



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2021 – 12:11 PM JST

PDB ID : 7DBL  
Title : Acyl-CoA hydrolase MpaH' mutant S139A in complex with MPA  
Authors : Li, S.Y.; You, C.  
Deposited on : 2020-10-20  
Resolution : 1.84 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 : 2.23.2  
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) : 2.23.2

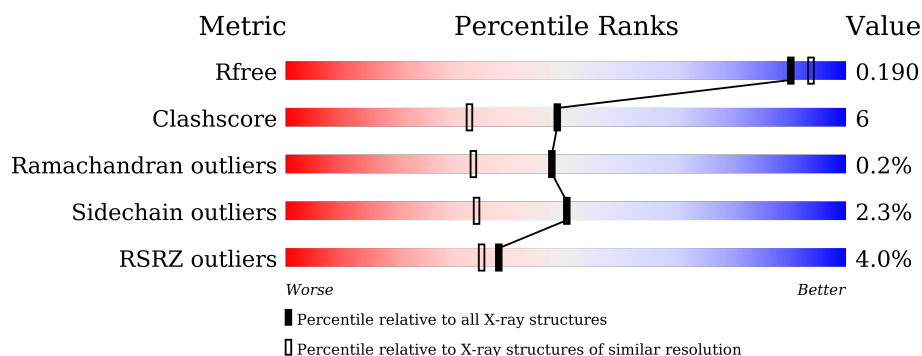
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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

Mol	Chain	Length	Quality of chain
1	A	433	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	B	433	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	C	433	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	D	433	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition [i](#)

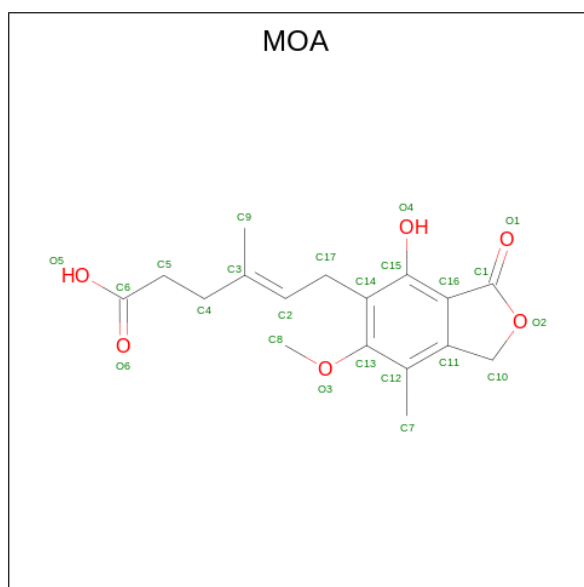
There are 3 unique types of molecules in this entry. The entry contains 14365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 acyl-CoA hydrolase MpaH'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3369	2143	593	615	18			
1	B	418	Total	C	N	O	S	0	0	0
			3342	2127	589	609	17			
1	C	418	Total	C	N	O	S	0	0	0
			3342	2127	589	609	17			
1	D	420	Total	C	N	O	S	0	0	0
			3351	2131	591	611	18			

- Molecule 2 is MYCOPHENOLIC ACID (three-letter code: MOA) (formula: C<sub>17</sub>H<sub>20</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	17	6		
2	B	1	Total	C	O	0	0
			23	17	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			23	17	6		
2	D	1	Total	C	O	0	0
			23	17	6		

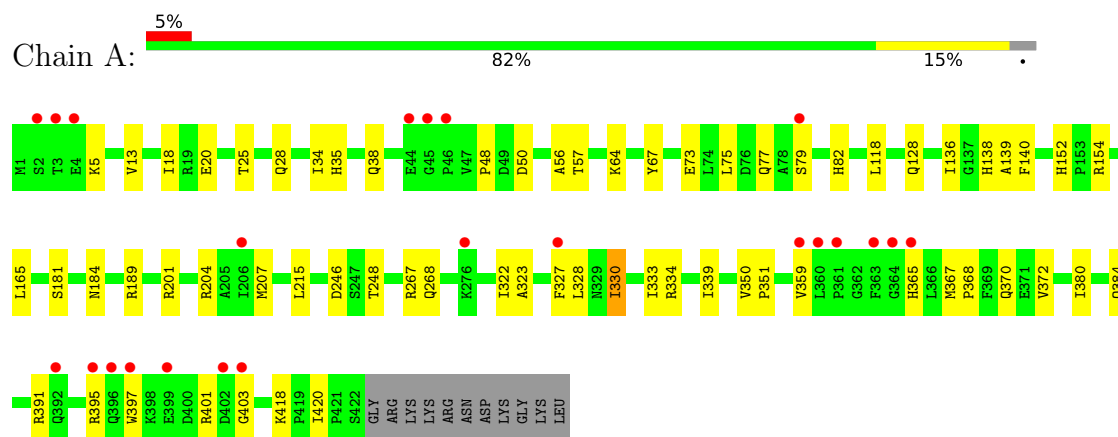
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	224	Total	O	0	0
			224	224		
3	C	210	Total	O	0	0
			210	210		
3	D	221	Total	O	0	0
			221	221		

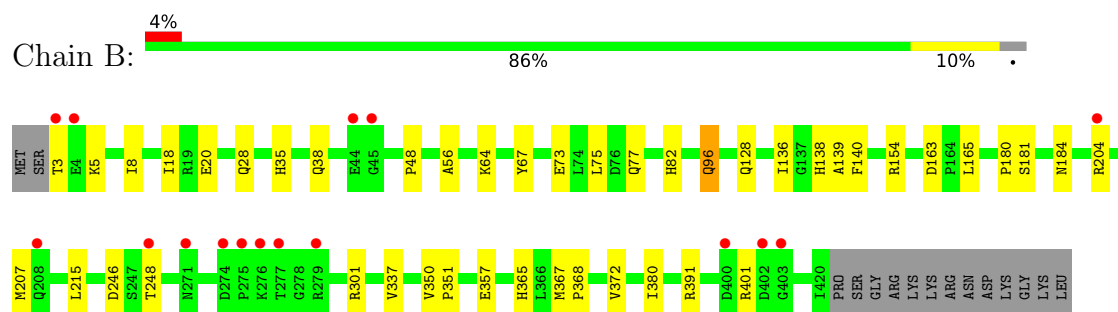
### 3 Residue-property plots [i](#)

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.

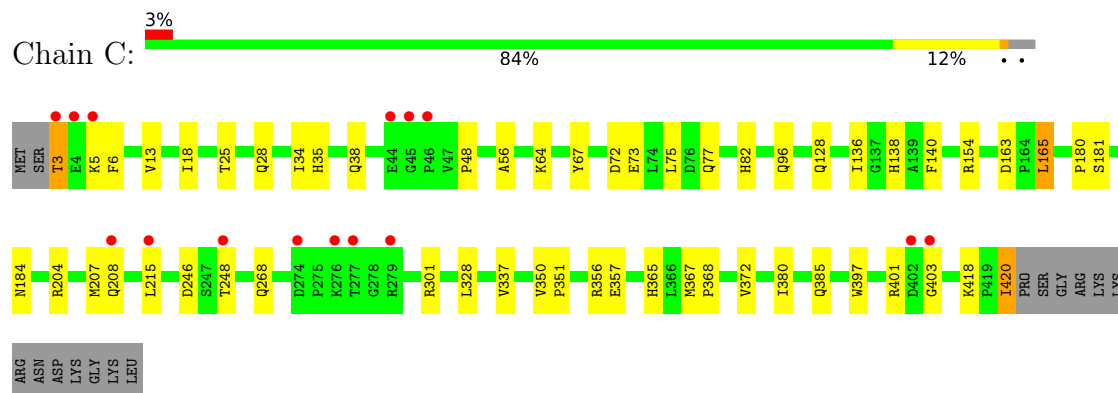
- Molecule 1: acyl-CoA hydrolase MpaH'



