



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:21 pm BST

PDB ID : 1P0Z  
Title : Sensor Kinase CitA binding domain  
Authors : Reinelt, S.; Hofmann, E.; Gerharz, T.; Bott, M.; Madden, D.R.  
Deposited on : 2003-04-11  
Resolution : 1.60 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

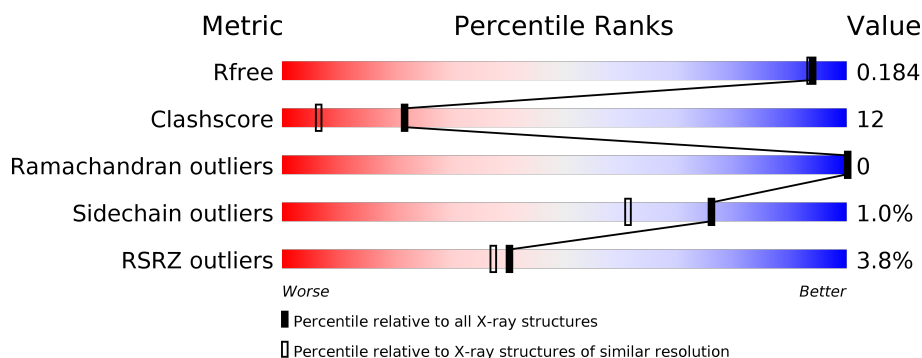
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	131	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	B	131	<div> <div>4%</div> <div>88%</div> <div>12%</div> </div>
1	C	131	<div> <div>%</div> <div>85%</div> <div>15%</div> <div>.</div> </div>
1	D	131	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	E	131	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>
1	F	131	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	131	
1	H	131	
1	I	131	
1	J	131	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MO7	B	1634	-	-	X	-
4	MO7	D	1642	-	-	X	-
4	MO7	F	1650	-	-	X	-
4	MO7	G	1654	-	-	X	-
4	MO7	H	1658	-	-	X	-
4	MO7	I	1662	-	-	X	-
4	MO7	J	1666	-	-	X	-
5	OMO	J	1667	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12523 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 Sensor kinase citA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	7	0
			1050	652	188	206	4			
1	B	131	Total	C	N	O	S	0	6	0
			1041	646	186	204	5			
1	C	131	Total	C	N	O	S	0	10	0
			1078	667	195	211	5			
1	D	131	Total	C	N	O	S	0	4	0
			1033	640	187	202	4			
1	E	131	Total	C	N	O	S	0	6	0
			1047	650	190	203	4			
1	F	131	Total	C	N	O	S	0	7	0
			1057	655	193	204	5			
1	G	131	Total	C	N	O	S	0	6	0
			1042	645	187	205	5			
1	H	131	Total	C	N	O	S	0	6	0
			1047	648	190	204	5			
1	I	131	Total	C	N	O	S	0	3	0
			1019	630	184	201	4			
1	J	131	Total	C	N	O	S	0	6	0
			1046	647	190	204	5			

There are 20 discrepancies between the modelled and reference sequences:

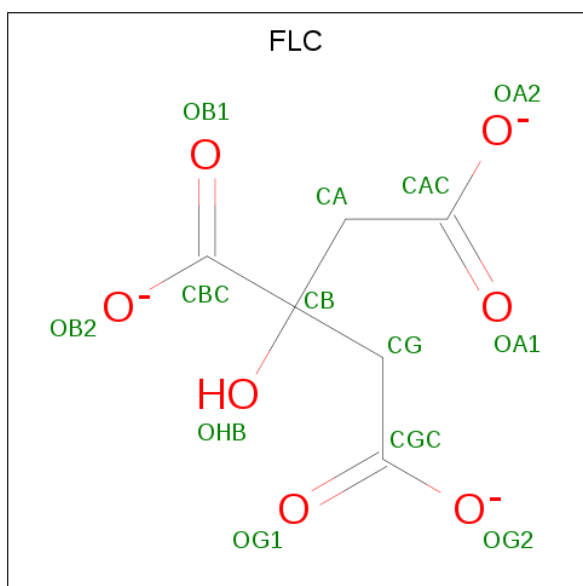
Chain	Residue	Modelled	Actual	Comment	Reference
A	134	HIS	ASN	EXPRESSION TAG	UNP P52687
A	135	HIS	TRP	EXPRESSION TAG	UNP P52687
B	134	HIS	ASN	EXPRESSION TAG	UNP P52687
B	135	HIS	TRP	EXPRESSION TAG	UNP P52687
C	134	HIS	ASN	EXPRESSION TAG	UNP P52687
C	135	HIS	TRP	EXPRESSION TAG	UNP P52687
D	134	HIS	ASN	EXPRESSION TAG	UNP P52687
D	135	HIS	TRP	EXPRESSION TAG	UNP P52687
E	134	HIS	ASN	EXPRESSION TAG	UNP P52687

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Chain	Residue	Modelled	Actual	Comment	Reference
E	135	HIS	TRP	EXPRESSION TAG	UNP P52687
F	134	HIS	ASN	EXPRESSION TAG	UNP P52687
F	135	HIS	TRP	EXPRESSION TAG	UNP P52687
G	134	HIS	ASN	EXPRESSION TAG	UNP P52687
G	135	HIS	TRP	EXPRESSION TAG	UNP P52687
H	134	HIS	ASN	EXPRESSION TAG	UNP P52687
H	135	HIS	TRP	EXPRESSION TAG	UNP P52687
I	134	HIS	ASN	EXPRESSION TAG	UNP P52687
I	135	HIS	TRP	EXPRESSION TAG	UNP P52687
J	134	HIS	ASN	EXPRESSION TAG	UNP P52687
J	135	HIS	TRP	EXPRESSION TAG	UNP P52687

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

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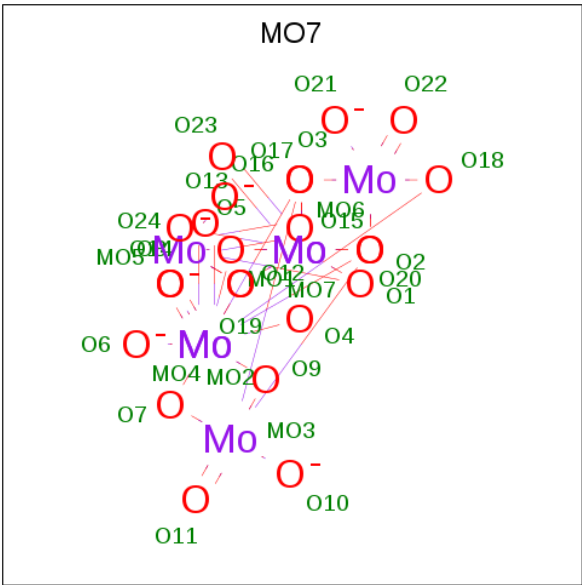
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

