



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:18 am BST

PDB ID : 3O2X  
Title : MMP-13 in complex with selective tetrazole core inhibitor  
Authors : Kiefer, J.R.; Barta, T.E.; Becker, D.P.; Mathis, K.J.; Williams, J.  
Deposited on : 2010-07-22  
Resolution : 1.90 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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

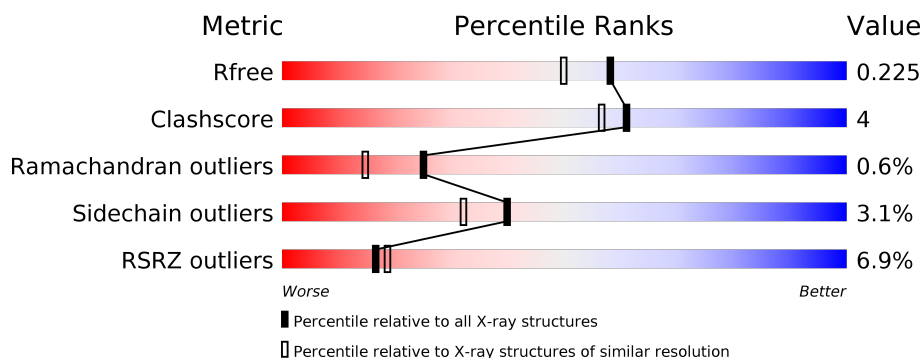
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	164	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> <div>•</div> </div>
1	B	164	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> <div>•</div> </div>
1	C	164	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> <div>•</div> </div>
1	D	164	<div> <div>7%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> <div>•</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6167 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.

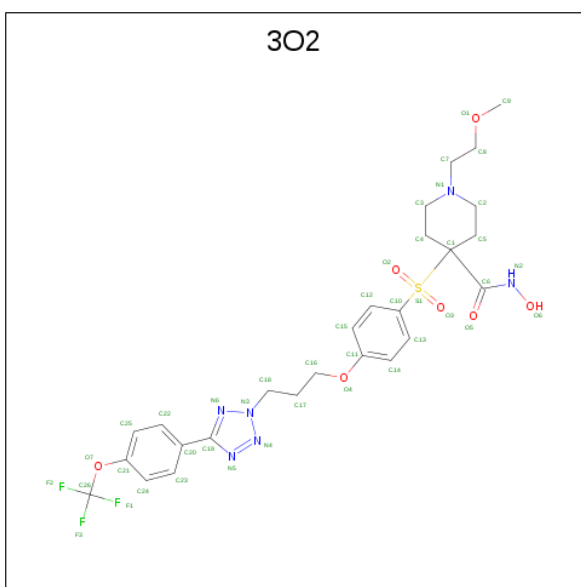
- Molecule 1 is a protein called Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	2	0
			1314	848	213	248	5			
1	B	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			
1	C	164	Total	C	N	O	S	0	2	0
			1314	850	213	246	5			
1	D	164	Total	C	N	O	S	0	0	0
			1300	841	211	243	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1104	ALA	-	expression tag	UNP P45452
B	2104	ALA	-	expression tag	UNP P45452
C	1104	ALA	-	expression tag	UNP P45452
D	2104	ALA	-	expression tag	UNP P45452

- Molecule 2 is N-hydroxy-1-(2-methoxyethyl)-4-{[4-(3-{5-[4-(trifluoromethoxy)phenyl]-2H-tetrazol-2-yl}propoxy)phenyl]sulfonyl}piperidine-4-carboxamide (three-letter code: 3O2) (formula: C<sub>26</sub>H<sub>31</sub>F<sub>3</sub>N<sub>6</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			43	26	3	6	7	1		
2	B	1	Total	C	F	N	O	S	0	0
			43	26	3	6	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			43	26	3	6	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			43	26	3	6	7	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



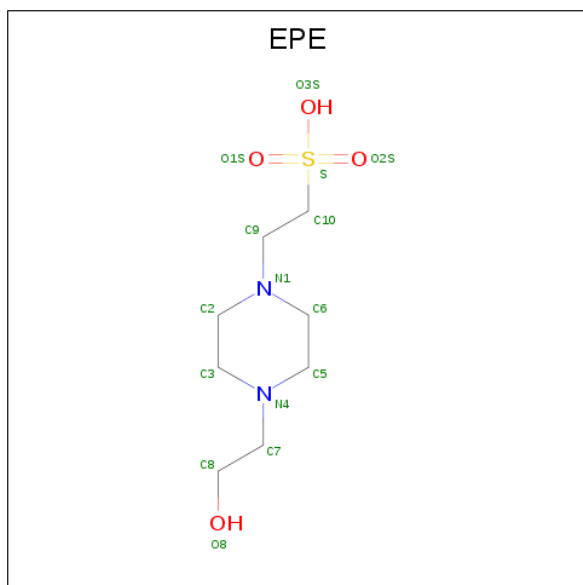
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

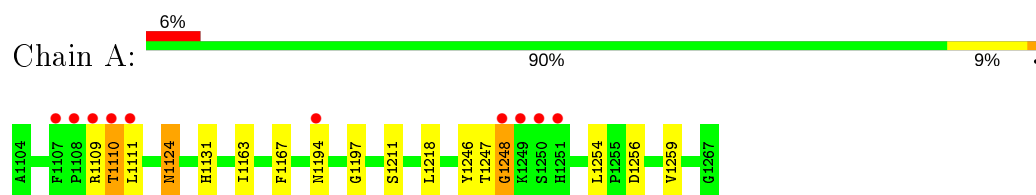
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	173	Total	O	0	0
			173	173		
7	B	151	Total	O	0	0
			151	151		
7	C	180	Total	O	0	0
			180	180		
7	D	178	Total	O	0	0
			178	178		

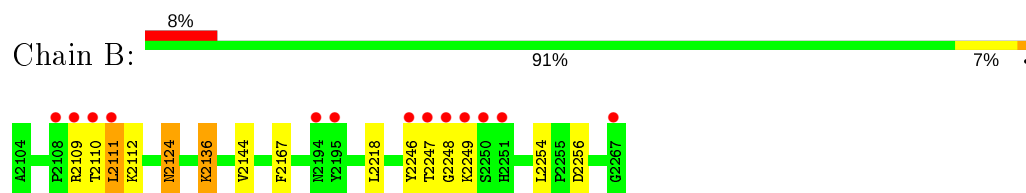
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