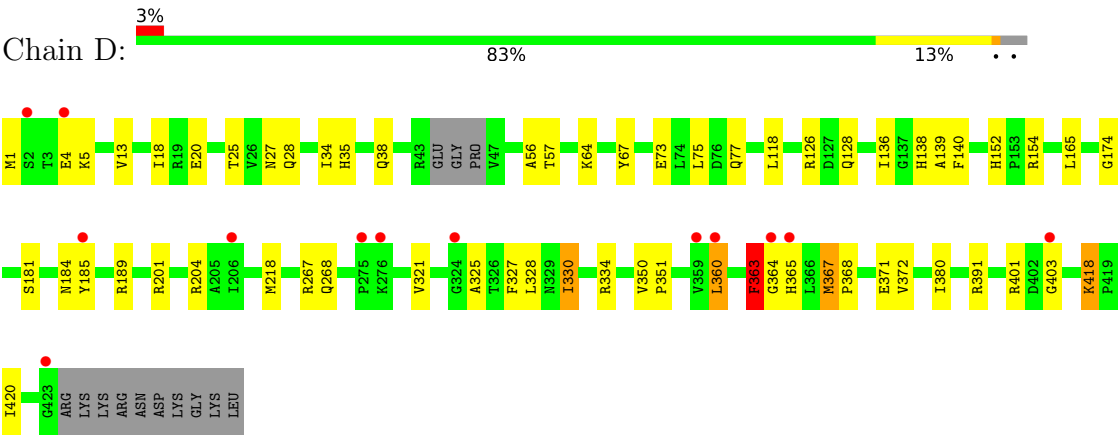
- Molecule 1: acyl-CoA hydrolase MpaH'



- Molecule 1: acyl-CoA hydrolase MpaH'



● Molecule 1: acyl-CoA hydrolase MpaH'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.82Å 92.78Å 160.76Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	48.08 – 1.84 48.08 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.08-1.84) 99.4 (48.08-1.84)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.179 , 0.205 0.188 , 0.190	Depositor DCC
$R_{free}$ test set	8113 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.72	0/3460	0.86	4/4710 (0.1%)
1	B	0.73	0/3432	0.83	2/4672 (0.0%)
1	C	0.72	0/3432	0.83	1/4672 (0.0%)
1	D	0.75	1/3439 (0.0%)	0.86	5/4678 (0.1%)
All	All	0.73	1/13763 (0.0%)	0.85	12/18732 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	D	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	364	GLY	C-O	11.37	1.41	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	363	PHE	CB-CA-C	6.61	123.63	110.40
1	A	267	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	267	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	391	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	126	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	334	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	391	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	C	356	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	267	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	189	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ALA	Peptide
1	A	403	GLY	Peptide
1	C	403	GLY	Peptide
1	D	363	PHE	Mainchain,Peptide
1	D	403	GLY	Peptide

## 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	3369	0	3337	50	0
1	B	3342	0	3308	35	0
1	C	3342	0	3308	48	0
1	D	3351	0	3317	49	0
2	A	23	0	19	5	0
2	B	23	0	19	2	0
2	C	23	0	18	1	0
2	D	23	0	19	2	0
3	A	214	0	0	2	0
3	B	224	0	0	0	0
3	C	210	0	0	1	0
3	D	221	0	0	3	0
All	All	14365	0	13345	160	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 6.