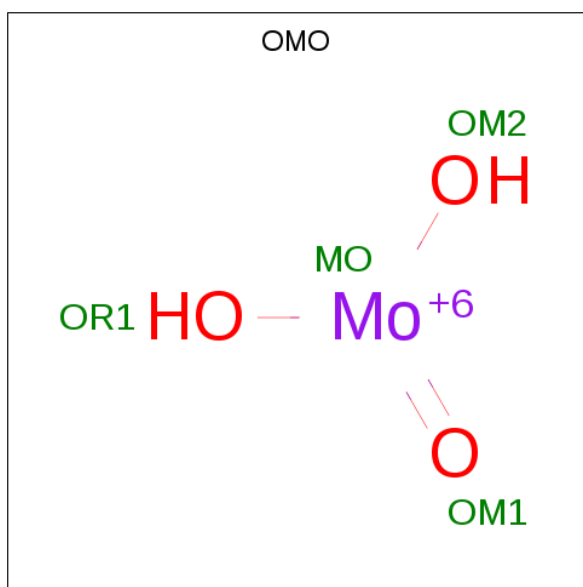
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Na	0	0
			1	1		
3	J	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	I	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is bis(mu4-oxo)-bis(mu3-oxo)-octakis(mu2-oxo)-dodecaoxo-heptamolybdenum (VI) (three-letter code: MO7) (formula: Mo<sub>7</sub>O<sub>24</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Mo	O	0	0
			31	7	24		
4	B	1	Total	Mo	O	0	0
			31	7	24		
4	C	1	Total	Mo	O	0	0
			31	7	24		
4	D	1	Total	Mo	O	0	0
			31	7	24		
4	E	1	Total	Mo	O	0	0
			31	7	24		
4	F	1	Total	Mo	O	0	0
			31	7	24		
4	G	1	Total	Mo	O	0	0
			31	7	24		
4	H	1	Total	Mo	O	0	0
			31	7	24		
4	I	1	Total	Mo	O	0	0
			31	7	24		
4	J	1	Total	Mo	O	0	0
			31	7	24		

- Molecule 5 is MO(VI)(=O)(OH)2 CLUSTER (three-letter code: OMO) (formula: H<sub>2</sub>MoO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Mo	O	0	0
			4	1	3		
5	B	1	Total	Mo	O	0	0
			4	1	3		
5	C	1	Total	Mo	O	0	0
			4	1	3		
5	D	1	Total	Mo	O	0	0
			4	1	3		
5	E	1	Total	Mo	O	0	0
			4	1	3		
5	F	1	Total	Mo	O	0	0
			4	1	3		
5	G	1	Total	Mo	O	0	0
			4	1	3		
5	H	1	Total	Mo	O	0	0
			4	1	3		
5	I	1	Total	Mo	O	0	0
			4	1	3		
5	J	1	Total	Mo	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	167	Total	O	0	0
			167	167		

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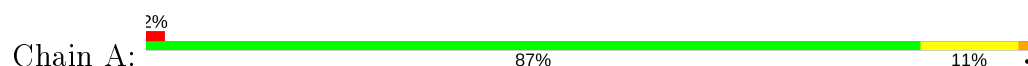
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	177	Total 177	O 177	0	0
6	D	193	Total 193	O 193	0	0
6	E	170	Total 170	O 170	0	0
6	F	172	Total 172	O 172	0	0
6	G	126	Total 126	O 126	0	0
6	H	139	Total 139	O 139	0	0
6	I	133	Total 133	O 133	0	0
6	J	123	Total 123	O 123	0	0

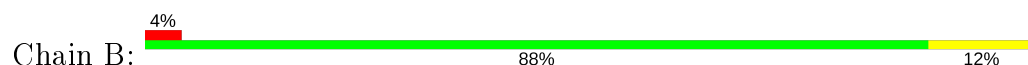
### 3 Residue-property plots [i](#)

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.

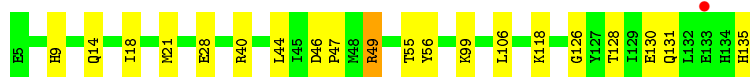
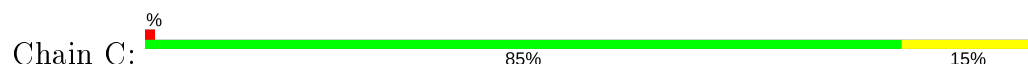
- Molecule 1: Sensor kinase citA



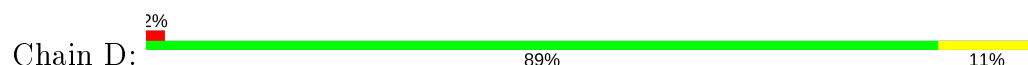
- Molecule 1: Sensor kinase citA



- Molecule 1: Sensor kinase citA



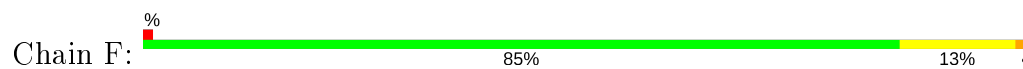
- Molecule 1: Sensor kinase citA



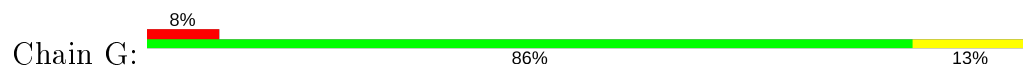
- Molecule 1: Sensor kinase citA



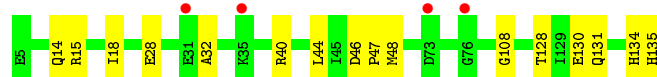
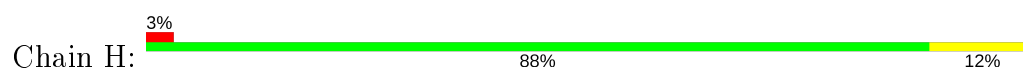
- Molecule 1: Sensor kinase citA



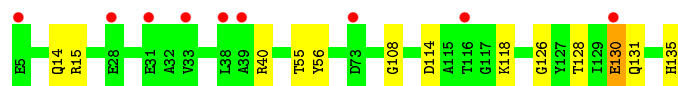
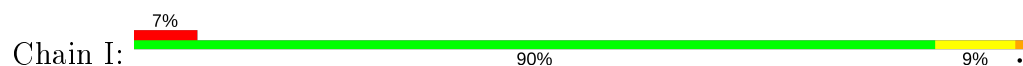
• Molecule 1: Sensor kinase citA