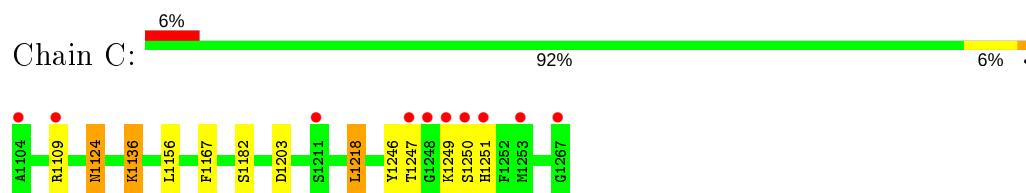
- Molecule 1: Collagenase 3



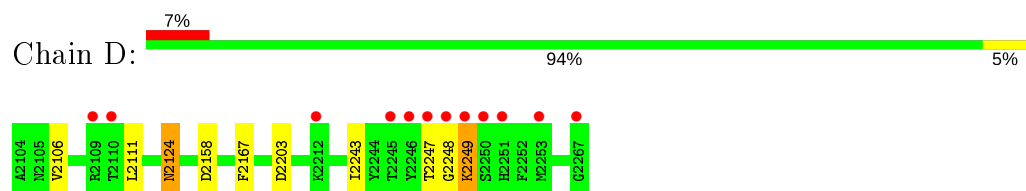
- Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



- Molecule 1: Collagenase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.86 Å 95.26 Å 120.08 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 1.90 19.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.1 (19.72-1.90) 84.1 (19.72-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.31 (at 1.90 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.210 0.192 , 0.225	Depositor DCC
$R_{free}$ test set	2879 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 41.9	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	0.94	EDS
Total number of atoms	6167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8373e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EPE, ZN, 3O2, CA, SO4

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	0.33	0/1360	0.49	0/1848
1	B	0.35	0/1346	0.52	0/1829
1	C	0.34	0/1360	0.50	0/1848
1	D	0.33	0/1346	0.49	0/1829
All	All	0.34	0/5412	0.50	0/7354

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2247	THR	Peptide

### 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	1314	0	1218	11	0
1	B	1300	0	1211	15	0
1	C	1314	0	1225	14	0
1	D	1300	0	1211	8	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
2	C	43	0	30	1	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	15	0	0	0	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
7	A	173	0	0	0	0
7	B	151	0	0	1	0
7	C	180	0	0	1	0
7	D	178	0	0	2	0
All	All	6167	0	5009	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1124:ASN:HD21	1:C:1167:PHE:H	1.06	0.95
1:D:2124:ASN:HD21	1:D:2167:PHE:H	1.07	0.95
1:A:1218:LEU:HD22	1:A:1246:TYR:HB2	1.56	0.88
1:B:2109:ARG:HB3	1:B:2110:THR:HA	1.63	0.81
1:B:2109:ARG:CB	1:B:2110:THR:HA	2.15	0.75
1:D:2111:LEU:HD23	7:D:860:HOH:O	1.92	0.69
1:C:1156:LEU:HD13	1:D:2243:ILE:HD13	1.77	0.66
1:C:1250:SER:CB	1:C:1251:HIS:HA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2124:ASN:HD21	1:B:2167:PHE:H	1.44	0.63
1:C:1218[B]:LEU:HD12	1:C:1246:TYR:HB2	1.82	0.62
1:B:2124:ASN:ND2	1:B:2167:PHE:H	1.99	0.60
1:D:2124:ASN:ND2	1:D:2167:PHE:H	1.88	0.59
1:A:1218:LEU:CD2	1:A:1246:TYR:HB2	2.29	0.59
1:B:2111:LEU:HD22	1:B:2112:LYS:HG2	1.85	0.59
1:B:2136:LYS:HD3	1:B:2136:LYS:N	2.17	0.59
1:C:1218[A]:LEU:HD21	2:C:1801:3O2:H17	1.86	0.56
1:A:1124:ASN:HD21	1:A:1167:PHE:H	1.54	0.55
1:D:2248:GLY:O	1:D:2249:LYS:CB	2.55	0.54
1:C:1250:SER:CB	1:C:1251:HIS:CA	2.86	0.53
1:A:1124:ASN:ND2	1:A:1167:PHE:H	2.07	0.52
1:C:1124:ASN:ND2	1:C:1167:PHE:H	1.90	0.52
1:C:1250:SER:HB2	1:C:1251:HIS:HA	1.90	0.51
1:D:2124:ASN:HD21	1:D:2167:PHE:N	1.91	0.51
1:C:1250:SER:HB3	1:C:1251:HIS:C	2.32	0.50
1:B:2246:TYR:HB3	1:B:2247:THR:HA	1.94	0.50
1:D:2106:VAL:HG22	7:D:794:HOH:O	2.12	0.49
1:D:2124:ASN:HD22	1:D:2124:ASN:C	2.16	0.48
1:C:1136:LYS:N	1:C:1136:LYS:HD3	2.29	0.47
1:C:1250:SER:HB3	1:C:1251:HIS:HA	1.97	0.47
1:C:1247:THR:HG23	1:C:1249:LYS:H	1.78	0.47
1:A:1247:THR:HG22	7:B:320:HOH:O	2.15	0.47
1:A:1109:ARG:HB3	1:A:1110:THR:CA	2.45	0.46
1:B:2218:LEU:HD13	1:B:2246:TYR:O	2.15	0.46
1:A:1218:LEU:HD22	1:A:1246:TYR:CB	2.38	0.45
1:C:1250:SER:HB3	1:C:1251:HIS:CA	2.46	0.45
1:B:2247:THR:N	1:B:2248:GLY:HA2	2.32	0.45
1:A:1211:SER:HB3	1:A:1248:GLY:HA2	1.99	0.45
1:B:2218:LEU:CD1	1:B:2246:TYR:O	2.65	0.45
1:B:2111:LEU:HD22	1:B:2112:LYS:CG	2.46	0.44
1:B:2144:VAL:CG1	1:B:2254:LEU:HD13	2.48	0.44
1:A:1109:ARG:HB3	1:A:1110:THR:CB	2.49	0.43
1:C:1247:THR:HG22	7:C:392:HOH:O	2.18	0.42
1:B:2110:THR:OG1	1:B:2111:LEU:N	2.52	0.42
1:A:1254:LEU:HD23	1:A:1259:VAL:HG22	2.01	0.42
1:A:1163:ILE:HG23	1:A:1197:GLY:O	2.19	0.42
1:B:2247:THR:N	1:B:2248:GLY:CA	2.83	0.41
1:B:2248:GLY:N	1:B:2249:LYS:HA	2.37	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	164/164 (100%)	155 (94%)	7 (4%)	2 (1%)	13	4
1	B	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	C	164/164 (100%)	156 (95%)	7 (4%)	1 (1%)	25	15
1	D	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	15
All	All	652/656 (99%)	617 (95%)	31 (5%)	4 (1%)	25	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2249	LYS
1	A	1194	ASN
1	A	1248	GLY
1	C	1109	ARG