All (160) 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:420:ILE:HD12	1:D:185:TYR:CZ	2.17	0.80
1:C:3:THR:HG23	1:C:72:ASP:OD1	1.82	0.80
1:D:330:ILE:CD1	1:D:334:ARG:HD2	2.16	0.74
1:B:246:ASP:OD1	1:B:248:THR:HG22	1.88	0.74
1:A:246:ASP:OD1	1:A:248:THR:HG22	1.88	0.73
1:D:27:ASN:HB3	3:D:738:HOH:O	1.86	0.73
1:C:246:ASP:OD1	1:C:248:THR:HG22	1.89	0.73
1:D:5:LYS:HB3	1:D:75:LEU:HD23	1.71	0.71
1:C:28:GLN:HE22	1:D:154:ARG:HH12	1.39	0.71
1:A:5:LYS:HB3	1:A:75:LEU:HD23	1.73	0.70
1:C:154:ARG:HH12	1:D:28:GLN:HE22	1.41	0.69
1:D:5:LYS:CB	1:D:75:LEU:HD23	2.24	0.68
1:C:420:ILE:HD12	1:D:185:TYR:CE1	2.28	0.68
1:A:327:PHE:HE1	2:A:501:MOA:C13	2.08	0.67
1:A:327:PHE:CE1	2:A:501:MOA:O3	2.48	0.67
1:A:5:LYS:CB	1:A:75:LEU:HD23	2.25	0.66
1:A:328:LEU:HD13	1:A:333:ILE:CD1	2.25	0.66
1:D:330:ILE:HD13	1:D:334:ARG:HD2	1.77	0.66
1:C:5:LYS:HB3	1:C:75:LEU:HD23	1.78	0.66
1:B:38:GLN:HE22	1:B:128:GLN:HE22	1.44	0.65
1:C:5:LYS:CB	1:C:75:LEU:HD23	2.26	0.65
1:A:154:ARG:HH12	1:B:28:GLN:HE22	1.43	0.65
1:A:327:PHE:HE2	1:A:365:HIS:CE1	2.14	0.65
1:A:38:GLN:HE22	1:A:128:GLN:HE22	1.45	0.64
1:A:420:ILE:HD13	1:B:180:PRO:HB2	1.79	0.64
1:B:5:LYS:CB	1:B:75:LEU:HD23	2.28	0.64
1:C:67:TYR:OH	1:C:138:HIS:HD2	1.81	0.63
1:A:67:TYR:OH	1:A:138:HIS:HD2	1.82	0.63
1:D:165:LEU:HD11	1:D:327:PHE:CE1	2.34	0.63
1:B:67:TYR:OH	1:B:138:HIS:HD2	1.81	0.63
1:A:28:GLN:HE22	1:B:154:ARG:HH12	1.46	0.63
1:D:35:HIS:HD2	1:D:64:LYS:NZ	1.97	0.62
1:D:67:TYR:OH	1:D:138:HIS:HD2	1.83	0.62
1:B:35:HIS:HD2	1:B:64:LYS:NZ	1.97	0.62
1:A:165:LEU:HD12	1:A:328:LEU:HD21	1.81	0.62
1:A:35:HIS:HD2	1:A:64:LYS:NZ	1.99	0.61
1:C:35:HIS:HD2	1:C:64:LYS:NZ	1.98	0.60
1:A:370:GLN:C	3:A:601:HOH:O	2.38	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:HG21	1:A:330:ILE:HD13	1.83	0.60
1:A:328:LEU:HD13	1:A:333:ILE:HD11	1.84	0.60
1:B:77:GLN:HB2	1:B:380:ILE:CD1	2.32	0.59
1:C:401:ARG:NH1	3:C:601:HOH:O	2.31	0.59
1:D:38:GLN:HE22	1:D:128:GLN:HE22	1.49	0.59
1:A:327:PHE:CE1	2:A:501:MOA:C13	2.85	0.59
1:B:5:LYS:HB3	1:B:75:LEU:HD23	1.84	0.59
1:A:77:GLN:HB2	1:A:380:ILE:CD1	2.34	0.58
1:C:38:GLN:HE22	1:C:128:GLN:HE22	1.52	0.58
1:C:77:GLN:HB2	1:C:380:ILE:CD1	2.34	0.58
1:C:181:SER:H	1:C:184:ASN:ND2	2.03	0.57
1:D:165:LEU:HD12	1:D:328:LEU:HD21	1.87	0.57
1:C:3:THR:CG2	1:C:72:ASP:OD1	2.53	0.56
1:B:35:HIS:CD2	1:B:96:GLN:HG2	2.40	0.56
1:D:77:GLN:HB2	1:D:380:ILE:CD1	2.36	0.56
1:D:27:ASN:OD1	3:D:601:HOH:O	2.18	0.55
1:D:181:SER:H	1:D:184:ASN:ND2	2.03	0.55
1:B:181:SER:H	1:B:184:ASN:ND2	2.03	0.55
1:C:3:THR:HG21	1:C:6:PHE:HD1	1.72	0.55
1:A:181:SER:H	1:A:184:ASN:ND2	2.03	0.54
1:C:73:GLU:HG3	1:C:372:VAL:HG12	1.88	0.54
1:D:35:HIS:HD2	1:D:64:LYS:HZ1	1.56	0.54
1:B:181:SER:H	1:B:184:ASN:HD22	1.56	0.54
1:A:330:ILE:HD12	1:A:330:ILE:O	2.07	0.54
1:B:77:GLN:CB	1:B:380:ILE:HD13	2.37	0.54
1:B:77:GLN:HB2	1:B:380:ILE:HD13	1.89	0.54
1:B:73:GLU:HG3	1:B:372:VAL:HG12	1.89	0.54
1:D:321:VAL:HG13	1:D:360:LEU:HD22	1.89	0.53
1:D:330:ILE:HD11	1:D:334:ARG:HD2	1.90	0.53
1:A:139:ALA:HB1	2:A:501:MOA:C6	2.39	0.53
1:C:181:SER:H	1:C:184:ASN:HD22	1.55	0.53
1:D:365:HIS:CD2	2:D:501:MOA:O5	2.62	0.53
1:A:181:SER:H	1:A:184:ASN:HD22	1.57	0.53
1:A:201:ARG:NH1	1:A:204:ARG:HG3	2.24	0.52
1:D:165:LEU:HD11	1:D:327:PHE:HE1	1.76	0.51
1:C:154:ARG:HH22	1:D:28:GLN:HE21	1.58	0.51
1:D:181:SER:H	1:D:184:ASN:HD22	1.57	0.51
1:C:418:LYS:HD3	1:D:174:GLY:O	2.10	0.51
1:C:28:GLN:NE2	1:D:154:ARG:HH12	2.06	0.51
1:D:321:VAL:CG1	1:D:360:LEU:HD22	2.41	0.51
1:B:138:HIS:HE1	1:B:365:HIS:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLN:HB2	1:C:380:ILE:HD13	1.94	0.50
1:A:138:HIS:HE1	1:A:365:HIS:O	1.94	0.50
1:D:139:ALA:HB1	2:D:501:MOA:C6	2.42	0.50
1:C:420:ILE:HD12	1:D:185:TYR:CE2	2.47	0.50
1:C:138:HIS:HE1	1:C:365:HIS:O	1.94	0.50
1:A:154:ARG:HH12	1:B:28:GLN:NE2	2.10	0.49
1:C:180:PRO:HB2	1:D:420:ILE:HD13	1.94	0.49
1:D:13:VAL:HG22	1:D:34:ILE:HG13	1.93	0.49
1:D:165:LEU:HD11	1:D:327:PHE:CZ	2.48	0.49
1:B:5:LYS:HB2	1:B:75:LEU:HD23	1.95	0.48
1:C:77:GLN:CB	1:C:380:ILE:HD13	2.43	0.48
1:C:35:HIS:HD2	1:C:64:LYS:HZ1	1.59	0.48
1:C:28:GLN:HE21	1:D:154:ARG:HH22	1.61	0.48
1:C:207:MET:CE	1:C:215:LEU:HD22	2.44	0.48
1:C:401:ARG:NH2	1:D:25:THR:O	2.47	0.48
1:C:3:THR:CG2	1:C:6:PHE:HD1	2.27	0.48
1:C:165:LEU:HD13	1:C:328:LEU:HD22	1.96	0.48
1:D:152:HIS:HD2	3:D:730:HOH:O	1.97	0.48
1:A:154:ARG:HH22	1:B:28:GLN:HE21	1.61	0.47
1:C:13:VAL:HG22	1:C:34:ILE:HG13	1.96	0.47
1:C:25:THR:O	1:D:401:ARG:NH2	2.47	0.47
1:C:5:LYS:HB2	1:C:75:LEU:HD23	1.96	0.47
1:A:13:VAL:HG22	1:A:34:ILE:HG13	1.95	0.47
1:C:3:THR:HG21	1:C:6:PHE:CD1	2.49	0.47
1:C:207:MET:HE3	1:C:215:LEU:HD22	1.96	0.47
1:D:367:MET:N	1:D:368:PRO:CD	2.76	0.47
1:A:35:HIS:HD2	1:A:64:LYS:HZ1	1.61	0.47
1:A:207:MET:HE3	1:A:215:LEU:HD22	1.97	0.47
1:A:207:MET:HE3	1:A:215:LEU:CD2	2.45	0.46
1:A:367:MET:N	1:A:368:PRO:CD	2.78	0.46
1:A:73:GLU:HG3	1:A:372:VAL:HG12	1.96	0.46
1:A:327:PHE:HE1	2:A:501:MOA:C12	2.29	0.46
1:A:77:GLN:HB2	1:A:380:ILE:HD13	1.96	0.46
1:D:77:GLN:HB2	1:D:380:ILE:HD13	1.98	0.46
1:A:25:THR:O	1:B:401:ARG:NH2	2.49	0.46
1:D:73:GLU:HG3	1:D:372:VAL:HG12	1.98	0.45
1:C:56:ALA:HA	1:C:136:ILE:O	2.16	0.45
1:A:56:ALA:HA	1:A:136:ILE:O	2.17	0.45
1:B:56:ALA:HA	1:B:136:ILE:O	2.17	0.45
1:C:301:ARG:HG2	2:C:501:MOA:O1	2.17	0.45
1:D:56:ALA:HA	1:D:136:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:HIS:HD2	1:B:64:LYS:HZ1	1.65	0.45
1:B:38:GLN:HE22	1:B:128:GLN:NE2	2.12	0.45
1:A:79:SER:OG	1:A:384:GLN:OE1	2.34	0.44
1:A:391:ARG:O	1:A:395:ARG:HG3	2.17	0.44
1:D:201:ARG:NH2	1:D:204:ARG:HG3	2.32	0.44
1:D:77:GLN:CB	1:D:380:ILE:HD13	2.47	0.44
1:A:50:ASP:OD1	1:A:50:ASP:N	2.50	0.43
1:A:152:HIS:HD2	3:A:694:HOH:O	1.99	0.43
1:D:5:LYS:HB2	1:D:75:LEU:HD23	1.99	0.43
1:B:337:VAL:HG11	1:B:357:GLU:HB3	2.01	0.43
1:C:48:PRO:HG2	1:C:82:HIS:CD2	2.53	0.43
1:B:301:ARG:HG2	2:B:501:MOA:O1	2.18	0.43
1:C:154:ARG:HH22	1:D:28:GLN:NE2	2.16	0.43
1:B:48:PRO:HG2	1:B:82:HIS:CG	2.54	0.43
1:C:154:ARG:HH12	1:D:28:GLN:NE2	2.10	0.43
1:D:325:ALA:O	1:D:363:PHE:HA	2.18	0.43
1:A:28:GLN:HE21	1:B:154:ARG:HH22	1.65	0.43
1:A:28:GLN:NE2	1:B:154:ARG:HH12	2.14	0.42
1:A:77:GLN:CB	1:A:380:ILE:HD13	2.49	0.42
1:A:350:VAL:N	1:A:351:PRO:CD	2.83	0.42
1:C:337:VAL:HG11	1:C:357:GLU:HB3	2.02	0.42
1:B:3:THR:HB	1:B:8:ILE:HD11	2.02	0.42
1:B:139:ALA:HB2	1:B:365:HIS:CE1	2.55	0.42
1:A:48:PRO:HG2	1:A:82:HIS:CG	2.54	0.42
1:C:367:MET:N	1:C:368:PRO:CD	2.83	0.42
1:B:350:VAL:N	1:B:351:PRO:CD	2.83	0.42
1:C:38:GLN:HE22	1:C:128:GLN:NE2	2.15	0.42
1:B:207:MET:CE	1:B:215:LEU:HD22	2.51	0.41
1:A:397:TRP:CZ2	1:A:401:ARG:HD2	2.55	0.41
1:B:139:ALA:HB1	2:B:501:MOA:C6	2.50	0.41
1:C:350:VAL:N	1:C:351:PRO:CD	2.83	0.41
1:A:327:PHE:HE2	1:A:365:HIS:ND1	2.19	0.41
1:D:57:THR:CG2	1:D:118:LEU:HD11	2.51	0.41
1:D:350:VAL:N	1:D:351:PRO:CD	2.84	0.41
1:D:418:LYS:HB3	1:D:418:LYS:HE3	1.98	0.41
1:A:5:LYS:HB2	1:A:75:LEU:HD23	2.00	0.41
1:B:367:MET:N	1:B:368:PRO:CD	2.84	0.41
1:C:397:TRP:CZ2	1:C:401:ARG:HD2	2.56	0.41
1:C:48:PRO:HG2	1:C:82:HIS:CG	2.56	0.40
1:A:57:THR:CG2	1:A:118:LEU:HD11	2.52	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	420/433 (97%)	406 (97%)	13 (3%)	1 (0%)	47	33
1	B	416/433 (96%)	406 (98%)	9 (2%)	1 (0%)	47	33
1	C	416/433 (96%)	407 (98%)	8 (2%)	1 (0%)	47	33
1	D	416/433 (96%)	401 (96%)	14 (3%)	1 (0%)	47	33
All	All	1668/1732 (96%)	1620 (97%)	44 (3%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	B	18	ILE
1	C	18	ILE
1	D	18	ILE

