-N26	5.12	121.06	117.25
2	B	301	OX0	C24-C25-N26	4.89	104.48	101.24
2	D	301	OX0	C29-C30-N09	4.88	115.67	111.23
2	F	301	OX0	C24-C25-N26	4.80	104.42	101.24
2	A	301	OX0	C14-N13-C12	4.75	124.83	117.80
2	F	301	OX0	C10-C11-C28	-4.35	116.74	120.62
2	D	301	OX0	C24-N23-C22	-4.26	98.40	105.49
2	F	301	OX0	C29-C28-N26	4.25	120.41	117.25
2	G	301	OX0	C14-N13-C12	4.21	124.03	117.80
2	D	301	OX0	C24-C25-N26	4.21	104.02	101.24
2	A	301	OX0	C30-C29-C28	4.00	116.01	108.47
2	D	301	OX0	C25-C24-N23	3.94	112.37	106.40
2	F	301	OX0	C24-N23-C22	-3.82	99.13	105.49
2	D	301	OX0	O27-C12-C11	-3.79	117.85	125.08
2	A	301	OX0	C29-C28-N26	3.72	120.02	117.25
2	B	301	OX0	C14-N13-C12	3.60	123.12	117.80
2	A	301	OX0	C10-C11-C28	-3.57	117.44	120.62
2	C	301	OX0	C08-N09-C30	-3.53	103.22	111.06
2	G	301	OX0	C29-C28-N26	3.44	119.81	117.25
2	E	301	OX0	C10-N09-C30	-3.44	105.50	109.95
2	C	301	OX0	O27-C12-C11	-3.35	118.70	125.08
2	E	301	OX0	O27-C12-C11	-3.34	118.72	125.08
2	B	301	OX0	C24-N23-C22	-3.32	99.96	105.49
2	D	301	OX0	O27-C12-N13	3.30	125.58	119.98
2	F	301	OX0	C25-C24-N23	3.27	111.35	106.40
2	C	301	OX0	C29-C28-N26	3.25	119.67	117.25
2	E	301	OX0	C21-C15-C16	3.17	123.15	118.17
2	C	301	OX0	C30-C29-C28	3.16	114.42	108.47
2	D	301	OX0	C29-C28-N26	3.13	119.58	117.25
2	B	301	OX0	C25-C24-N23	3.10	111.11	106.40
2	G	301	OX0	C24-N23-C22	-3.02	100.47	105.49
2	A	301	OX0	C08-N09-C30	-2.98	104.42	111.06
2	G	301	OX0	O27-C12-C11	-2.96	119.44	125.08
2	F	301	OX0	O27-C12-C11	-2.93	119.48	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	OX0	C04-C03-C02	-2.93	116.27	120.65
2	B	301	OX0	C25-N26-C22	2.92	116.48	110.94
2	C	301	OX0	C24-N23-C22	-2.91	100.65	105.49
2	F	301	OX0	N26-C22-N13	2.89	123.77	118.50
2	E	301	OX0	C14-N13-C12	2.88	122.06	117.80
2	F	301	OX0	C25-N26-C22	2.87	116.40	110.94
2	D	301	OX0	C31-C03-C02	2.78	123.64	120.09
2	E	301	OX0	C08-N09-C30	-2.76	104.92	111.06
2	C	301	OX0	C17-C16-C15	-2.74	117.25	121.03
2	G	301	OX0	C08-N09-C10	2.74	114.14	110.53
2	D	301	OX0	C04-C03-C02	-2.73	116.57	120.65
2	G	301	OX0	C11-C12-N13	2.71	119.94	115.17
2	B	301	OX0	O27-C12-C11	-2.68	119.96	125.08
2	F	301	OX0	C30-C29-C28	2.68	113.52	108.47
2	A	301	OX0	O27-C12-C11	-2.66	120.02	125.08
2	B	301	OX0	C08-N09-C30	-2.65	105.16	111.06
2	D	301	OX0	C25-N26-C22	2.64	115.95	110.94
2	C	301	OX0	C31-C03-C02	-2.60	116.75	120.09
2	C	301	OX0	C10-C11-C28	-2.60	118.30	120.62
2	D	301	OX0	C21-C15-C16	2.59	122.23	118.17
2	G	301	OX0	C08-N09-C30	-2.55	105.38	111.06
2	F	301	OX0	C11-C12-N13	2.55	119.66	115.17
2	B	301	OX0	C30-C29-C28	2.53	113.24	108.47
2	F	301	OX0	C29-C30-N09	2.53	113.53	111.23
2	D	301	OX0	N26-C22-N13	2.51	123.08	118.50
2	E	301	OX0	N26-C22-N13	2.49	123.04	118.50
2	C	301	OX0	C25-N26-C22	2.48	115.66	110.94
2	C	301	OX0	C21-C15-C16	2.47	122.06	118.17
2	G	301	OX0	C30-C29-C28	2.47	113.12	108.47
2	F	301	OX0	C11-C28-N26	-2.43	117.98	120.63
2	E	301	OX0	C20-C21-C15	-2.41	117.71	121.03
2	E	301	OX0	C25-N26-C22	2.39	115.47	110.94
2	E	301	OX0	C30-C29-C28	2.37	112.93	108.47
2	C	301	OX0	N26-C22-N13	2.35	122.78	118.50
2	G	301	OX0	C25-C24-N23	2.34	109.95	106.40
2	B	301	OX0	C10-C11-C28	-2.32	118.55	120.62
2	A	301	OX0	C24-N23-C22	-2.31	101.65	105.49
2	E	301	OX0	C11-C12-N13	2.28	119.19	115.17
2	A	301	OX0	N26-C22-N13	2.27	122.64	118.50
2	G	301	OX0	N26-C22-N13	2.26	122.63	118.50
2	C	301	OX0	C11-C12-N13	2.22	119.07	115.17
2	G	301	OX0	C21-C15-C16	2.21	121.65	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	OX0	C08-N09-C10	2.21	113.44	110.53
2	B	301	OX0	C21-C15-C16	2.19	121.61	118.17
2	A	301	OX0	C04-C03-C02	-2.17	117.41	120.65
2	C	301	OX0	C25-C24-N23	2.15	109.66	106.40
2	B	301	OX0	C04-C03-C02	-2.13	117.47	120.65
2	B	301	OX0	N26-C22-N13	2.12	122.37	118.50
2	G	301	OX0	C04-C03-C02	-2.12	117.48	120.65
2	A	301	OX0	C11-C12-N13	2.11	118.88	115.17
2	B	301	OX0	C29-C28-N26	2.10	118.82	117.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	OX0	C01-C02-C03-C04
2	B	301	OX0	C01-C02-C03-C31
2	E	301	OX0	C01-C02-C03-C04
2	F	301	OX0	C01-C02-C03-C04
2	G	301	OX0	C01-C02-C03-C04

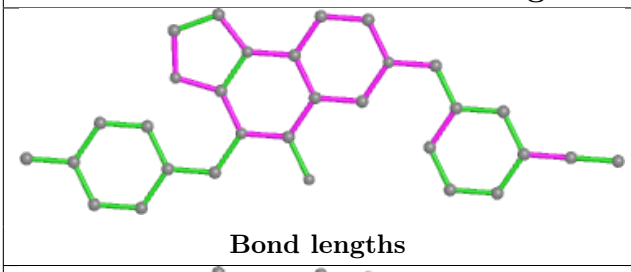
There are no ring outliers.