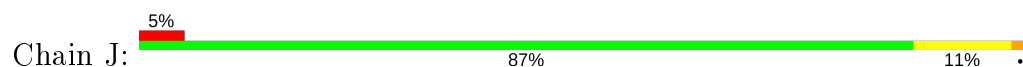
• Molecule 1: Sensor kinase citA



• Molecule 1: Sensor kinase citA



• Molecule 1: Sensor kinase citA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.61Å 84.33Å 97.71Å 112.83° 107.36° 93.74°	Depositor
Resolution (Å)	38.03 – 1.60 38.03 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (38.03-1.60) 96.0 (38.03-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.168 , 0.190 0.162 , 0.184	Depositor DCC
$R_{free}$ test set	6704 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FLC, MO7, OMO

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	0.65	0/1063	0.81	0/1432
1	B	0.71	0/1054	0.83	0/1419
1	C	0.73	0/1091	0.81	0/1468
1	D	0.69	0/1046	0.84	0/1408
1	E	0.64	0/1060	0.75	0/1426
1	F	0.70	0/1070	0.86	3/1439 (0.2%)
1	G	0.63	0/1055	0.75	0/1420
1	H	0.61	0/1060	0.75	1/1426 (0.1%)
1	I	0.64	0/1032	0.76	1/1391 (0.1%)
1	J	0.63	0/1059	0.78	0/1426
All	All	0.66	0/10590	0.79	5/14255 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	36	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	F	36	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	F	108	GLY	N-CA-C	-5.08	100.40	113.10
1	I	108	GLY	N-CA-C	-5.06	100.45	113.10
1	H	108	GLY	N-CA-C	-5.04	100.50	113.10

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1050	0	1052	23	0
1	B	1041	0	1043	17	0
1	C	1078	0	1078	20	0
1	D	1033	0	1034	18	0
1	E	1047	0	1055	13	0
1	F	1057	0	1063	21	0
1	G	1042	0	1040	24	0
1	H	1047	0	1048	18	0
1	I	1019	0	1017	11	0
1	J	1046	0	1048	28	0
2	A	13	0	4	0	0
2	B	13	0	4	0	0
2	C	13	0	4	0	0
2	D	13	0	4	0	0
2	E	13	0	4	0	0
2	F	13	0	4	0	0
2	G	13	0	4	0	0
2	H	13	0	4	0	0
2	I	13	0	4	0	0
2	J	13	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	31	0	0	6	0
4	B	31	0	0	7	0
4	C	31	0	0	6	0
4	D	31	0	0	8	0
4	E	31	0	0	5	0
4	F	31	0	0	7	0
4	G	31	0	0	7	0
4	H	31	0	0	7	0
4	I	31	0	0	7	0
4	J	31	0	0	7	0
5	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	4	0	0	0	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
5	G	4	0	0	0	0
5	H	4	0	0	0	0
5	I	4	0	0	1	0
5	J	4	0	0	2	0
6	A	173	0	0	9	0
6	B	167	0	0	5	0
6	C	177	0	0	11	0
6	D	193	0	0	7	0
6	E	170	0	0	4	0
6	F	172	0	0	10	0
6	G	126	0	0	10	0
6	H	139	0	0	7	0
6	I	133	0	0	3	0
6	J	123	0	0	9	0
All	All	12523	0	10518	257	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 12.