### 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	140/139 (101%)	134 (96%)	6 (4%)	29	19
1	B	138/139 (99%)	134 (97%)	4 (3%)	42	35
1	C	140/139 (101%)	134 (96%)	6 (4%)	29	19
1	D	138/139 (99%)	135 (98%)	3 (2%)	52	47
All	All	556/556 (100%)	537 (97%)	19 (3%)	40	28

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1110	THR
1	A	1111	LEU
1	A	1124	ASN
1	A	1131	HIS
1	A	1256[A]	ASP
1	A	1256[B]	ASP
1	B	2111	LEU
1	B	2124	ASN
1	B	2136	LYS
1	B	2256	ASP
1	C	1124	ASN
1	C	1136	LYS
1	C	1182	SER
1	C	1203	ASP
1	C	1218[A]	LEU
1	C	1218[B]	LEU
1	D	2124	ASN
1	D	2158	ASP
1	D	2203	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1124	ASN
1	A	1131	HIS
1	B	2124	ASN
1	C	1124	ASN
1	C	1131	HIS
1	D	2124	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 16 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	D	5	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	6	-	4,4,4	0.14	0	6,6,6	0.09	0
6	EPE	A	400	-	12,12,15	0.94	1 (8%)	14,16,20	1.62	3 (21%)
6	EPE	B	400	-	12,12,15	0.97	1 (8%)	14,16,20	1.63	4 (28%)
2	3O2	C	1801	3	41,46,46	0.92	1 (2%)	53,66,66	1.27	5 (9%)
5	SO4	D	8	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	B	4	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	A	2	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	A	9	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	C	1	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	B	3	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	7	-	4,4,4	0.13	0	6,6,6	0.09	0
2	3O2	B	1801	3	41,46,46	0.94	2 (4%)	53,66,66	1.32	8 (15%)
2	3O2	D	1801	3	41,46,46	0.95	2 (4%)	53,66,66	1.18	5 (9%)
2	3O2	A	1801	3	41,46,46	0.94	2 (4%)	53,66,66	1.31	8 (15%)

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
6	EPE	A	400	-	-	1/6/14/19	0/1/1/1
6	EPE	B	400	-	-	1/6/14/19	0/1/1/1
2	3O2	C	1801	3	-	8/39/55/55	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3O2	B	1801	3	-	4/39/55/55	0/4/4/4
2	3O2	D	1801	3	-	7/39/55/55	0/4/4/4
2	3O2	A	1801	3	-	10/39/55/55	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1801	3O2	C19-N5	3.22	1.37	1.33
2	A	1801	3O2	C19-N5	3.18	1.37	1.33
2	C	1801	3O2	C19-N5	3.18	1.37	1.33
2	D	1801	3O2	C19-N5	3.00	1.37	1.33
6	B	400	EPE	C10-S	2.86	1.81	1.77
6	A	400	EPE	C10-S	2.84	1.81	1.77
2	B	1801	3O2	O7-C26	2.13	1.43	1.31
2	D	1801	3O2	O7-C26	2.06	1.43	1.31
2	A	1801	3O2	O7-C26	2.03	1.43	1.31

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1801	3O2	C16-O4-C11	-3.92	107.69	117.93
2	B	1801	3O2	C4-C3-N1	-3.73	107.55	111.23
2	A	1801	3O2	C16-O4-C11	-3.59	108.53	117.93
2	A	1801	3O2	C4-C3-N1	-3.52	107.77	111.23
2	C	1801	3O2	C4-C3-N1	-3.20	108.08	111.23
6	A	400	EPE	C5-N4-C3	3.12	119.32	110.34
6	B	400	EPE	C5-N4-C3	3.10	119.26	110.34
2	B	1801	3O2	O2-S1-C10	-3.10	104.51	108.27
2	D	1801	3O2	O3-S1-C10	-2.98	104.67	108.27
6	A	400	EPE	O2S-S-C10	2.91	110.42	106.92
2	B	1801	3O2	C16-O4-C11	-2.91	110.32	117.93
2	B	1801	3O2	C5-C2-N1	-2.86	108.41	111.23
2	D	1801	3O2	O3-S1-C1	2.82	110.72	107.67
2	D	1801	3O2	C16-O4-C11	-2.78	110.65	117.93
2	C	1801	3O2	O3-S1-C10	-2.71	104.98	108.27
2	A	1801	3O2	O3-S1-C10	-2.70	105.00	108.27
2	A	1801	3O2	C17-C18-N3	-2.60	106.55	111.70
2	A	1801	3O2	O3-S1-C1	2.54	110.42	107.67
2	D	1801	3O2	C4-C3-N1	-2.40	108.87	111.23
2	B	1801	3O2	C26-O7-C21	-2.39	110.11	118.01
2	A	1801	3O2	C5-C2-N1	-2.36	108.91	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	400	EPE	O3S-S-C10	2.35	109.57	105.77
2	D	1801	3O2	O2-S1-C10	-2.34	105.44	108.27
2	C	1801	3O2	C5-C2-N1	-2.33	108.93	111.23
6	B	400	EPE	O2S-S-C10	2.31	109.69	106.92
2	C	1801	3O2	C1-C6-N2	-2.30	112.56	116.37
2	B	1801	3O2	C8-C7-N1	-2.27	107.13	113.31
6	B	400	EPE	O1S-S-C10	2.25	109.62	106.92
2	B	1801	3O2	O3-S1-C10	-2.24	105.56	108.27
6	A	400	EPE	O1S-S-C10	2.22	109.59	106.92
2	B	1801	3O2	N6-C19-N5	2.21	113.54	111.85
2	A	1801	3O2	O2-S1-C10	-2.09	105.74	108.27
2	A	1801	3O2	C12-C10-S1	-2.06	117.58	119.37