4 monomers are involved in 4 short contacts:

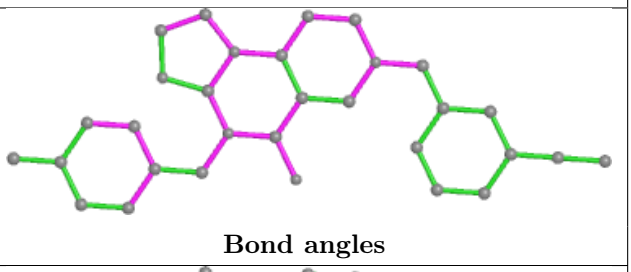
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	OX0	1	0
2	C	301	OX0	1	0
2	A	301	OX0	1	0
2	B	301	OX0	1	0

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 then 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.

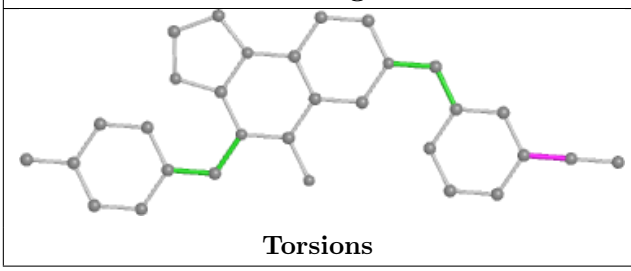
Ligand OX0 E 301



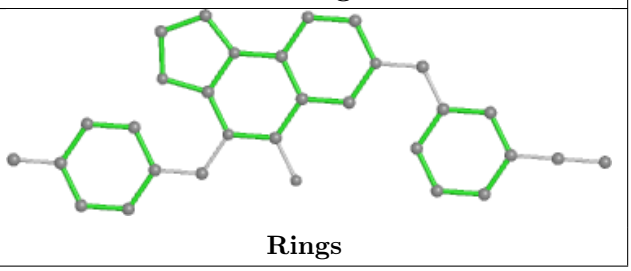
Bond lengths



Bond angles

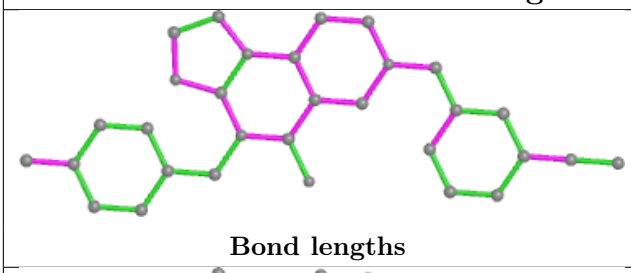


Torsions



Rings

Ligand OX0 C 301



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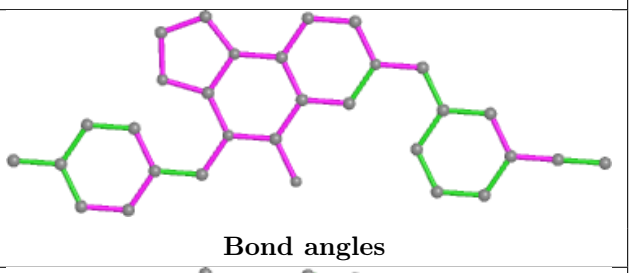
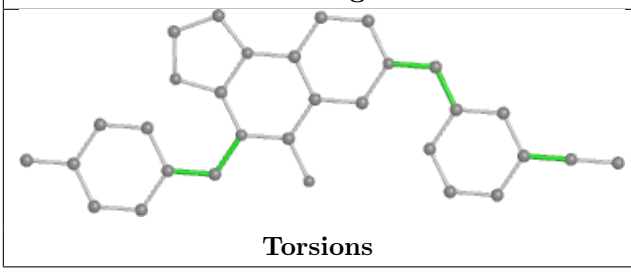


Bond angles



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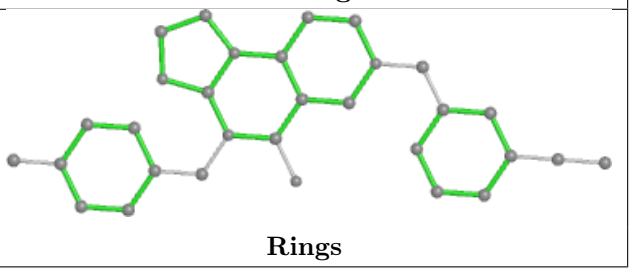
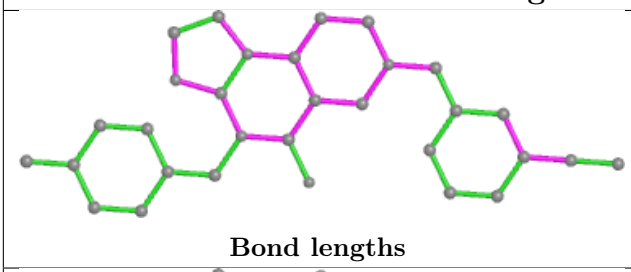


Rings

Ligand OX0 F 301



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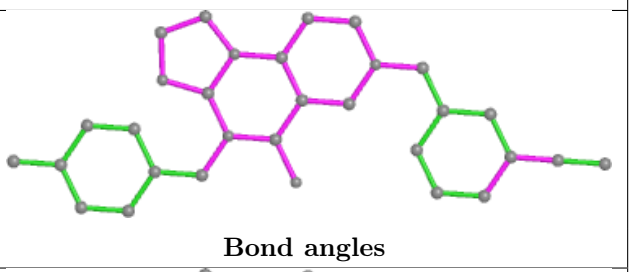
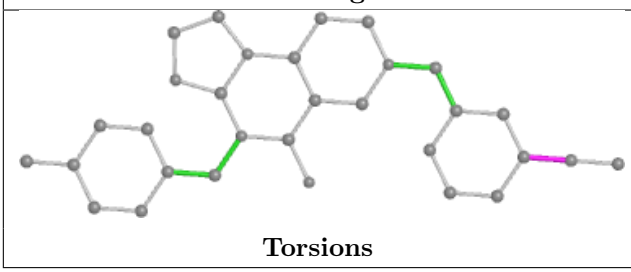