All (257) 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:D:49[B]:ARG:HD3	6:D:1780:HOH:O	1.50	1.10
1:H:131:GLN:HG3	6:H:1792:HOH:O	1.58	1.03
1:A:42:LYS:HE2	6:A:1802:HOH:O	1.62	0.98
1:H:128[B]:THR:HG21	1:H:131:GLN:NE2	1.81	0.94
1:A:80:GLU:HG3	6:A:1799:HOH:O	1.72	0.87
1:G:22[B]:GLN:HG3	6:G:1693:HOH:O	1.74	0.87
1:G:128[B]:THR:HG21	1:G:131:GLN:NE2	1.93	0.83
1:C:99[A]:LYS:HE3	6:C:1790:HOH:O	1.78	0.83
1:J:49[B]:ARG:HH11	1:J:49[B]:ARG:HG2	1.44	0.82
1:G:128[B]:THR:HG21	1:G:131:GLN:CD	2.04	0.78
4:B:1634:MO7:O11	4:B:1634:MO7:MO3	1.56	0.76
4:C:1638:MO7:MO2	4:C:1638:MO7:O6	1.57	0.76
1:I:130:GLU:OE1	1:I:131:GLN:HG3	1.87	0.75
4:F:1650:MO7:O6	4:F:1650:MO7:MO2	1.57	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:1666:MO7:O1	4:J:1666:MO7:MO1	1.58	0.75
1:F:9:HIS:HB2	1:F:106[B]:LEU:HD11	1.69	0.75
1:C:40[A]:ARG:HD2	6:C:1764:HOH:O	1.87	0.74
1:I:14:GLN:NE2	6:I:1717:HOH:O	2.21	0.74
4:J:1666:MO7:MO6	4:J:1666:MO7:O21	1.58	0.74
4:C:1638:MO7:MO6	4:C:1638:MO7:O21	1.59	0.73
4:H:1658:MO7:O21	4:H:1658:MO7:MO6	1.60	0.73
1:J:72:PRO:HA	1:J:75[B]:ILE:HD13	1.71	0.73
4:I:1662:MO7:MO1	4:I:1662:MO7:O1	1.60	0.73
1:E:131:GLN:HG2	6:E:1797:HOH:O	1.89	0.72
4:D:1642:MO7:O21	4:D:1642:MO7:MO6	1.60	0.72
1:G:49:ARG:HD3	6:G:1730:HOH:O	1.87	0.72
4:A:1630:MO7:MO1	4:A:1630:MO7:O1	1.62	0.71
4:G:1654:MO7:O10	4:G:1654:MO7:MO3	1.60	0.71
4:I:1662:MO7:O21	4:I:1662:MO7:MO6	1.61	0.71
1:D:14:GLN:NE2	6:D:1726:HOH:O	2.24	0.70
1:G:128[B]:THR:HG23	1:G:131:GLN:HB2	1.72	0.70
4:J:1666:MO7:O6	4:J:1666:MO7:MO2	1.62	0.70
4:J:1666:MO7:O10	4:J:1666:MO7:MO3	1.61	0.70
4:G:1654:MO7:O21	4:G:1654:MO7:MO6	1.63	0.70
4:D:1642:MO7:O1	4:D:1642:MO7:MO1	1.61	0.70
1:D:49[A]:ARG:HG3	6:D:1787:HOH:O	1.92	0.70
4:H:1658:MO7:O6	4:H:1658:MO7:MO2	1.61	0.70
4:F:1650:MO7:O1	4:F:1650:MO7:MO1	1.63	0.70
4:F:1650:MO7:O21	4:F:1650:MO7:MO6	1.61	0.70
1:A:112[B]:ILE:HD11	1:A:123:VAL:HG23	1.73	0.69
4:C:1638:MO7:O1	4:C:1638:MO7:MO1	1.62	0.69
1:J:49[B]:ARG:HG2	1:J:49[B]:ARG:NH1	2.07	0.69
4:A:1630:MO7:MO6	4:A:1630:MO7:O21	1.63	0.69
1:H:134:HIS:CD2	6:H:1780:HOH:O	2.45	0.69
4:G:1654:MO7:O1	4:G:1654:MO7:MO1	1.62	0.69
4:A:1630:MO7:MO2	4:A:1630:MO7:O6	1.64	0.69
5:B:1635:OMO:OR1	5:B:1635:OMO:MO	1.64	0.69
1:B:134:HIS:HE1	6:B:1792:HOH:O	1.74	0.69
4:J:1666:MO7:O16	4:J:1666:MO7:MO5	1.63	0.69
1:J:28:GLU:CD	1:J:28:GLU:H	1.96	0.69
1:B:55:THR:HG21	1:B:128[B]:THR:HG23	1.76	0.68
1:B:130:GLU:OE1	1:B:131:GLN:HG3	1.92	0.68
4:I:1662:MO7:O6	4:I:1662:MO7:MO2	1.63	0.68
4:I:1662:MO7:O10	4:I:1662:MO7:MO3	1.65	0.68
4:H:1658:MO7:MO1	4:H:1658:MO7:O1	1.65	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1658:MO7:O10	4:H:1658:MO7:MO3	1.63	0.68
1:B:55:THR:HG21	1:B:128[B]:THR:CG2	2.25	0.67
4:G:1654:MO7:O16	4:G:1654:MO7:MO5	1.65	0.67
4:D:1642:MO7:MO2	4:D:1642:MO7:O6	1.65	0.67
4:B:1634:MO7:MO6	4:B:1634:MO7:O22	1.66	0.66
4:B:1634:MO7:MO6	4:B:1634:MO7:O21	1.66	0.66
5:F:1651:OMO:OM2	5:F:1651:OMO:MO	1.67	0.66
1:J:131:GLN:HG3	6:J:1792:HOH:O	1.96	0.65
4:I:1662:MO7:O16	4:I:1662:MO7:MO5	1.68	0.65
1:J:15:ARG:HD3	6:J:1786:HOH:O	1.97	0.65
4:G:1654:MO7:O6	4:G:1654:MO7:MO2	1.67	0.65
1:C:55:THR:HG21	1:C:128[B]:THR:HG23	1.79	0.65
1:D:49[A]:ARG:NE	1:D:70:VAL:HG12	2.12	0.65
5:J:1667:OMO:OM2	5:J:1667:OMO:MO	1.68	0.65
4:E:1646:MO7:MO6	4:E:1646:MO7:O21	1.67	0.65
4:F:1650:MO7:O10	4:F:1650:MO7:MO3	1.68	0.65
4:C:1638:MO7:MO3	4:C:1638:MO7:O10	1.65	0.65
4:C:1638:MO7:O15	4:C:1638:MO7:MO5	1.68	0.65
4:B:1634:MO7:O1	4:B:1634:MO7:MO1	1.68	0.64
1:A:134:HIS:HE1	6:A:1767:HOH:O	1.80	0.64
1:F:14:GLN:NE2	6:F:1699:HOH:O	2.30	0.64
1:H:14:GLN:NE2	6:H:1746:HOH:O	2.30	0.64
5:C:1639:OMO:OM2	5:C:1639:OMO:MO	1.68	0.64
1:B:7:ARG:HD2	6:B:1769:HOH:O	1.97	0.64
1:H:128[B]:THR:CG2	1:H:131:GLN:HB2	2.28	0.63
4:E:1646:MO7:O11	4:E:1646:MO7:MO3	1.70	0.63
1:F:133:GLU:HG3	6:F:1786:HOH:O	1.97	0.63
1:A:28:GLU:OE2	1:A:40:ARG:NH2	2.31	0.63
1:A:24:SER:HB2	1:A:112[B]:ILE:HD13	1.81	0.62
4:E:1646:MO7:MO1	4:E:1646:MO7:O1	1.68	0.62
4:E:1646:MO7:O6	4:E:1646:MO7:MO2	1.69	0.62
1:H:128[B]:THR:HG21	1:H:131:GLN:CD	2.20	0.62
4:B:1634:MO7:MO2	4:B:1634:MO7:O6	1.71	0.62
1:H:128[B]:THR:HG23	1:H:131:GLN:HB2	1.80	0.62
4:H:1658:MO7:O16	4:H:1658:MO7:MO5	1.71	0.62
4:H:1658:MO7:O11	4:H:1658:MO7:MO3	1.71	0.62