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	400	EPE	C10-C9-N1-C2
6	B	400	EPE	C10-C9-N1-C2
2	C	1801	3O2	C4-C1-S1-O3
2	C	1801	3O2	C16-C17-C18-N3
2	D	1801	3O2	C4-C1-S1-O3
2	D	1801	3O2	C16-C17-C18-N3
2	B	1801	3O2	C4-C1-S1-O3
2	B	1801	3O2	C16-C17-C18-N3
2	C	1801	3O2	N1-C7-C8-O1
2	D	1801	3O2	N1-C7-C8-O1
2	C	1801	3O2	C7-C8-O1-C9
2	A	1801	3O2	C15-C11-O4-C16
2	A	1801	3O2	C7-C8-O1-C9
2	A	1801	3O2	C14-C11-O4-C16
2	C	1801	3O2	C8-C7-N1-C2
2	D	1801	3O2	C8-C7-N1-C3
2	A	1801	3O2	O4-C16-C17-C18
2	A	1801	3O2	C16-C17-C18-N3
2	C	1801	3O2	C8-C7-N1-C3
2	D	1801	3O2	C8-C7-N1-C2
2	C	1801	3O2	C4-C1-S1-C10
2	D	1801	3O2	C4-C1-S1-C10
2	B	1801	3O2	C4-C1-S1-C10
2	A	1801	3O2	C4-C1-S1-O3
2	A	1801	3O2	C8-C7-N1-C2

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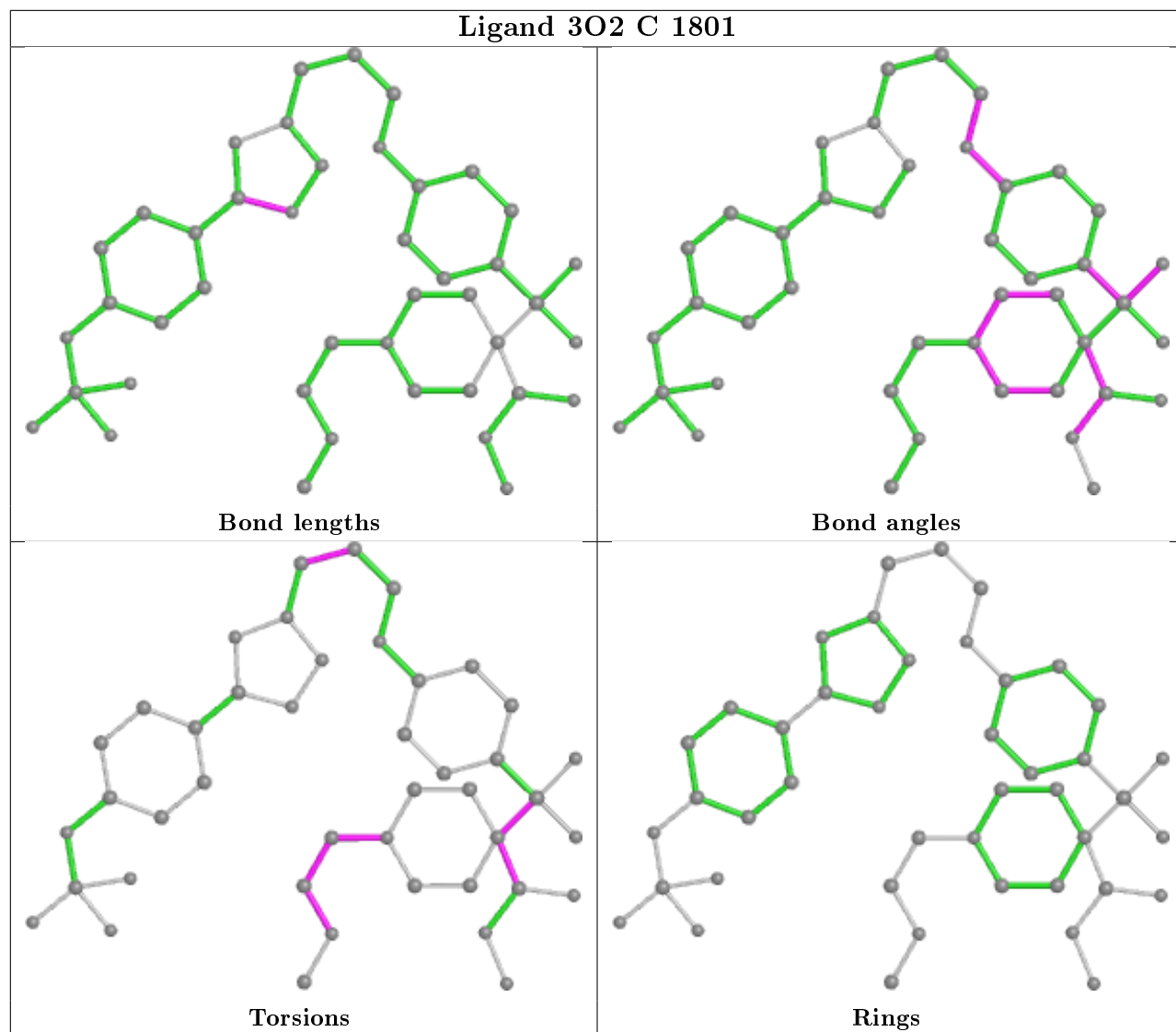
Mol	Chain	Res	Type	Atoms
2	C	1801	3O2	C4-C1-C6-O5
2	D	1801	3O2	C4-C1-C6-O5
2	A	1801	3O2	C4-C1-C6-O5
2	B	1801	3O2	C4-C1-C6-O5
2	A	1801	3O2	C4-C1-S1-C10
2	A	1801	3O2	C8-C7-N1-C3