Bond angles



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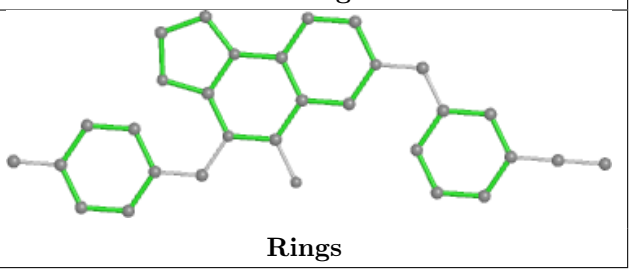
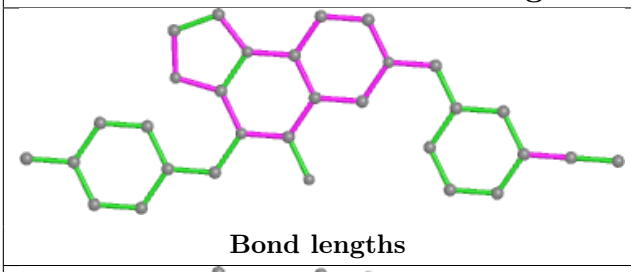


Rings

Ligand OX0 D 301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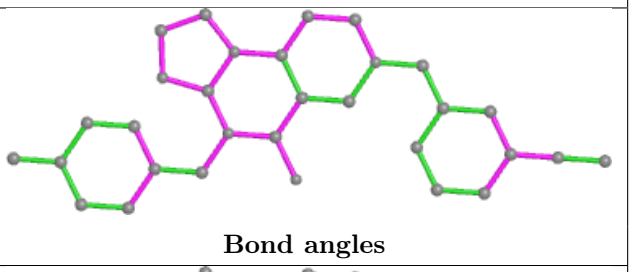
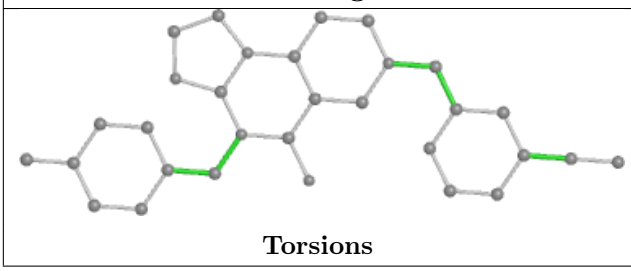

Bond angles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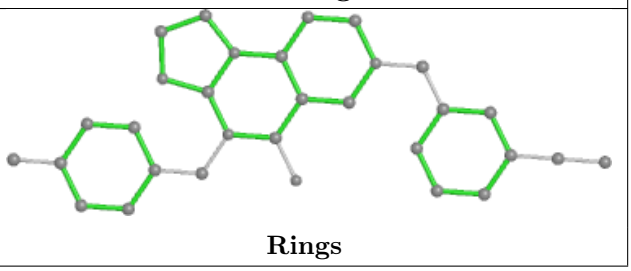
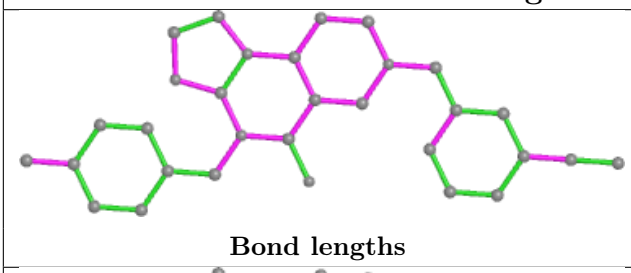
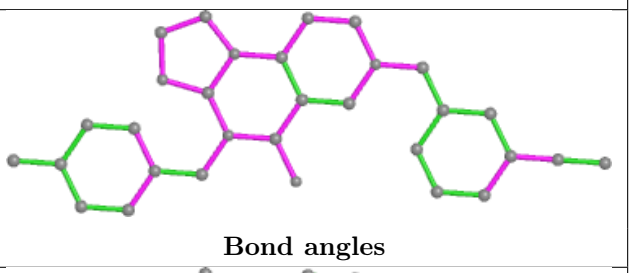
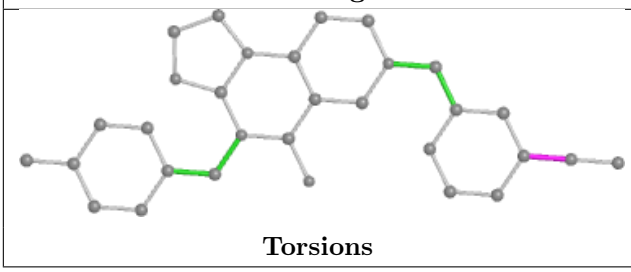

Rings

Ligand OX0 G 301


Bond lengths


Bond angles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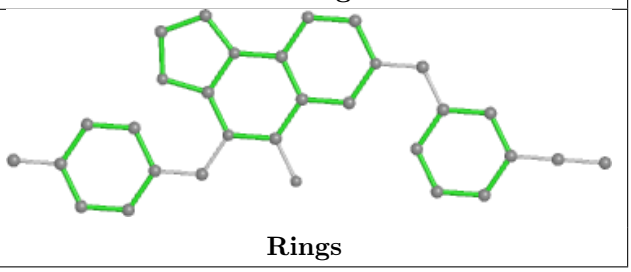
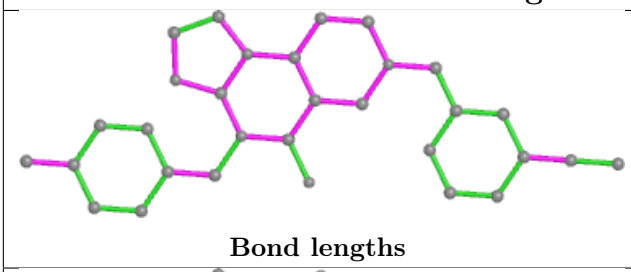