1:C:49:ARG:HH11	1:C:49:ARG:HG2	1.64	0.62
1:F:135:HIS:HE1	6:F:1772:HOH:O	1.82	0.62
4:B:1634:MO7:MO4	4:B:1634:MO7:O13	1.70	0.62
1:J:128[A]:THR:HG21	6:J:1773:HOH:O	1.99	0.62
4:D:1642:MO7:O10	4:D:1642:MO7:MO3	1.70	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1667:OMO:MO	5:J:1667:OMO:OM1	1.71	0.61
4:D:1642:MO7:O11	4:D:1642:MO7:MO3	1.72	0.61
1:D:49[A]:ARG:CZ	1:D:70:VAL:HG12	2.30	0.61
4:G:1654:MO7:O11	4:G:1654:MO7:MO3	1.70	0.61
5:A:1631:OMO:MO	5:A:1631:OMO:OR1	1.71	0.61
4:A:1630:MO7:O10	4:A:1630:MO7:MO3	1.72	0.61
4:D:1642:MO7:O16	4:D:1642:MO7:MO5	1.72	0.61
4:F:1650:MO7:O16	4:F:1650:MO7:MO5	1.71	0.61
1:D:128[B]:THR:HG21	6:D:1712:HOH:O	2.00	0.61
5:I:1663:OMO:MO	5:I:1663:OMO:OM2	1.70	0.61
4:B:1634:MO7:O10	4:B:1634:MO7:MO3	1.72	0.61
1:H:134:HIS:HD2	6:H:1780:HOH:O	1.83	0.60
1:E:92[B]:LYS:HE2	6:G:1672:HOH:O	2.01	0.60
5:E:1647:OMO:MO	5:E:1647:OMO:OR1	1.72	0.60
4:F:1650:MO7:O15	4:F:1650:MO7:MO5	1.72	0.60
4:A:1630:MO7:MO3	4:A:1630:MO7:O11	1.72	0.60
4:A:1630:MO7:MO5	4:A:1630:MO7:O16	1.73	0.60
1:A:55:THR:HG21	1:A:128[B]:THR:HG23	1.83	0.60
4:C:1638:MO7:MO7	4:C:1638:MO7:O24	1.72	0.60
4:D:1642:MO7:O15	4:D:1642:MO7:MO5	1.73	0.60
1:G:48[A]:MET:HE1	6:G:1775:HOH:O	2.02	0.59
1:J:14:GLN:NE2	6:J:1744:HOH:O	2.35	0.59
1:E:49:ARG:HG2	6:E:1734:HOH:O	2.02	0.59
4:I:1662:MO7:MO5	4:I:1662:MO7:O15	1.73	0.59
1:J:49[B]:ARG:NH2	1:J:55:THR:O	2.36	0.59
1:B:49:ARG:HD3	1:B:68:TYR:OH	2.03	0.59
1:J:132:LEU:HB2	6:J:1780:HOH:O	2.03	0.59
4:J:1666:MO7:O15	4:J:1666:MO7:MO5	1.73	0.59
1:C:135:HIS:HE1	6:C:1805:HOH:O	1.85	0.58
1:A:14:GLN:NE2	6:A:1762:HOH:O	2.36	0.57
1:G:48[A]:MET:HA	1:G:48[A]:MET:CE	2.35	0.57
1:C:14:GLN:NE2	6:C:1808:HOH:O	2.38	0.57
1:J:128[B]:THR:OG1	1:J:131:GLN:HB2	2.05	0.56
1:H:32:ALA:HB2	1:H:40:ARG:HG3	1.87	0.56
1:F:131:GLN:NE2	6:F:1820:HOH:O	2.29	0.56
1:C:9:HIS:HB2	1:C:106[B]:LEU:HD11	1.87	0.56
1:F:55:THR:HG21	1:F:128[B]:THR:HG23	1.87	0.56
1:C:21[A]:MET:HE3	6:C:1813:HOH:O	2.05	0.56
1:I:114:ASP:OD2	1:I:118:LYS:HE2	2.06	0.56
1:J:49[B]:ARG:HG2	6:J:1751:HOH:O	2.05	0.56
1:J:75[B]:ILE:N	1:J:75[B]:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:HA	1:A:112[B]:ILE:CD1	2.37	0.54
1:A:55:THR:HG21	1:A:128[B]:THR:CG2	2.36	0.54
1:H:48[A]:MET:HA	1:H:48[A]:MET:CE	2.38	0.54
1:I:15:ARG:HD2	6:I:1711:HOH:O	2.08	0.54
1:A:112[B]:ILE:HD11	1:A:123:VAL:CG2	2.37	0.54
1:H:15[A]:ARG:HD2	6:H:1762:HOH:O	2.07	0.54
1:J:48[A]:MET:HE2	1:J:48[A]:MET:HA	1.90	0.54
1:G:49:ARG:CZ	1:G:70:VAL:HG12	2.37	0.54
1:A:26:MET:CE	6:A:1805:HOH:O	2.56	0.54
1:A:49:ARG:HD3	6:A:1753:HOH:O	2.07	0.53
1:A:49:ARG:CD	6:A:1752:HOH:O	2.56	0.53
1:E:9:HIS:HB2	1:E:106[B]:LEU:CD1	2.39	0.53
1:J:135:HIS:HD2	4:J:1666:MO7:O3	1.91	0.53
1:G:128[B]:THR:CG2	1:G:131:GLN:HB2	2.38	0.53
1:F:131:GLN:NE2	6:F:1777:HOH:O	2.41	0.52
1:C:28:GLU:CD	1:C:28:GLU:H	2.12	0.52
1:H:128[A]:THR:HG21	6:H:1782:HOH:O	2.10	0.52
1:E:128[B]:THR:HG21	6:E:1810:HOH:O	2.09	0.52
1:A:24:SER:CB	1:A:112[B]:ILE:HD13	2.40	0.52
1:D:134:HIS:CE1	6:D:1830:HOH:O	2.63	0.52
1:E:9:HIS:HB2	1:E:106[B]:LEU:HD11	1.91	0.51
1:C:44:LEU:HG	6:C:1764:HOH:O	2.11	0.51
1:G:14:GLN:NE2	6:G:1711:HOH:O	2.43	0.51
1:G:48[A]:MET:HE2	1:G:48[A]:MET:HA	1.92	0.51
1:A:49:ARG:HD3	6:A:1752:HOH:O	2.10	0.51
1:F:49:ARG:HG3	1:F:49:ARG:NH1	2.26	0.51
1:A:26:MET:HE1	6:A:1805:HOH:O	2.11	0.51
1:H:135:HIS:HE1	6:H:1778:HOH:O	1.93	0.51
1:G:28:GLU:CD	1:G:28:GLU:H	2.14	0.51
1:I:40:ARG:HD3	6:I:1736:HOH:O	2.11	0.51
1:A:130:GLU:OE2	1:A:131:GLN:HG3	2.11	0.50
1:J:14:GLN:O	1:J:18:ILE:HG12	2.12	0.50
1:B:128[B]:THR:HG21	6:B:1693:HOH:O	2.11	0.50
1:C:18[B]:ILE:HD12	6:C:1742:HOH:O	2.10	0.49
1:J:134:HIS:CE1	6:J:1780:HOH:O	2.65	0.49
1:F:40[B]:ARG:NH2	6:F:1769:HOH:O	2.45	0.49
1:E:135:HIS:HD2	4:E:1646:MO7:O3	1.95	0.49
1:J:28:GLU:CD	1:J:28:GLU:N	2.65	0.48
1:G:128[B]:THR:CG2	1:G:131:GLN:CD	2.81	0.48
1:J:49[B]:ARG:HE	1:J:70:VAL:CG1	2.27	0.48
1:F:28:GLU:OE1	1:F:40[A]:ARG:NH2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:THR:HG21	1:J:128[B]:THR:HG23	1.94	0.48
1:A:106[B]:LEU:HD23	1:A:106[B]:LEU:HA	1.79	0.47
1:A:24:SER:CA	1:A:112[B]:ILE:HD13	2.44	0.47
1:G:134:HIS:NE2	6:G:1737:HOH:O	2.35	0.47
1:D:46:ASP:HB2	1:D:47:PRO:HD3	1.97	0.47
1:F:49:ARG:HG2	6:F:1753:HOH:O	2.14	0.47
1:D:49[A]:ARG:HD2	1:D:70:VAL:CG1	2.45	0.47