### 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	369/378 (98%)	362 (98%)	7 (2%)	57	42
1	B	365/378 (97%)	359 (98%)	6 (2%)	62	49
1	C	365/378 (97%)	355 (97%)	10 (3%)	44	28
1	D	366/378 (97%)	355 (97%)	11 (3%)	41	23
All	All	1465/1512 (97%)	1431 (98%)	34 (2%)	50	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	140	PHE
1	A	268	GLN
1	A	330	ILE
1	A	339	ILE
1	A	359	VAL
1	A	418	LYS
1	B	20	GLU
1	B	96	GLN
1	B	140	PHE
1	B	163	ASP
1	B	165	LEU
1	B	204	ARG
1	C	3	THR
1	C	96	GLN
1	C	140	PHE
1	C	163	ASP
1	C	165	LEU
1	C	204	ARG
1	C	208	GLN
1	C	268	GLN
1	C	385	GLN
1	C	420	ILE
1	D	1	MET
1	D	4	GLU
1	D	20	GLU
1	D	140	PHE
1	D	218	MET
1	D	268	GLN
1	D	330	ILE
1	D	360	LEU
1	D	367	MET
1	D	371	GLU
1	D	418	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	35	HIS
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	95	ASN
1	A	128	GLN
1	A	138	HIS
1	A	152	HIS
1	A	184	ASN
1	A	268	GLN
1	B	28	GLN
1	B	35	HIS
1	B	77	GLN
1	B	95	ASN
1	B	128	GLN
1	B	138	HIS
1	B	152	HIS
1	B	184	ASN
1	B	208	GLN
1	C	28	GLN
1	C	35	HIS
1	C	77	GLN
1	C	82	HIS
1	C	95	ASN
1	C	128	GLN
1	C	138	HIS
1	C	152	HIS
1	C	184	ASN
1	C	208	GLN
1	C	268	GLN
1	D	28	GLN
1	D	35	HIS
1	D	77	GLN
1	D	95	ASN
1	D	128	GLN
1	D	138	HIS
1	D	152	HIS
1	D	184	ASN
1	D	268	GLN
1	D	365	HIS

### 5.3.3 RNA ⓘ

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](#)

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	MOA	D	501	-	21,24,24	3.59	9 (42%)	31,34,34	2.50	15 (48%)
2	MOA	C	501	-	21,24,24	2.93	9 (42%)	31,34,34	2.84	12 (38%)
2	MOA	B	501	-	21,24,24	2.84	8 (38%)	31,34,34	2.97	12 (38%)
2	MOA	A	501	-	21,24,24	3.26	7 (33%)	31,34,34	2.85	14 (45%)

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	MOA	D	501	-	-	3/10/21/21	0/2/2/2
2	MOA	C	501	-	-	0/10/21/21	0/2/2/2
2	MOA	B	501	-	-	0/10/21/21	0/2/2/2
2	MOA	A	501	-	-	0/10/21/21	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	MOA	O2-C1	7.84	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MOA	O2-C1	7.65	1.46	1.36
2	A	501	MOA	C13-C12	7.22	1.52	1.39
2	D	501	MOA	C13-C12	7.06	1.51	1.39
2	D	501	MOA	C13-C14	7.05	1.51	1.39
2	D	501	MOA	C15-C14	6.45	1.49	1.40
2	C	501	MOA	C13-C12	6.11	1.50	1.39
2	B	501	MOA	C13-C12	5.78	1.49	1.39
2	A	501	MOA	C15-C14	5.77	1.48	1.40
2	B	501	MOA	C13-C14	5.31	1.48	1.39
2	C	501	MOA	O2-C1	5.27	1.43	1.36
2	C	501	MOA	C13-C14	5.19	1.48	1.39
2	A	501	MOA	C13-C14	5.14	1.48	1.39
2	B	501	MOA	C15-C14	4.96	1.47	1.40
2	B	501	MOA	C11-C12	4.73	1.48	1.40
2	B	501	MOA	O2-C1	4.60	1.42	1.36
2	C	501	MOA	C15-C14	4.59	1.47	1.40
2	D	501	MOA	C16-C15	4.53	1.50	1.41
2	C	501	MOA	C11-C12	4.45	1.47	1.40
2	A	501	MOA	C16-C15	4.38	1.50	1.41
2	D	501	MOA	C11-C12	4.35	1.47	1.40
2	A	501	MOA	C11-C12	4.17	1.47	1.40
2	B	501	MOA	C16-C11	3.69	1.46	1.39
2	C	501	MOA	C16-C11	3.61	1.46	1.39
2	D	501	MOA	C16-C11	3.47	1.45	1.39
2	C	501	MOA	C16-C15	3.38	1.48	1.41
2	A	501	MOA	C16-C11	3.12	1.45	1.39
2	B	501	MOA	C10-C11	2.71	1.53	1.50
2	C	501	MOA	C10-C11	2.67	1.53	1.50
2	B	501	MOA	C16-C15	2.47	1.46	1.41
2	D	501	MOA	C4-C3	2.11	1.55	1.51
2	D	501	MOA	C2-C3	2.10	1.38	1.33
2	C	501	MOA	C17-C14	2.04	1.53	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MOA	C15-C16-C11	9.52	127.45	121.85
2	C	501	MOA	C15-C16-C11	8.20	126.67	121.85
2	C	501	MOA	O2-C1-O1	6.52	128.08	121.13
2	A	501	MOA	C15-C16-C11	6.38	125.60	121.85
2	B	501	MOA	O2-C1-O1	6.00	127.53	121.13
2	C	501	MOA	C16-C11-C12	-5.68	117.60	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MOA	O1-C1-C16	-5.48	120.73	131.04
2	B	501	MOA	O1-C1-C16	-5.35	120.97	131.04
2	A	501	MOA	C14-C17-C2	-5.33	103.72	112.17
2	A	501	MOA	O2-C1-O1	4.91	126.37	121.13
2	D	501	MOA	C14-C17-C2	4.84	119.83	112.17
2	B	501	MOA	C16-C11-C12	-4.83	118.36	122.66
2	D	501	MOA	C17-C14-C15	-4.37	115.07	120.82
2	A	501	MOA	C9-C3-C4	4.23	122.39	115.27
2	D	501	MOA	C15-C16-C11	4.00	124.20	121.85
2	D	501	MOA	C11-C16-C1	-3.98	103.59	108.42
2	A	501	MOA	C16-C15-C14	-3.97	114.05	121.39
2	A	501	MOA	O1-C1-C16	-3.80	123.89	131.04
2	B	501	MOA	O2-C1-C16	3.79	111.33	108.26
2	D	501	MOA	O2-C1-O1	3.78	125.16	121.13
2	D	501	MOA	O1-C1-C16	-3.71	124.06	131.04
2	B	501	MOA	C16-C15-C14	-3.71	114.54	121.39
2	A	501	MOA	C11-C16-C1	-3.63	104.01	108.42
2	A	501	MOA	C4-C3-C2	-3.58	113.87	121.12
2	A	501	MOA	O3-C13-C12	3.51	123.75	118.83
2	C	501	MOA	O2-C1-C16	3.42	111.03	108.26
2	B	501	MOA	C14-C17-C2	-3.20	107.09	112.17
2	D	501	MOA	O2-C1-C16	3.12	110.79	108.26
2	D	501	MOA	C4-C5-C6	3.08	117.83	112.67
2	A	501	MOA	C7-C12-C13	3.07	126.01	121.30
2	A	501	MOA	C15-C14-C13	3.03	121.59	117.76
2	A	501	MOA	C10-C11-C16	3.01	112.13	107.88
2	C	501	MOA	O3-C13-C14	-2.92	113.57	118.83
2	C	501	MOA	C17-C2-C3	-2.87	122.78	127.24
2	D	501	MOA	C16-C15-C14	-2.87	116.08	121.39
2	D	501	MOA	C9-C3-C2	-2.85	116.36	123.68
2	D	501	MOA	C10-C11-C16	2.85	111.90	107.88
2	C	501	MOA	C14-C17-C2	-2.84	107.66	112.17
2	C	501	MOA	C16-C15-C14	-2.82	116.18	121.39
2	B	501	MOA	C11-C16-C1	-2.78	105.05	108.42
2	A	501	MOA	O3-C13-C14	-2.77	113.85	118.83
2	D	501	MOA	C7-C12-C13	2.62	125.33	121.30
2	A	501	MOA	C16-C11-C12	-2.37	120.55	122.66
2	B	501	MOA	C17-C2-C3	-2.37	123.57	127.24
2	C	501	MOA	C11-C16-C1	-2.31	105.62	108.42
2	C	501	MOA	C10-C11-C12	2.30	132.56	129.60
2	D	501	MOA	C16-C11-C12	-2.22	120.68	122.66
2	D	501	MOA	C15-C16-C1	2.21	132.21	129.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MOA	C17-C14-C15	-2.19	117.93	120.82
2	D	501	MOA	C7-C12-C11	-2.16	117.29	120.42
2	B	501	MOA	C4-C3-C2	2.14	125.44	121.12
2	C	501	MOA	O3-C13-C12	2.10	121.77	118.83
2	B	501	MOA	O3-C13-C14	-2.09	115.07	118.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