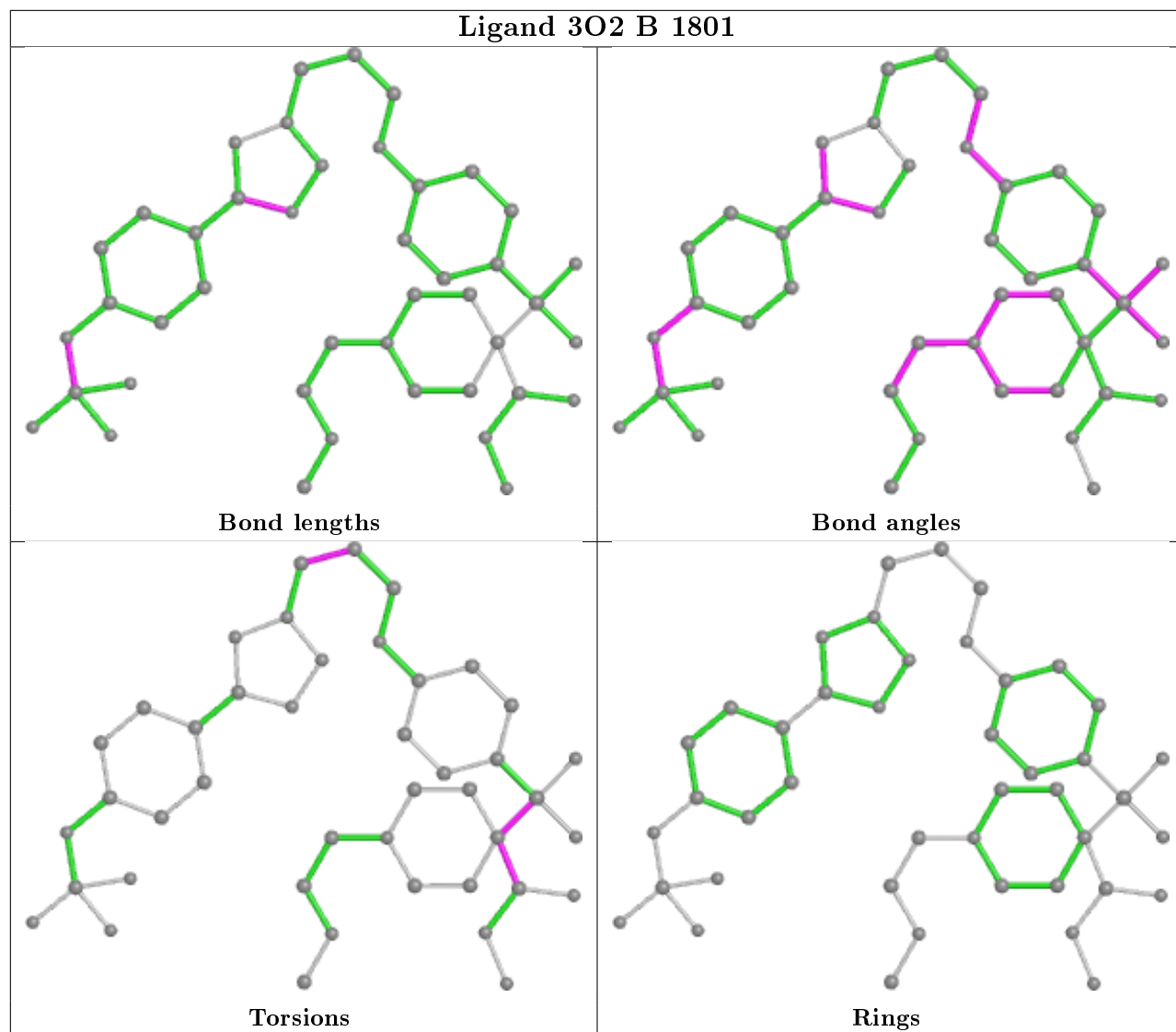
There are no ring outliers.