1:F:9:HIS:HB2	1:F:106[B]:LEU:CD1	2.41	0.47
1:G:128[A]:THR:HG21	6:G:1773:HOH:O	2.15	0.47
1:B:73:ASP:OD1	1:D:36:ARG:HD2	2.15	0.47
1:I:55:THR:HG21	1:I:128[B]:THR:HG23	1.97	0.46
1:D:135:HIS:HD2	4:D:1642:MO7:O3	1.97	0.46
1:E:49:ARG:HD2	1:E:70:VAL:HG12	1.97	0.46
1:E:18[B]:ILE:O	1:E:18[B]:ILE:HD13	2.16	0.46
1:C:131:GLN:HG2	6:C:1767:HOH:O	2.15	0.46
1:E:46:ASP:N	1:E:47:PRO:HD2	2.31	0.46
1:J:49[B]:ARG:HE	1:J:70:VAL:HG12	1.80	0.46
1:B:9:HIS:HB2	1:B:106[B]:LEU:CD1	2.46	0.46
1:D:49[B]:ARG:HD2	6:D:1787:HOH:O	2.16	0.46
1:D:56:TYR:CZ	1:D:126:GLY:HA3	2.51	0.45
1:I:128[B]:THR:OG1	1:I:131:GLN:HB2	2.15	0.45
1:G:15:ARG:HD3	6:G:1770:HOH:O	2.16	0.45
1:G:135:HIS:HD2	4:G:1654:MO7:O3	1.99	0.45
1:D:31:GLU:HA	1:D:34:GLN:HE21	1.80	0.45
1:F:18[A]:ILE:HD12	6:F:1763:HOH:O	2.16	0.45
1:I:130:GLU:CD	1:I:131:GLN:HG3	2.35	0.45
1:H:14:GLN:O	1:H:18:ILE:HG12	2.17	0.45
1:J:48[A]:MET:CE	1:J:48[A]:MET:HA	2.46	0.45
1:F:15[B]:ARG:HD2	6:F:1727:HOH:O	2.16	0.44
1:H:28:GLU:H	1:H:28:GLU:CD	2.20	0.44
1:G:52:SER:O	6:G:1727:HOH:O	2.21	0.44
1:E:14:GLN:NE2	6:E:1722:HOH:O	2.51	0.44
1:F:31:GLU:HG2	1:F:40[B]:ARG:HH12	1.83	0.44
1:C:55:THR:HG21	1:C:128[B]:THR:CG2	2.46	0.44
1:F:135:HIS:HD2	4:F:1650:MO7:O3	2.01	0.44
1:B:74:GLU:HA	1:B:74:GLU:OE1	2.18	0.43
1:G:56:TYR:CZ	1:G:126:GLY:HA3	2.54	0.43
1:B:14:GLN:NE2	6:B:1703:HOH:O	2.50	0.43
1:C:40[A]:ARG:NH1	6:C:1764:HOH:O	2.50	0.43
1:C:56:TYR:CZ	1:C:126:GLY:HA3	2.54	0.43
1:F:55:THR:HG21	1:F:128[B]:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:HA	1:A:112[B]:ILE:HD13	2.01	0.43
1:H:46:ASP:N	1:H:47:PRO:CD	2.82	0.43
1:B:106[B]:LEU:HA	1:B:106[B]:LEU:HD23	1.83	0.42
1:C:128[B]:THR:HG21	6:C:1691:HOH:O	2.18	0.42
1:F:49:ARG:HG3	1:F:49:ARG:HH11	1.83	0.42
1:F:130:GLU:OE1	1:F:131:GLN:HG2	2.19	0.42
1:F:56:TYR:CZ	1:F:126:GLY:HA3	2.54	0.42
1:D:55:THR:HG21	1:D:128[B]:THR:HG23	2.01	0.42
1:B:71:ASN:HA	1:B:72:PRO:HD2	1.83	0.42
1:J:132:LEU:O	6:J:1780:HOH:O	2.20	0.42
1:J:128[A]:THR:CG2	6:J:1773:HOH:O	2.65	0.42
1:B:73:ASP:OD2	1:D:36:ARG:HD2	2.20	0.42
1:C:28:GLU:CD	1:C:28:GLU:N	2.73	0.42
1:E:18[B]:ILE:CD1	1:E:22:GLN:CD	2.89	0.42
1:E:28:GLU:H	1:E:28:GLU:CD	2.24	0.42
1:J:56:TYR:CZ	1:J:126:GLY:HA3	2.55	0.42
1:I:56:TYR:CZ	1:I:126:GLY:HA3	2.55	0.41
1:G:99:LYS:HA	1:G:104:SER:HA	2.03	0.41
1:J:49[B]:ARG:NH1	1:J:49[B]:ARG:CG	2.80	0.41
1:B:73:ASP:CG	1:D:36:ARG:HD2	2.41	0.41
1:A:116:THR:HG22	1:G:116:THR:HA	2.02	0.41
1:H:135:HIS:HD2	4:H:1658:MO7:O3	2.03	0.41
1:I:114:ASP:C	1:I:114:ASP:OD1	2.58	0.41
1:C:106[A]:LEU:HA	1:C:106[A]:LEU:HD12	1.94	0.41
1:G:128[B]:THR:HG23	1:G:131:GLN:CB	2.47	0.41
1:J:72:PRO:O	1:J:75[B]:ILE:HD13	2.21	0.41
1:I:135:HIS:HD2	4:I:1662:MO7:O3	2.04	0.41
1:C:118:LYS:HE2	6:C:1713:HOH:O	2.20	0.41
1:B:21[A]:MET:HE3	6:B:1759:HOH:O	2.20	0.41
1:C:46:ASP:HB2	1:C:47:PRO:HD3	2.01	0.41
1:G:49:ARG:HG2	6:G:1730:HOH:O	2.20	0.41
1:B:55:THR:HG21	1:B:128[B]:THR:HG21	1.98	0.41
1:J:75[B]:ILE:N	1:J:75[B]:ILE:CD1	2.84	0.41
1:H:44:LEU:O	1:H:47:PRO:HD2	2.20	0.40
1:F:133:GLU:CG	6:F:1786:HOH:O	2.65	0.40
1:A:116:THR:O	1:A:116:THR:HG22	2.21	0.40
1:D:49[B]:ARG:CD	6:D:1780:HOH:O	2.33	0.40
1:G:130:GLU:HG3	1:G:131:GLN:HG3	2.03	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	136/131 (104%)	135 (99%)	1 (1%)	0	100	100
1	B	135/131 (103%)	134 (99%)	1 (1%)	0	100	100
1	C	139/131 (106%)	138 (99%)	1 (1%)	0	100	100
1	D	133/131 (102%)	133 (100%)	0	0	100	100
1	E	135/131 (103%)	135 (100%)	0	0	100	100
1	F	136/131 (104%)	135 (99%)	1 (1%)	0	100	100
1	G	135/131 (103%)	135 (100%)	0	0	100	100
1	H	135/131 (103%)	135 (100%)	0	0	100	100
1	I	132/131 (101%)	131 (99%)	1 (1%)	0	100	100
1	J	135/131 (103%)	135 (100%)	0	0	100	100
All	All	1351/1310 (103%)	1346 (100%)	5 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/108 (106%)	112 (98%)	2 (2%)	59	36
1	B	113/108 (105%)	113 (100%)	0	100	100
1	C	117/108 (108%)	115 (98%)	2 (2%)	60	38
1	D	111/108 (103%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	113/108 (105%)	113 (100%)	0	100	100
1	F	114/108 (106%)	112 (98%)	2 (2%)	59	36
1	G	113/108 (105%)	112 (99%)	1 (1%)	78	65
1	H	113/108 (105%)	112 (99%)	1 (1%)	78	65
1	I	110/108 (102%)	109 (99%)	1 (1%)	78	65
1	J	113/108 (105%)	110 (97%)	3 (3%)	44	20
All	All	1131/1080 (105%)	1119 (99%)	12 (1%)	76	57