Rings

Ligand OX0 A 301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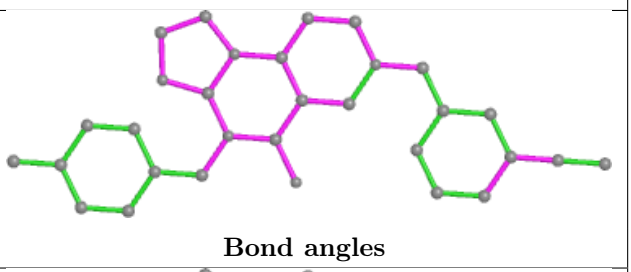
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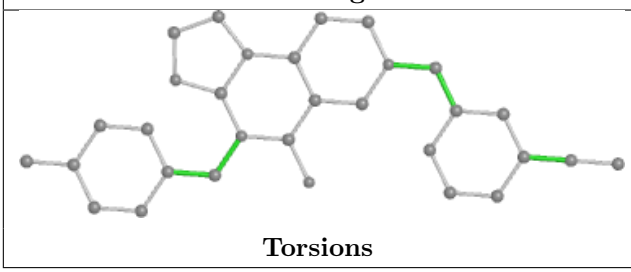
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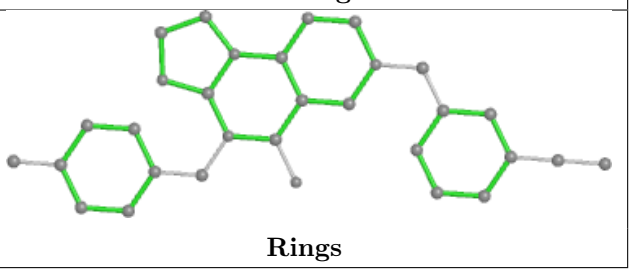
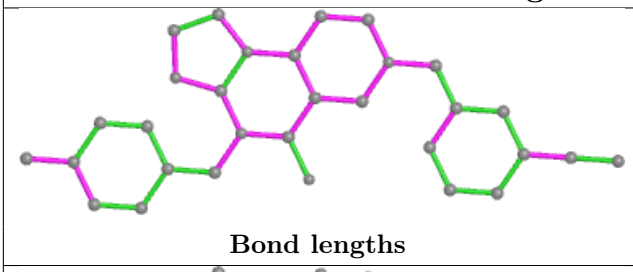

Rings

Ligand OX0 B 301



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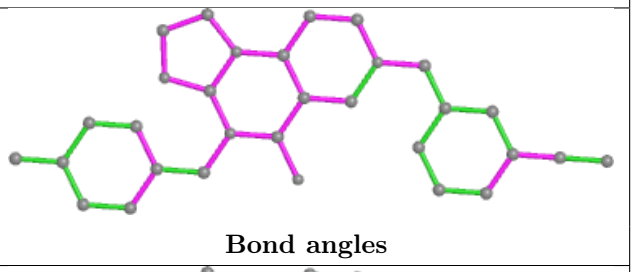
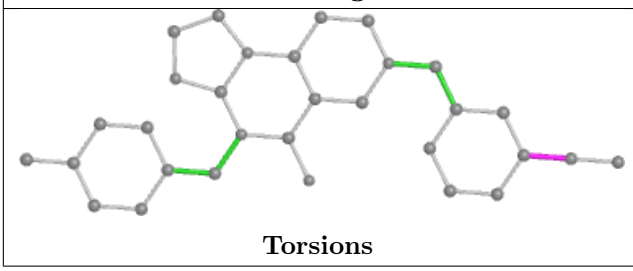


Bond angles



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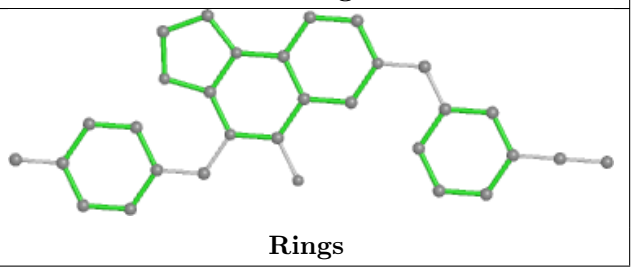

Rings

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

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, 95^{th} 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	174/221 (78%)	0.25	8 (4%) 32 31	30, 41, 69, 90	0
1	B	173/221 (78%)	0.12	6 (3%) 44 42	28, 37, 59, 76	0
1	C	173/221 (78%)	0.35	15 (8%) 10 8	29, 38, 62, 108	0
1	D	175/221 (79%)	0.21	9 (5%) 28 26	27, 36, 68, 95	0
1	E	175/221 (79%)	0.40	19 (10%) 5 5	29, 38, 65, 97	0
1	F	177/221 (80%)	0.22	11 (6%) 20 19	27, 37, 77, 96	0
1	G	174/221 (78%)	0.33	13 (7%) 14 13	31, 41, 62, 110	0
All	All	1221/1547 (78%)	0.27	81 (6%) 18 17	27, 39, 66, 110	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71	ARG	8.1
1	E	191	ILE	5.7
1	D	249	PRO	5.5
1	E	72	ALA	5.3
1	F	71	ARG	5.2
1	D	73	TYR	5.2
1	F	191	ILE	4.9
1	D	71	ARG	4.9
1	G	63	VAL	4.7
1	G	181	SER	4.7
1	C	71	ARG	4.5
1	B	181	SER	4.3
1	B	63	VAL	4.3
1	G	64	GLU	4.1
1	B	73	TYR	3.9
1	C	181	SER	3.9
1	A	192	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	71	ARG	3.8
1	C	73	TYR	3.7
1	F	69	GLY	3.7
1	C	64	GLU	3.7
1	G	73	TYR	3.7
1	B	249	PRO	3.5
1	E	63	VAL	3.5
1	B	72	ALA	3.5
1	E	189	THR	3.5
1	A	181	SER	3.4
1	A	218	GLN	3.4
1	B	192	ALA	3.4
1	F	63	VAL	3.4
1	E	119	ILE	3.3
1	C	63	VAL	3.2
1	A	73	TYR	3.2
1	C	247	HIS	3.1
1	E	158	LEU	3.1
1	F	64	GLU	3.1
1	A	63	VAL	3.1
1	F	192	ALA	3.1
1	C	119	ILE	3.0
1	D	70	GLU	2.9
1	G	119	ILE	2.9
1	F	73	TYR	2.9
1	G	247	HIS	2.8
1	A	64	GLU	2.8
1	F	70	GLU	2.8
1	D	192	ALA	2.8
1	E	61	ILE	2.7
1	C	158	LEU	2.7
1	E	247	HIS	2.6
1	E	86	CYS	2.6
1	E	133	TYR	2.6
1	G	218	GLN	2.6
1	C	72	ALA	2.5
1	G	246	VAL	2.5
1	E	245	LEU	2.4
1	C	140	LEU	2.4
1	E	181	SER	2.4
1	E	192	ALA	2.4
1	F	72	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	117	MET	2.4
1	C	157	LEU	2.4
1	E	140	LEU	2.4
1	D	63	VAL	2.4
1	C	86	CYS	2.3
1	D	181	SER	2.3
1	F	233	MET	2.3
1	G	85	VAL	2.3
1	E	157	LEU	2.3
1	G	72	ALA	2.2
1	G	192	ALA	2.2
1	E	188	ALA	2.2
1	C	133	TYR	2.2
1	E	73	TYR	2.2
1	E	103	LEU	2.2
1	D	156	SER	2.2
1	D	158	LEU	2.1
1	F	217	LEU	2.1
1	G	193	ILE	2.1
1	C	237	GLU	2.0
1	C	218	GLN	2.0
1	A	157	LEU	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 monosaccharides 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^{th} 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
2	OX0	A	301	31/31	0.91	0.14	41,50,63,71	0