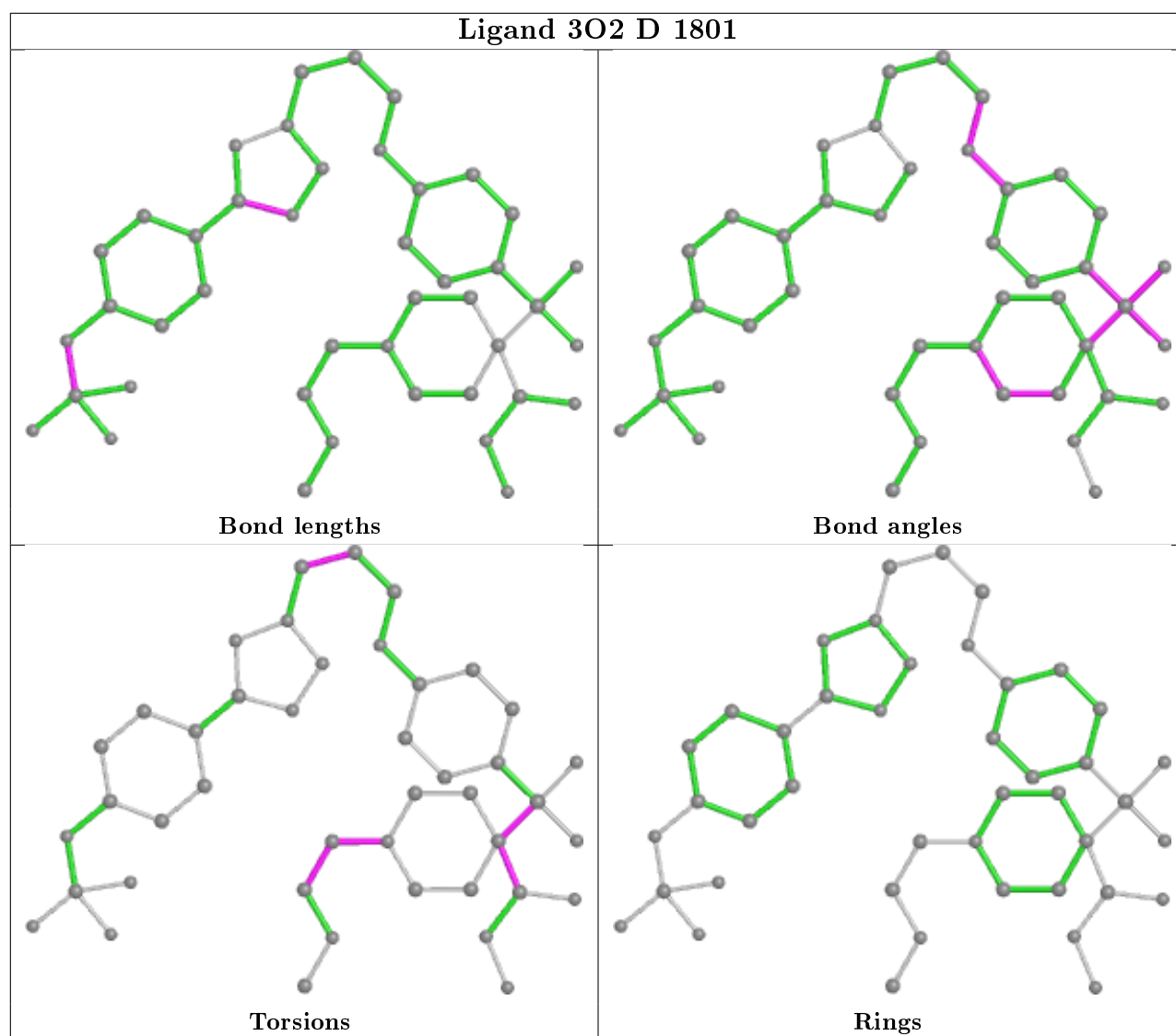
1 monomer is involved in 1 short contact:

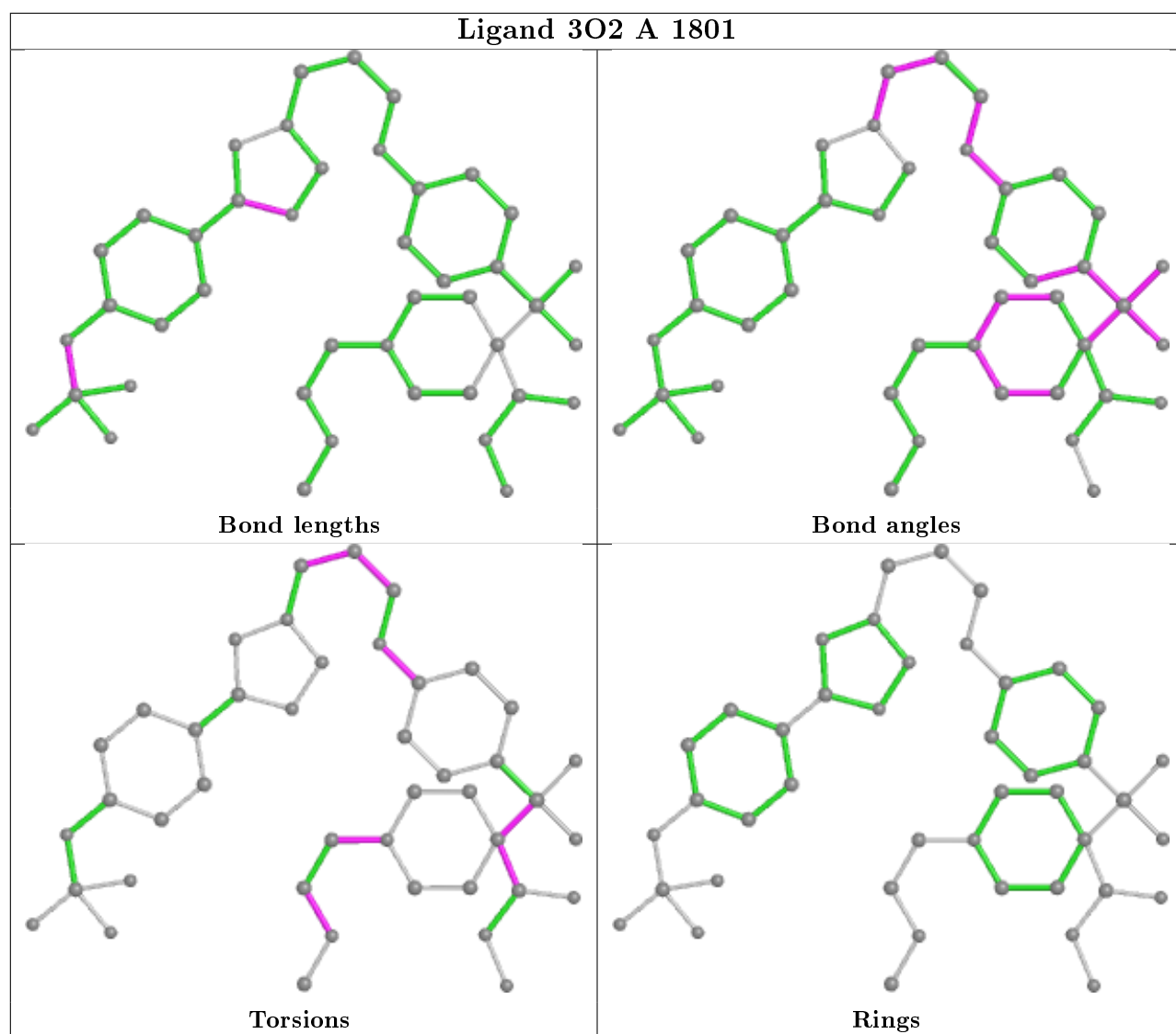
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1801	3O2	1	0