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	130	GLU
1	C	49	ARG
1	C	130	GLU
1	F	49	ARG
1	F	130	GLU
1	G	15	ARG
1	H	130	GLU
1	I	130	GLU
1	J	15	ARG
1	J	49[A]	ARG
1	J	49[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	B	131	GLN
1	B	135	HIS
1	C	11	GLN
1	C	34	GLN
1	C	135	HIS
1	D	34	GLN
1	D	135	HIS
1	E	135	HIS
1	F	131	GLN
1	F	135	HIS
1	G	14	GLN

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Mol	Chain	Res	Type
1	G	131	GLN
1	G	135	HIS
1	H	135	HIS
1	I	131	GLN
1	I	135	HIS
1	J	22	GLN
1	J	135	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 10 are monoatomic - leaving 30 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	OMO	B	1635	-	0,3,3	0.00	-	-		
2	FLC	I	1664	-	3,12,12	3.36	2 (66%)	3,17,17	1.15	0
5	OMO	D	1643	-	0,3,3	0.00	-	-		
2	FLC	A	1632	-	3,12,12	3.41	2 (66%)	3,17,17	1.35	0
2	FLC	C	1640	-	3,12,12	3.89	3 (100%)	3,17,17	0.47	0
2	FLC	G	1656	-	3,12,12	3.11	2 (66%)	3,17,17	0.44	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MO7	F	1650	-	20,42,42	4.45	10 (50%)	-		
5	OMO	A	1631	-	0,3,3	0.00	-	-		
4	MO7	J	1666	-	20,42,42	5.27	9 (45%)	-		
5	OMO	C	1639	-	0,3,3	0.00	-	-		
5	OMO	F	1651	-	0,3,3	0.00	-	-		
2	FLC	F	1652	-	3,12,12	3.33	3 (100%)	3,17,17	0.35	0
4	MO7	E	1646	-	20,42,42	3.22	9 (45%)	-		
5	OMO	G	1655	-	0,3,3	0.00	-	-		
2	FLC	J	1668	-	3,12,12	3.51	3 (100%)	3,17,17	0.41	0
2	FLC	D	1644	-	3,12,12	2.78	2 (66%)	3,17,17	1.04	0
5	OMO	J	1667	-	0,3,3	0.00	-	-		
4	MO7	I	1662	-	20,42,42	4.72	10 (50%)	-		
4	MO7	B	1634	-	20,42,42	3.82	8 (40%)	-		
4	MO7	D	1642	-	20,42,42	4.39	10 (50%)	-		
2	FLC	E	1648	-	3,12,12	3.30	2 (66%)	3,17,17	0.49	0
4	MO7	A	1630	-	20,42,42	3.98	10 (50%)	-		
2	FLC	H	1660	-	3,12,12	2.64	2 (66%)	3,17,17	0.37	0
4	MO7	C	1638	-	20,42,42	4.68	9 (45%)	-		
4	MO7	H	1658	-	20,42,42	3.89	9 (45%)	-		
4	MO7	G	1654	-	20,42,42	4.63	10 (50%)	-		
5	OMO	E	1647	-	0,3,3	0.00	-	-		
2	FLC	B	1636	-	3,12,12	3.58	2 (66%)	3,17,17	0.62	0
5	OMO	I	1663	-	0,3,3	0.00	-	-		
5	OMO	H	1659	-	0,3,3	0.00	-	-		