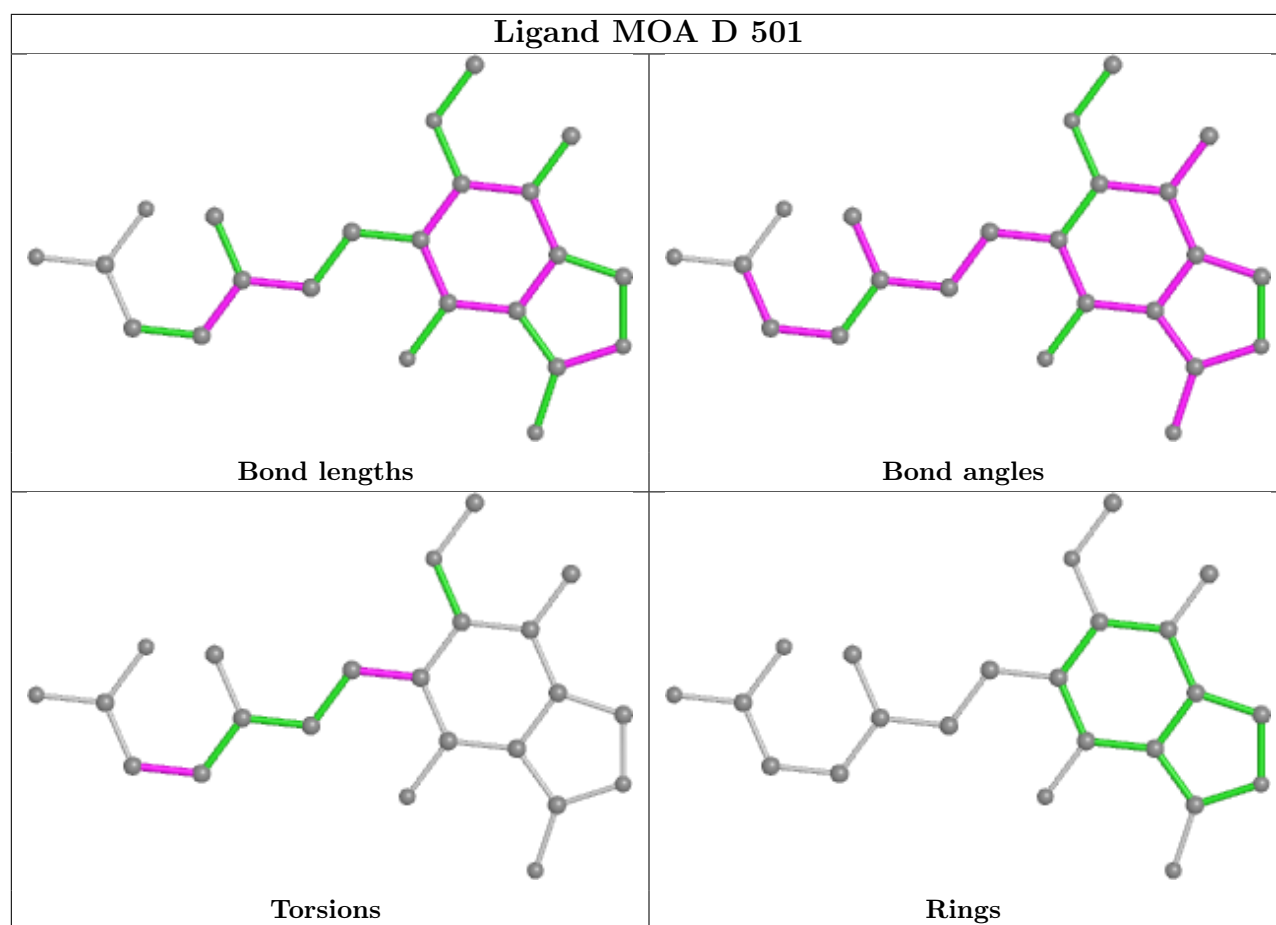
Mol	Chain	Res	Type	Atoms
2	D	501	MOA	C13-C14-C17-C2
2	D	501	MOA	C15-C14-C17-C2
2	D	501	MOA	C3-C4-C5-C6