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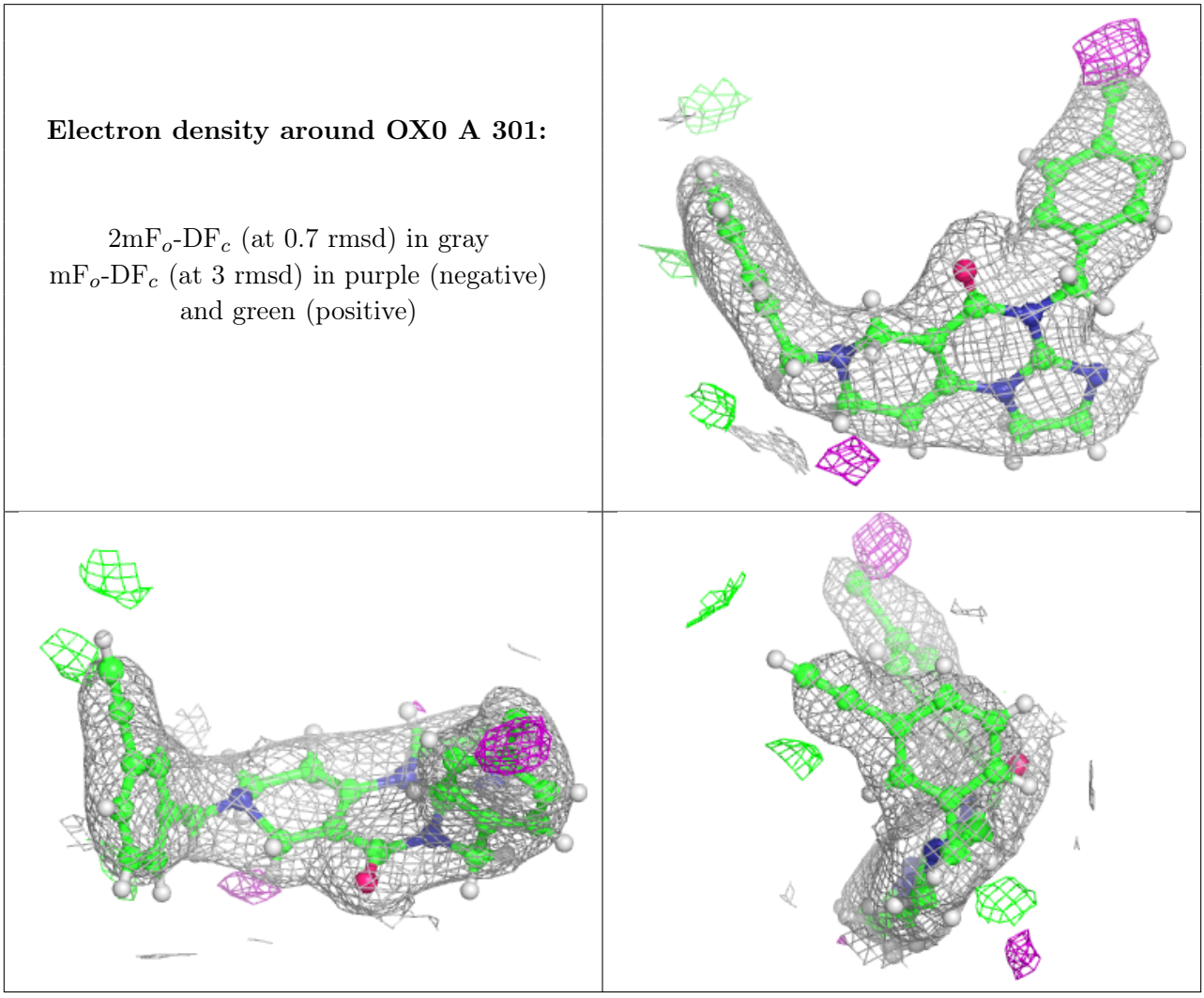
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OX0	E	301	31/31	0.92	0.13	33,42,51,65	0
2	OX0	C	301	31/31	0.93	0.14	34,42,55,65	0
2	OX0	B	301	31/31	0.93	0.14	34,44,55,65	0
2	OX0	F	301	31/31	0.93	0.13	35,44,54,64	0
2	OX0	G	301	31/31	0.93	0.12	35,43,54,68	0
2	OX0	D	301	31/31	0.94	0.12	34,43,56,59	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.