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 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, 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	164/164 (100%)	0.21	10 (6%) 21 24	4, 9, 20, 25	0
1	B	164/164 (100%)	0.37	13 (7%) 12 14	4, 9, 22, 27	0
1	C	164/164 (100%)	0.21	10 (6%) 21 24	5, 9, 17, 24	0
1	D	164/164 (100%)	0.25	12 (7%) 15 16	5, 9, 18, 27	0
All	All	656/656 (100%)	0.26	45 (6%) 16 19	4, 9, 20, 27	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2248	GLY	9.3
1	B	2247	THR	9.2
1	B	2249	LYS	9.1
1	D	2249	LYS	8.4
1	D	2246	TYR	7.6
1	B	2251	HIS	6.9
1	B	2250	SER	6.8
1	C	1250	SER	6.2
1	B	2109	ARG	5.8
1	C	1251	HIS	5.4
1	A	1109	ARG	5.3
1	D	2250	SER	5.2
1	A	1250	SER	5.1
1	D	2247	THR	4.9
1	A	1249	LYS	4.7
1	B	2111	LEU	4.6
1	A	1111	LEU	4.5
1	A	1248	GLY	4.4
1	C	1247	THR	4.4
1	C	1211	SER	4.3
1	A	1110	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	1249	LYS	4.0
1	A	1251	HIS	4.0
1	C	1104	ALA	4.0
1	D	2251	HIS	3.7
1	A	1108	PRO	3.5
1	B	2248	GLY	3.4
1	C	1248	GLY	3.3
1	C	1267	GLY	3.0
1	B	2195	TYR	2.8
1	D	2109	ARG	2.7
1	B	2108	PRO	2.6
1	B	2246	TYR	2.6
1	C	1253	MET	2.4
1	D	2212	LYS	2.4
1	D	2267	GLY	2.3
1	D	2253	MET	2.2
1	D	2110	THR	2.2
1	B	2267	GLY	2.2
1	A	1194	ASN	2.2
1	B	2194	ASN	2.2
1	D	2245	THR	2.2
1	B	2110	THR	2.0
1	A	1107	PHE	2.0
1	C	1109	ARG	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 carbohydrates 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.

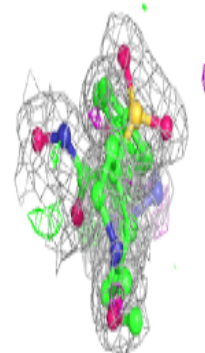
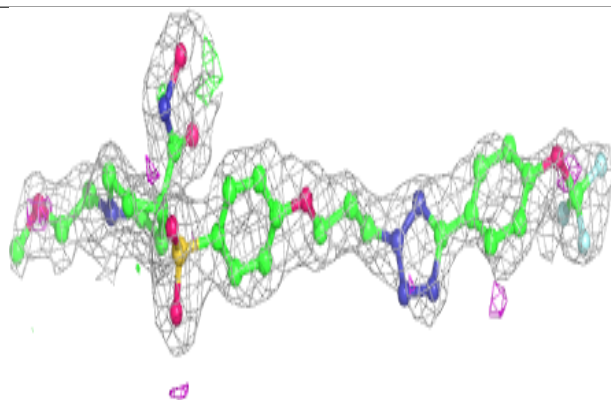
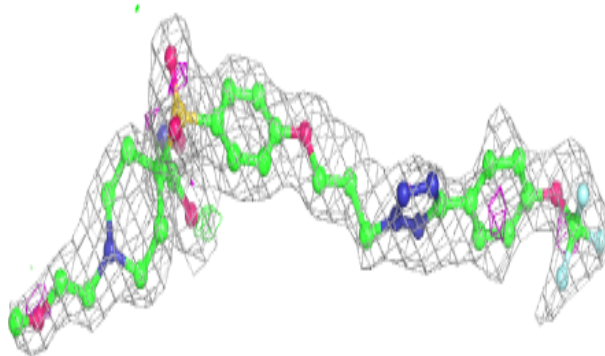
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3O2	B	1801	43/43	0.89	0.17	19,28,50,51	0
2	3O2	A	1801	43/43	0.90	0.15	11,15,20,24	0
2	3O2	C	1801	43/43	0.91	0.14	12,17,22,26	0
6	EPE	A	400	12/15	0.93	0.18	29,29,30,30	0
2	3O2	D	1801	43/43	0.93	0.13	15,22,30,31	0
6	EPE	B	400	12/15	0.94	0.15	37,37,37,37	0
5	SO4	A	9	5/5	0.95	0.18	47,48,48,48	0
5	SO4	C	1	5/5	0.96	0.16	41,41,41,42	0
5	SO4	A	7	5/5	0.96	0.14	45,46,46,46	0
5	SO4	B	6	5/5	0.96	0.13	40,41,41,41	0
5	SO4	A	2	5/5	0.96	0.13	47,47,48,48	0
5	SO4	B	4	5/5	0.97	0.12	39,39,39,40	0
5	SO4	D	8	5/5	0.97	0.20	33,33,34,34	0
4	CA	D	2996	1/1	0.97	0.15	37,37,37,37	0
5	SO4	B	3	5/5	0.97	0.17	45,45,46,46	0
4	CA	A	1996	1/1	0.98	0.17	37,37,37,37	0
5	SO4	D	5	5/5	0.98	0.13	36,36,36,36	0
4	CA	C	1996	1/1	0.98	0.16	35,35,35,35	0
4	CA	B	2996	1/1	0.99	0.13	34,34,34,34	0
4	CA	C	1997	1/1	0.99	0.04	8,8,8,8	0
3	ZN	C	1999	1/1	1.00	0.04	9,9,9,9	0
3	ZN	B	2999	1/1	1.00	0.05	14,14,14,14	0
4	CA	D	2997	1/1	1.00	0.04	7,7,7,7	0
3	ZN	B	2998	1/1	1.00	0.06	13,13,13,13	0
3	ZN	D	2998	1/1	1.00	0.04	12,12,12,12	0
3	ZN	A	1998	1/1	1.00	0.05	8,8,8,8	0
4	CA	A	1997	1/1	1.00	0.04	6,6,6,6	0
4	CA	B	2997	1/1	1.00	0.05	11,11,11,11	0
3	ZN	C	1998	1/1	1.00	0.04	8,8,8,8	0
3	ZN	D	2999	1/1	1.00	0.06	11,11,11,11	0
3	ZN	A	1999	1/1	1.00	0.06	8,8,8,8	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.