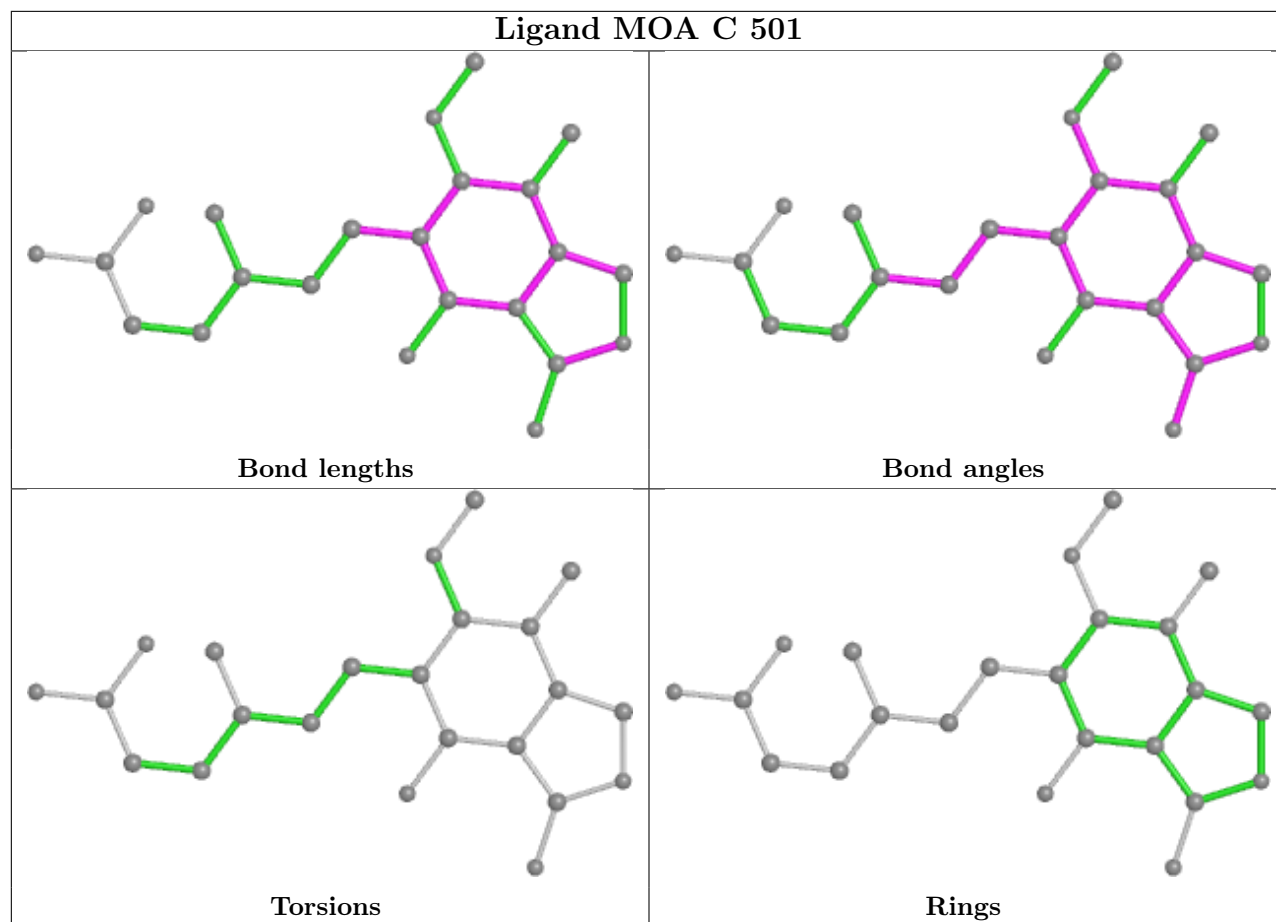
There are no ring outliers.

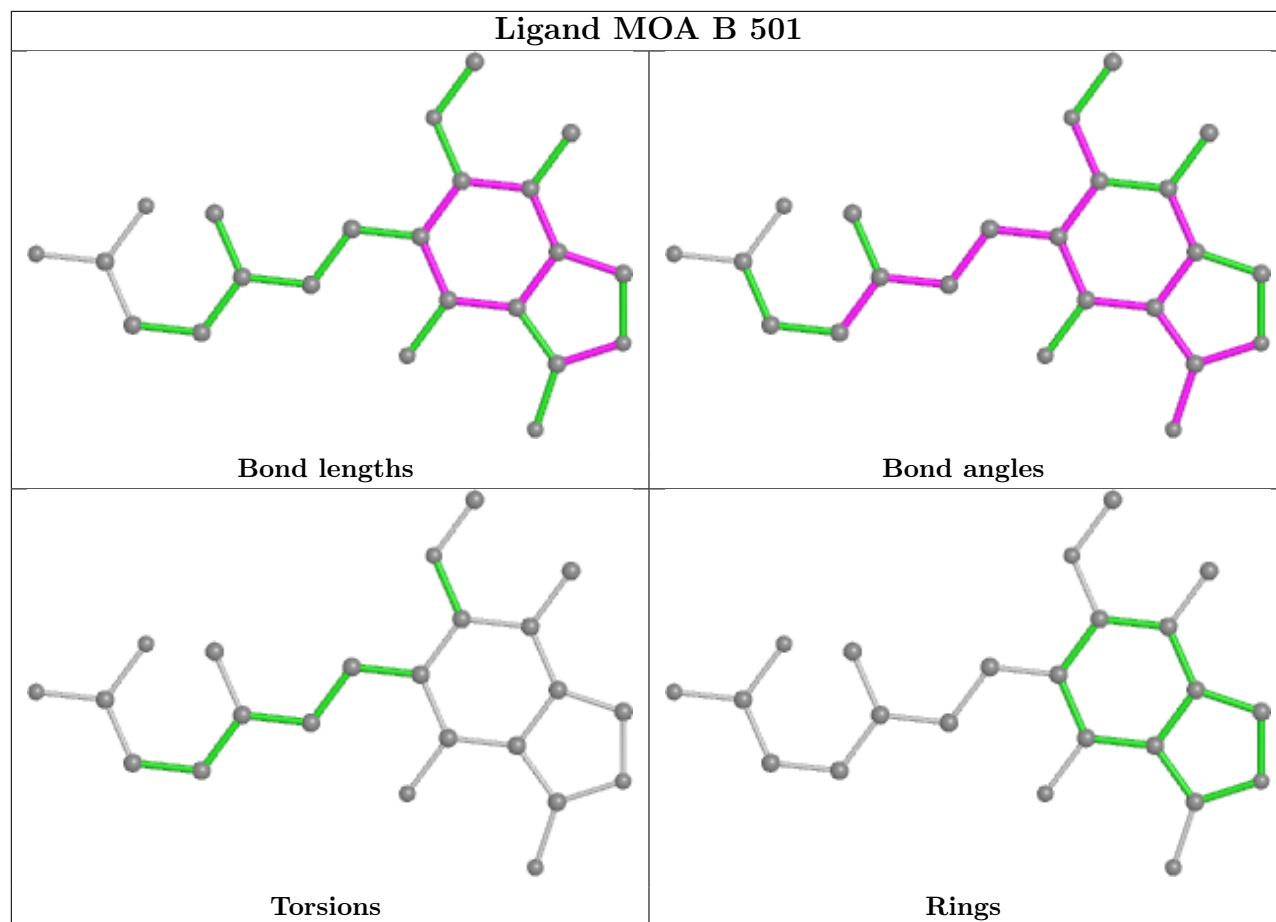
4 monomers are involved in 10 short contacts:

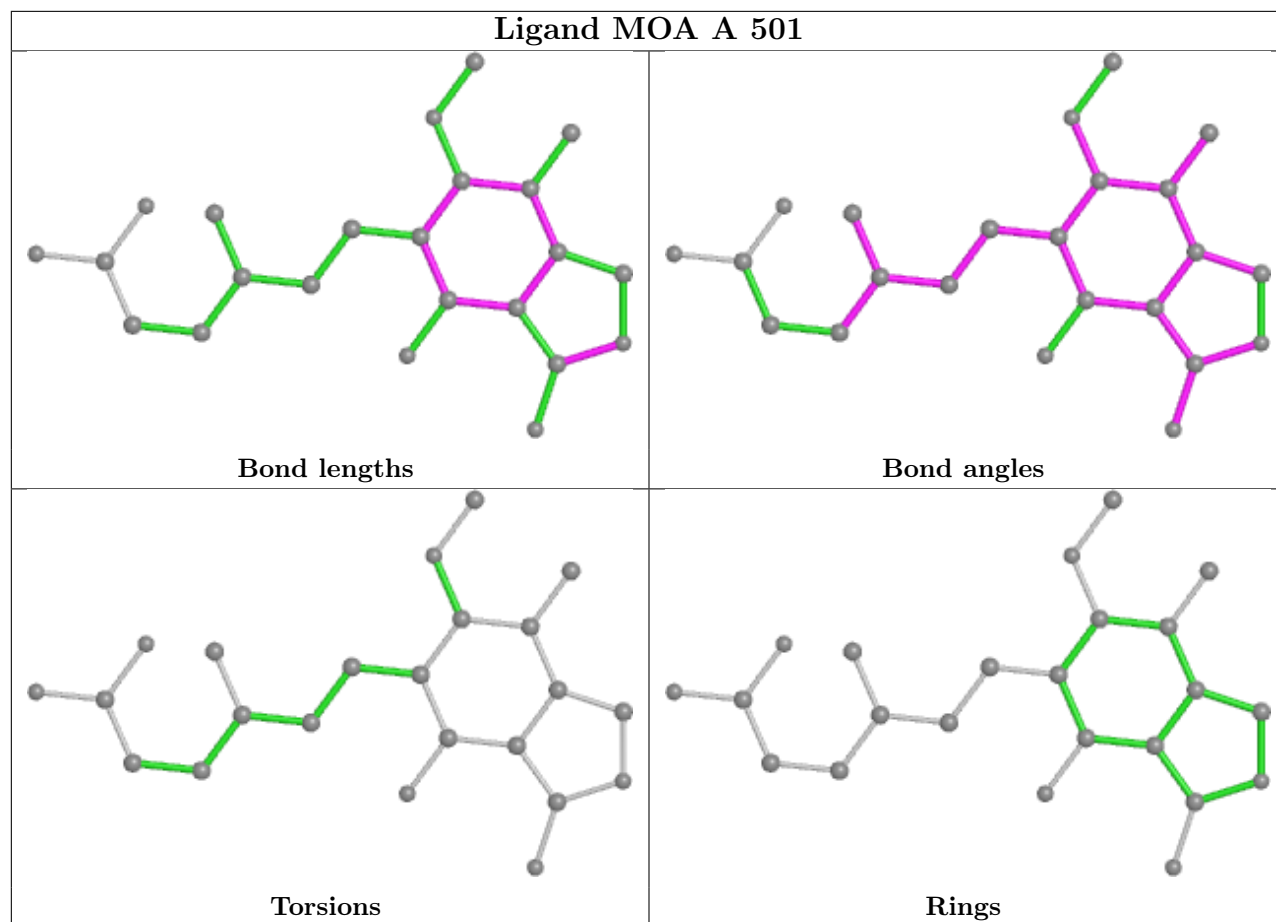
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	MOA	2	0
2	C	501	MOA	1	0
2	B	501	MOA	2	0
2	A	501	MOA	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [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	422/433 (97%)	0.12	23 (5%)	25 22	17, 24, 48, 76	0
1	B	418/433 (96%)	0.14	16 (3%)	40 37	16, 23, 48, 94	0
1	C	418/433 (96%)	0.05	15 (3%)	42 39	15, 23, 45, 86	0
1	D	420/433 (96%)	0.05	13 (3%)	49 46	16, 23, 43, 67	0
All	All	1678/1732 (96%)	0.09	67 (3%)	38 35	15, 24, 47, 94	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	6.9
1	C	4	GLU	5.8
1	B	276	LYS	5.1
1	A	4	GLU	4.7
1	A	360	LEU	4.5
1	D	4	GLU	4.5
1	D	423	GLY	4.4
1	A	361	PRO	4.3
1	A	359	VAL	4.2
1	C	45	GLY	4.1
1	B	3	THR	4.1
1	D	365	HIS	4.1
1	C	403	GLY	4.1
1	C	44	GLU	4.0
1	B	277	THR	3.9
1	A	276	LYS	3.9
1	D	360	LEU	3.8
1	D	403	GLY	3.7
1	A	44	GLU	3.5
1	D	206	ILE	3.5
1	C	5	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	276	LYS	3.4
1	C	276	LYS	3.4
1	B	403	GLY	3.3
1	A	403	GLY	3.2
1	C	46	PRO	3.2
1	A	363	PHE	3.2
1	A	46	PRO	3.2
1	B	248	THR	3.1
1	A	402	ASP	3.0
1	C	215	LEU	3.0
1	C	274	ASP	3.0
1	D	324	GLY	2.9
1	D	2	SER	2.9
1	B	44	GLU	2.9
1	B	208	GLN	2.9
1	D	185	TYR	2.9
1	C	277	THR	2.9
1	B	274	ASP	2.8
1	A	3	THR	2.7
1	C	3	THR	2.7
1	C	248	THR	2.7
1	A	79	SER	2.7
1	B	275	PRO	2.7
1	D	364	GLY	2.6
1	A	327	PHE	2.6
1	A	364	GLY	2.6
1	A	2	SER	2.5
1	C	208	GLN	2.4
1	A	45	GLY	2.4
1	C	279	ARG	2.4
1	A	365	HIS	2.4
1	D	275	PRO	2.4
1	B	279	ARG	2.3
1	B	204	ARG	2.3
1	A	392	GLN	2.3
1	B	402	ASP	2.3
1	A	396	GLN	2.2
1	A	395	ARG	2.2
1	B	271	ASN	2.2
1	A	397	TRP	2.2
1	A	399	GLU	2.1
1	C	402	ASP	2.1

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	2.1
1	D	359	VAL	2.1
1	B	45	GLY	2.1
1	A	206	ILE	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](#)

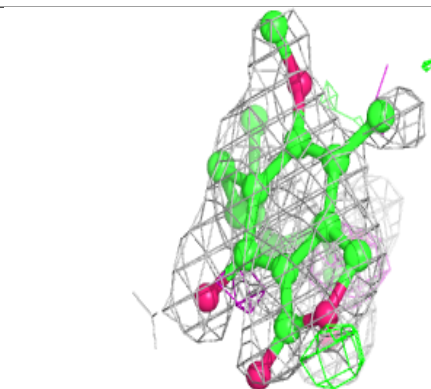
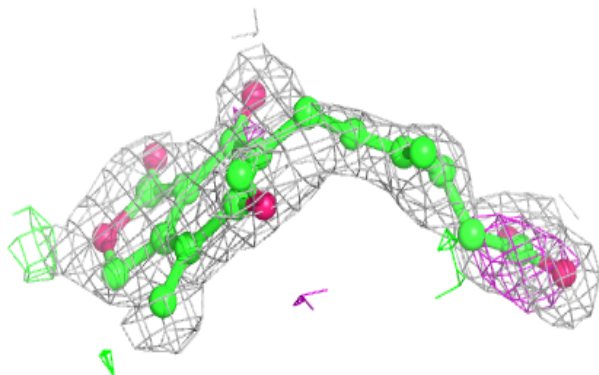
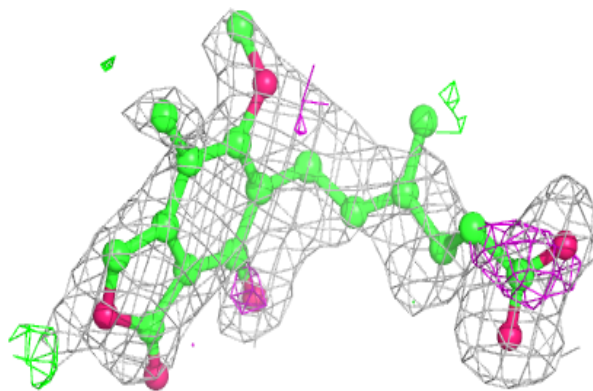
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MOA	A	501	23/23	0.83	0.22	20,52,60,68	0
2	MOA	D	501	23/23	0.84	0.24	20,57,63,70	0
2	MOA	B	501	23/23	0.93	0.10	21,30,35,38	0
2	MOA	C	501	23/23	0.94	0.11	21,28,34,38	0