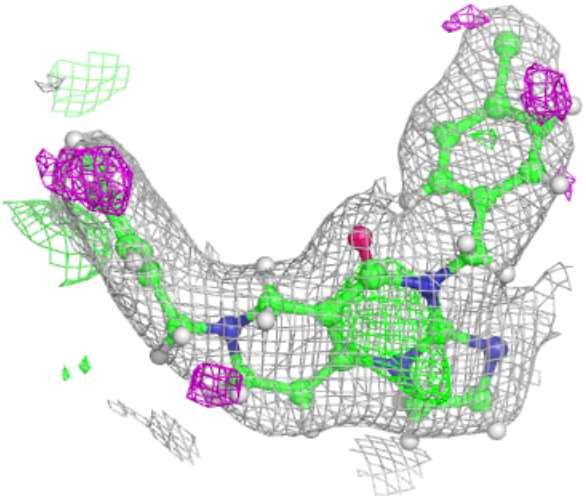
Electron density around OX0 A 301:

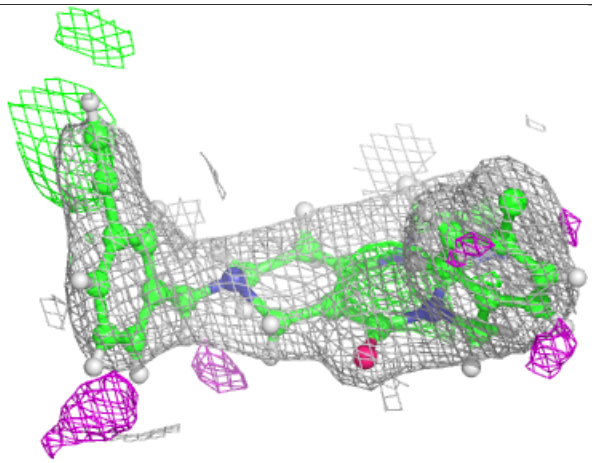
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

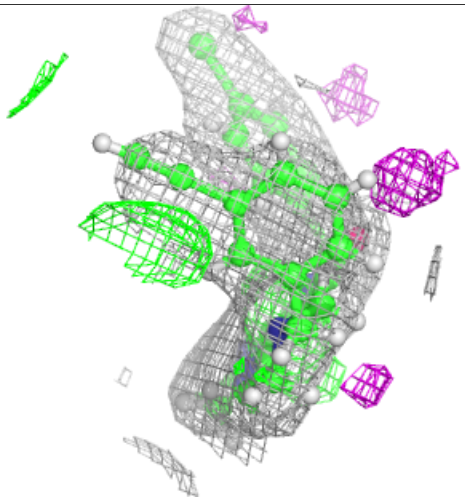


Electron density around OX0 E 301:

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

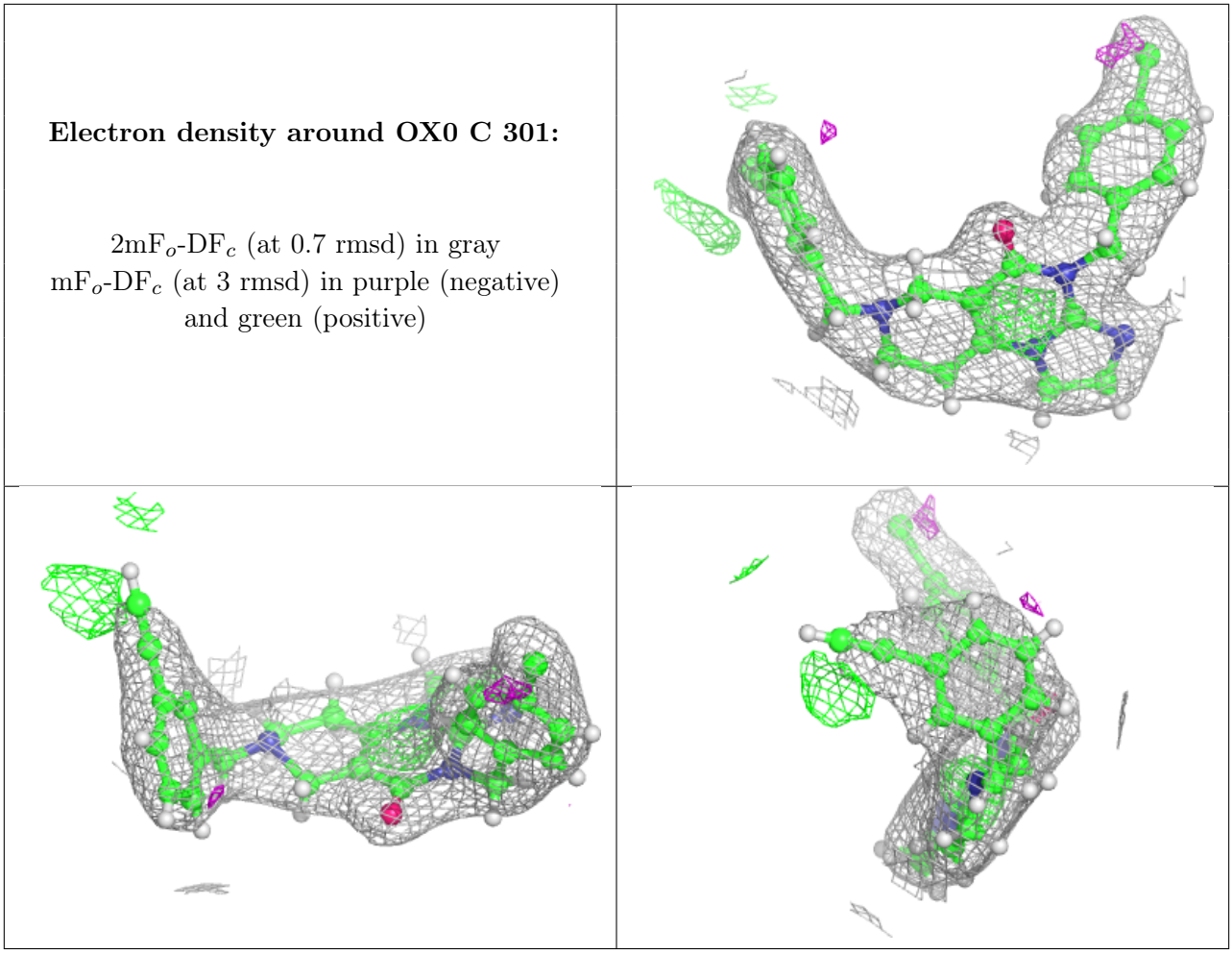






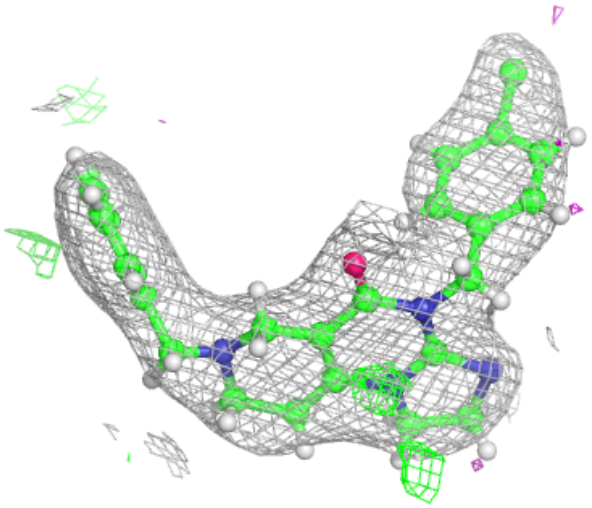
Electron density around OX0 C 301:

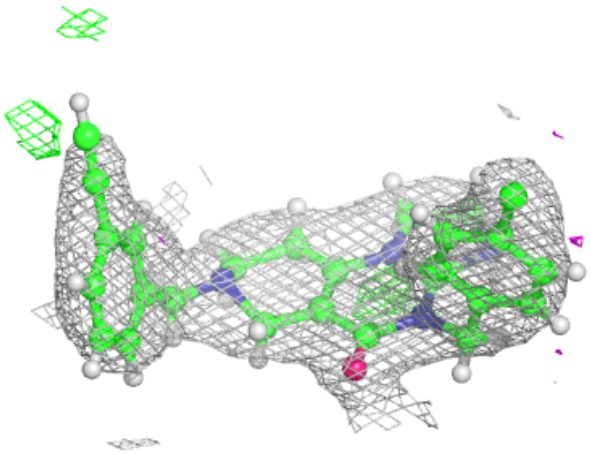
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

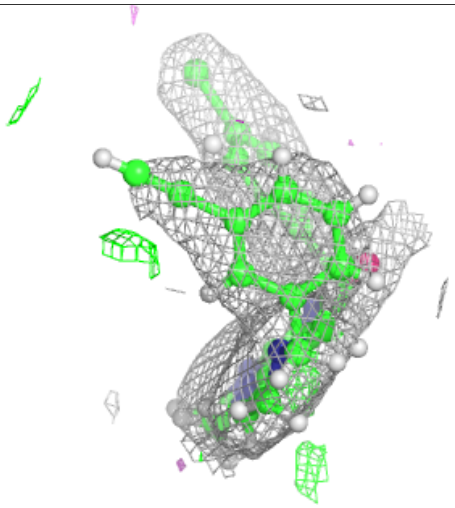


Electron density around OX0 B 301:

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

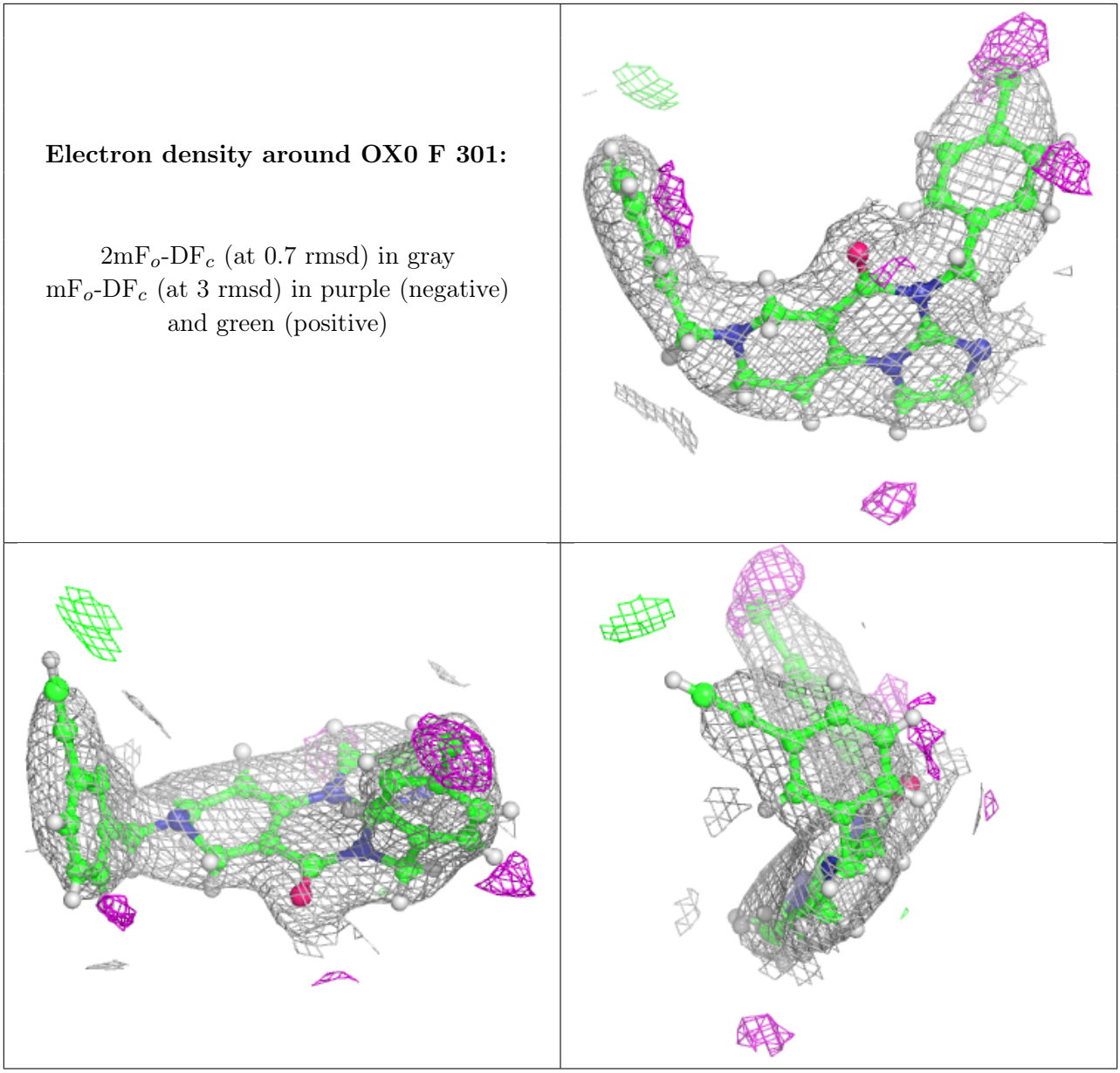






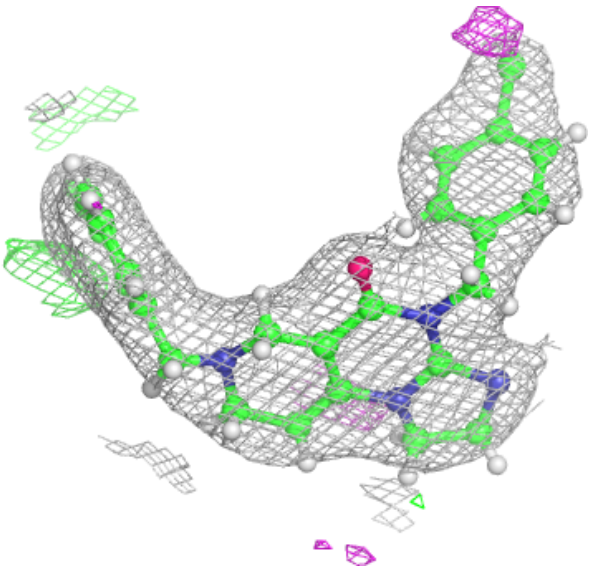
Electron density around OX0 F 301:

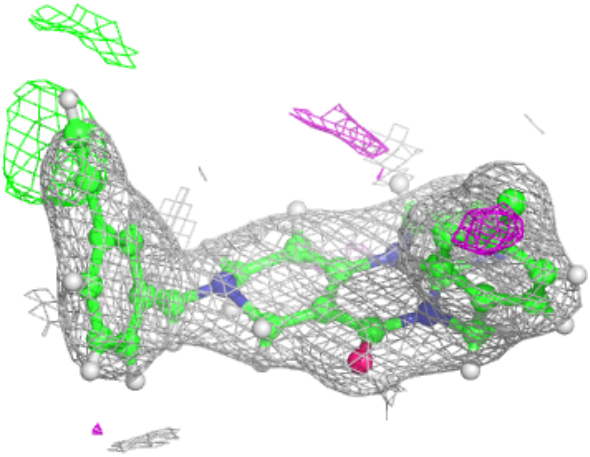
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

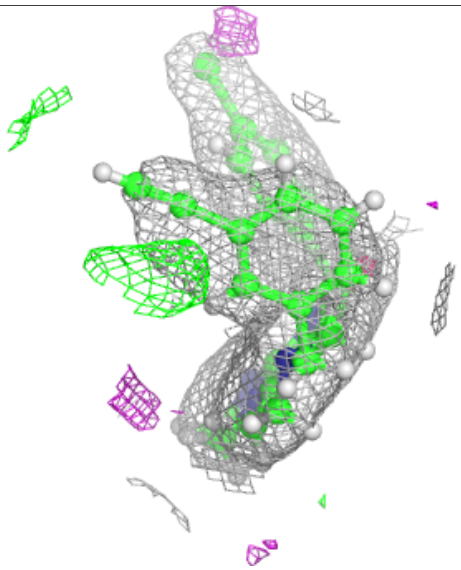


Electron density around OX0 G 301:

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

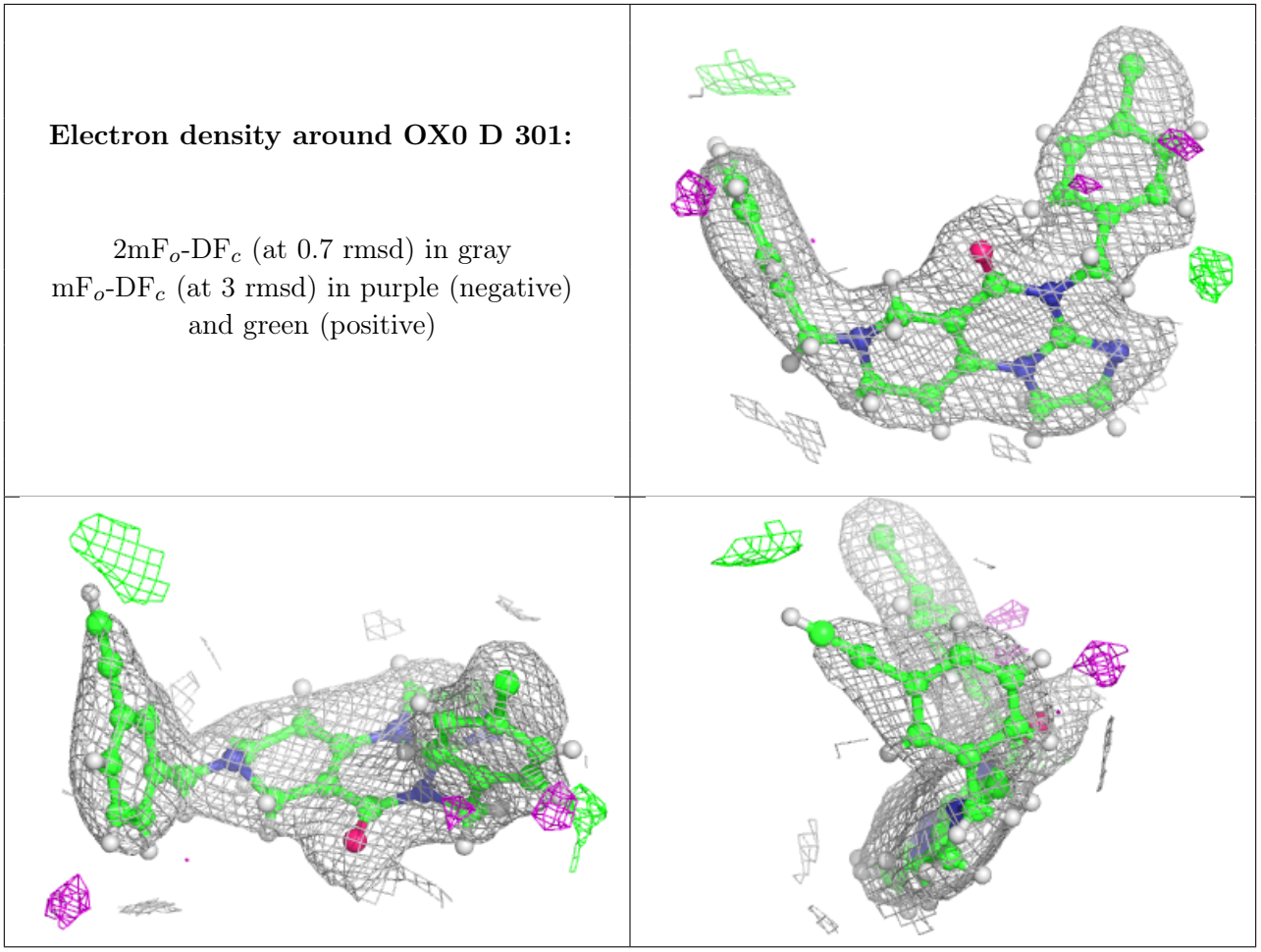






Electron density around OX0 D 301:

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



6.5 Other polymers

There are no such residues in this entry.