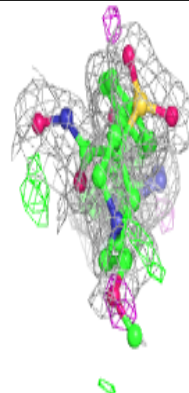
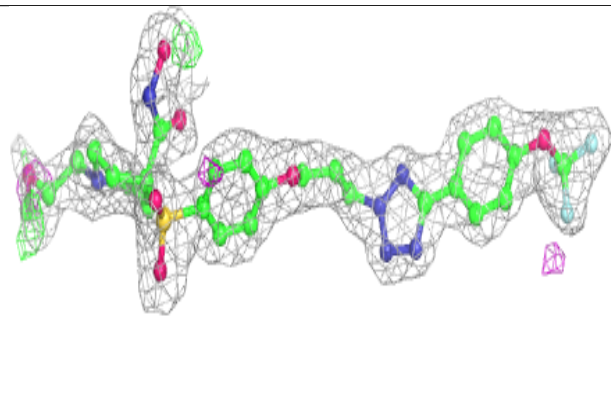
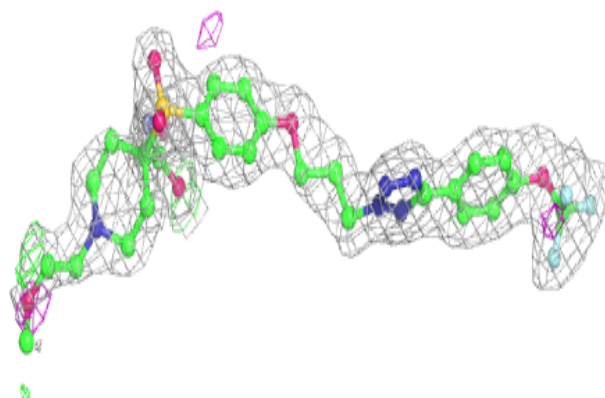


**Electron density around 3O2 B 1801:**

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

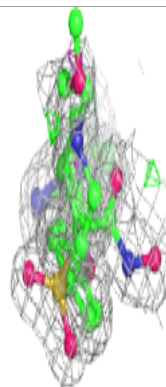
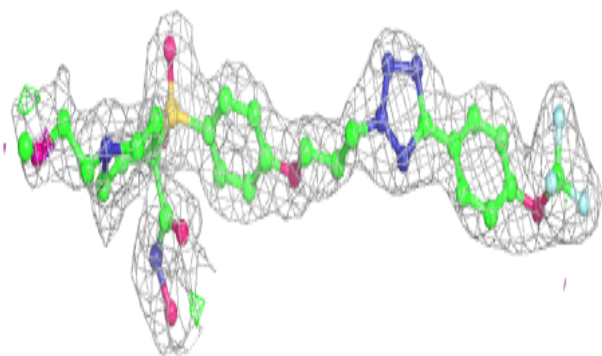
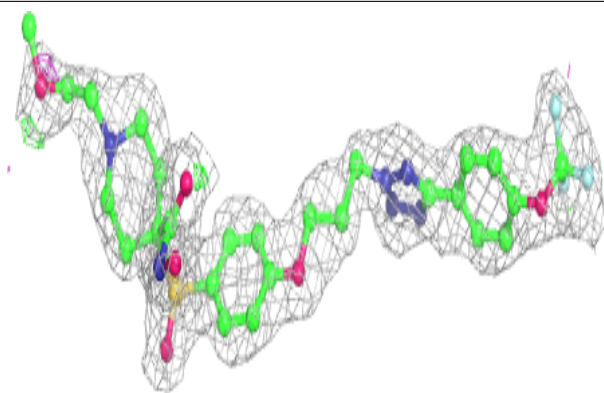
**Electron density around 3O2 A 1801:**

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

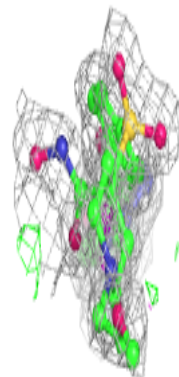
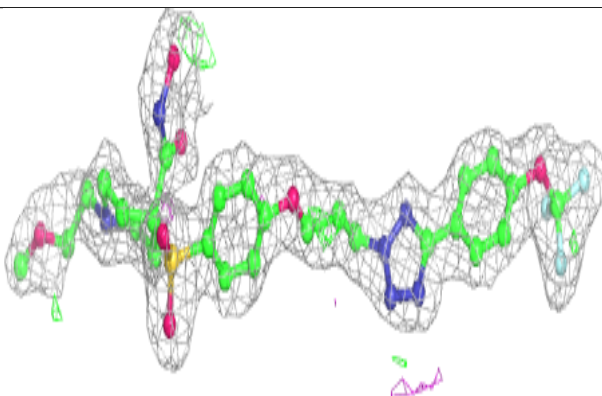
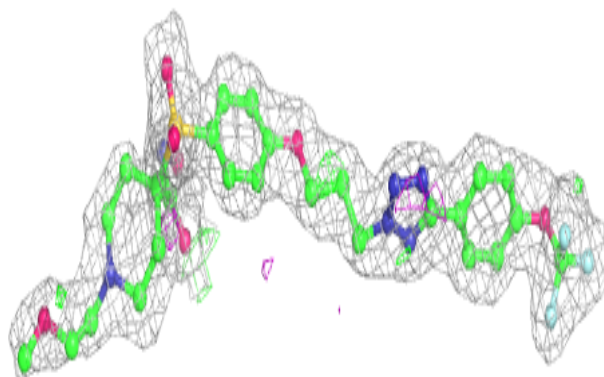


**Electron density around 3O2 C 1801:**

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

**Electron density around 3O2 D 1801:**

$2mF_o-DF_c$  (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.