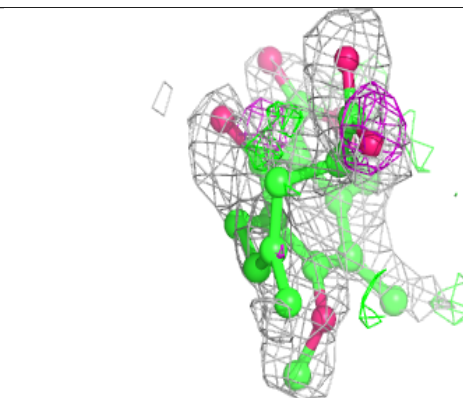
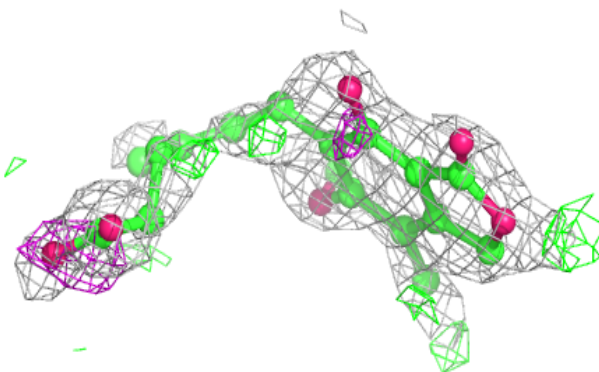
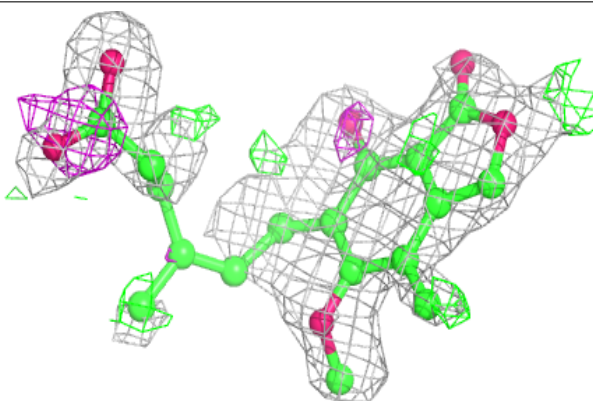
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around MOA A 501:**

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

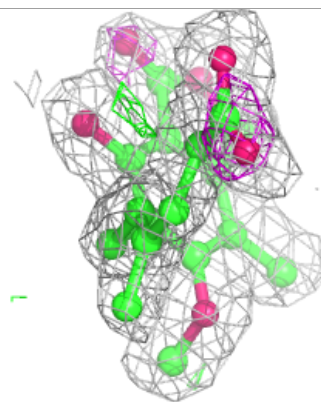
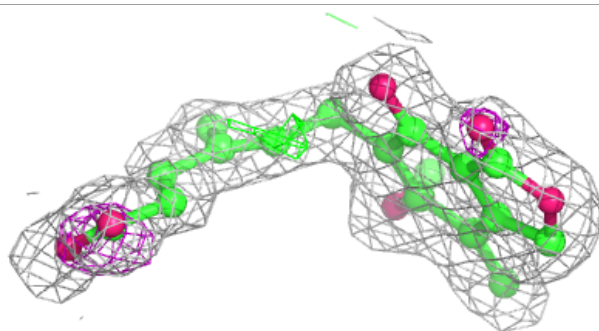
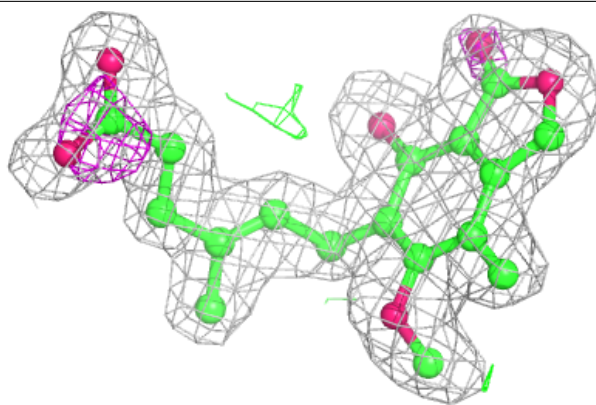
**Electron density around MOA D 501:**

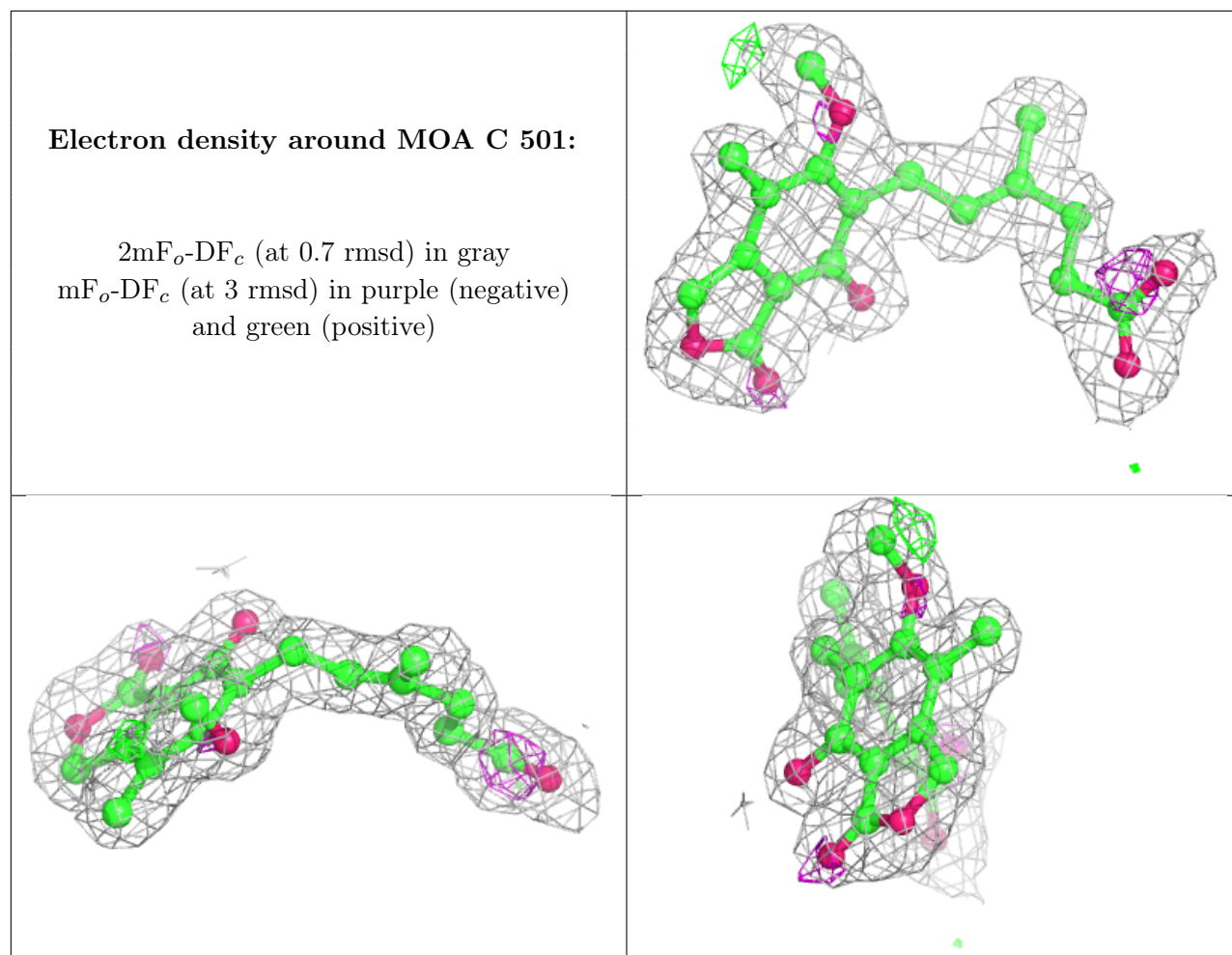
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MOA B 501:**

$2mF_o-DF_c$  (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.