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	FLC	H	1660	-	-	0/6/16/16	-
2	FLC	I	1664	-	-	0/6/16/16	-
2	FLC	D	1644	-	-	0/6/16/16	-
2	FLC	A	1632	-	-	0/6/16/16	-
2	FLC	C	1640	-	-	0/6/16/16	-
2	FLC	B	1636	-	-	0/6/16/16	-
2	FLC	G	1656	-	-	0/6/16/16	-
2	FLC	E	1648	-	-	0/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	F	1652	-	-	0/6/16/16	-
2	FLC	J	1668	-	-	0/6/16/16	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1666	MO7	O1-MO1	-15.53	1.58	1.74
4	I	1662	MO7	O1-MO1	-13.11	1.60	1.74
4	D	1642	MO7	O1-MO1	-12.20	1.61	1.74
4	A	1630	MO7	O1-MO1	-11.60	1.62	1.74
4	C	1638	MO7	O1-MO1	-11.46	1.62	1.74
4	G	1654	MO7	O1-MO1	-11.36	1.62	1.74
4	F	1650	MO7	O1-MO1	-10.16	1.63	1.74
4	D	1642	MO7	O23-MO7	9.37	1.84	1.68
4	C	1638	MO7	O23-MO7	9.16	1.84	1.68
4	B	1634	MO7	O4-MO1	9.12	1.83	1.74
4	F	1650	MO7	O23-MO7	9.02	1.84	1.68
4	J	1666	MO7	O13-MO4	8.67	1.83	1.68
4	G	1654	MO7	O23-MO7	8.49	1.83	1.68
4	J	1666	MO7	O23-MO7	8.48	1.83	1.68
4	H	1658	MO7	O1-MO1	-8.31	1.65	1.74
4	I	1662	MO7	O23-MO7	8.01	1.82	1.68
4	F	1650	MO7	O13-MO4	7.96	1.82	1.68
4	I	1662	MO7	O13-MO4	7.81	1.82	1.68
4	G	1654	MO7	O4-MO1	7.63	1.82	1.74
4	H	1658	MO7	O8-MO2	7.45	1.82	1.68
4	C	1638	MO7	O13-MO4	7.17	1.80	1.68
4	C	1638	MO7	O22-MO6	7.11	1.80	1.68
4	J	1666	MO7	O22-MO6	6.94	1.80	1.68
4	B	1634	MO7	O11-MO3	-6.56	1.56	1.68
4	J	1666	MO7	O11-MO3	6.53	1.79	1.68
4	H	1658	MO7	O4-MO1	6.47	1.81	1.74
4	G	1654	MO7	O8-MO2	6.35	1.80	1.68
4	H	1658	MO7	O23-MO7	6.00	1.78	1.68
4	G	1654	MO7	O15-MO5	5.91	1.79	1.68
4	F	1650	MO7	O22-MO6	5.88	1.78	1.68
4	E	1646	MO7	O4-MO1	5.84	1.80	1.74
4	B	1634	MO7	O8-MO2	5.82	1.79	1.68
4	B	1634	MO7	O1-MO1	-5.78	1.68	1.74
4	A	1630	MO7	O4-MO1	5.75	1.80	1.74
4	B	1634	MO7	O15-MO5	5.70	1.79	1.68
4	D	1642	MO7	O13-MO4	5.67	1.78	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1650	MO7	O8-MO2	5.62	1.79	1.68
4	G	1654	MO7	O22-MO6	5.57	1.78	1.68
4	E	1646	MO7	O8-MO2	5.55	1.79	1.68
4	A	1630	MO7	O23-MO7	5.53	1.78	1.68
4	C	1638	MO7	O8-MO2	5.52	1.78	1.68
4	I	1662	MO7	O4-MO2	5.48	2.55	1.95
4	E	1646	MO7	O23-MO7	5.36	1.77	1.68
4	E	1646	MO7	O1-MO1	-5.22	1.68	1.74
4	D	1642	MO7	O4-MO2	5.16	2.51	1.95
4	H	1658	MO7	O4-MO2	5.12	2.51	1.95
2	C	1640	FLC	CG-CB	4.98	1.61	1.54
4	E	1646	MO7	O22-MO6	4.96	1.77	1.68
4	D	1642	MO7	O1-MO5	4.96	2.49	1.95
4	C	1638	MO7	O1-MO5	4.91	2.48	1.95
4	A	1630	MO7	O1-MO5	4.86	2.48	1.95
4	I	1662	MO7	O8-MO2	4.82	1.77	1.68
4	I	1662	MO7	O11-MO3	4.72	1.76	1.68
4	C	1638	MO7	O4-MO2	4.69	2.46	1.95
2	G	1656	FLC	CA-CB	4.66	1.61	1.54
4	J	1666	MO7	O1-MO5	4.66	2.46	1.95
4	F	1650	MO7	O1-MO5	4.65	2.45	1.95
4	C	1638	MO7	O11-MO3	4.65	1.76	1.68
4	A	1630	MO7	O13-MO4	4.60	1.76	1.68
4	H	1658	MO7	O15-MO5	4.60	1.77	1.68
4	B	1634	MO7	O4-MO2	4.59	2.45	1.95
4	H	1658	MO7	O13-MO4	4.55	1.76	1.68
4	I	1662	MO7	O22-MO6	4.52	1.76	1.68
4	D	1642	MO7	O22-MO6	4.45	1.76	1.68
2	J	1668	FLC	CA-CB	4.41	1.61	1.54
2	E	1648	FLC	CA-CB	4.40	1.61	1.54
4	I	1662	MO7	O4-MO1	4.39	1.78	1.74
4	A	1630	MO7	O22-MO6	4.39	1.76	1.68
4	J	1666	MO7	O4-MO2	4.37	2.42	1.95
4	A	1630	MO7	O4-MO2	4.35	2.42	1.95
2	B	1636	FLC	CG-CB	4.35	1.61	1.54
4	E	1646	MO7	O15-MO5	4.32	1.76	1.68
4	G	1654	MO7	O1-MO5	4.32	2.42	1.95
2	I	1664	FLC	CA-CB	4.32	1.61	1.54
4	I	1662	MO7	O1-MO5	4.30	2.42	1.95
4	A	1630	MO7	O8-MO2	4.26	1.76	1.68
4	B	1634	MO7	O23-MO7	4.21	1.75	1.68
4	B	1634	MO7	O1-MO5	4.18	2.40	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1650	MO7	O4-MO2	4.17	2.40	1.95
2	B	1636	FLC	CA-CB	4.17	1.60	1.54
4	F	1650	MO7	O4-MO1	4.17	1.78	1.74
2	A	1632	FLC	CG-CB	4.17	1.60	1.54
2	A	1632	FLC	CA-CB	4.16	1.60	1.54
4	G	1654	MO7	O13-MO4	4.09	1.75	1.68
4	E	1646	MO7	O1-MO5	4.00	2.38	1.95
4	J	1666	MO7	O8-MO2	3.92	1.75	1.68
4	D	1642	MO7	O4-MO1	3.73	1.78	1.74
4	H	1658	MO7	O1-MO5	3.69	2.35	1.95
4	D	1642	MO7	O8-MO2	3.65	1.75	1.68
2	I	1664	FLC	CG-CB	3.52	1.59	1.54
4	C	1638	MO7	O4-MO1	3.50	1.78	1.74
2	C	1640	FLC	OHB-CB	3.49	1.48	1.43
2	E	1648	FLC	CG-CB	3.48	1.59	1.54
2	H	1660	FLC	CA-CB	3.46	1.59	1.54
2	F	1652	FLC	OHB-CB	3.46	1.48	1.43
2	F	1652	FLC	CA-CB	3.35	1.59	1.54
2	D	1644	FLC	CG-CB	3.35	1.59	1.54
4	F	1650	MO7	O11-MO3	3.34	1.74	1.68
4	E	1646	MO7	O4-MO2	3.34	2.31	1.95
4	E	1646	MO7	O13-MO4	3.32	1.74	1.68
4	G	1654	MO7	O4-MO2	3.21	2.30	1.95
2	D	1644	FLC	CA-CB	3.21	1.59	1.54
2	J	1668	FLC	OHB-CB	3.19	1.48	1.43
2	F	1652	FLC	CG-CB	3.17	1.59	1.54
4	H	1658	MO7	O22-MO6	3.04	1.73	1.68
2	C	1640	FLC	CA-CB	2.91	1.59	1.54
2	H	1660	FLC	CG-CB	2.89	1.59	1.54
4	A	1630	MO7	O15-MO5	2.87	1.73	1.68
2	J	1668	FLC	CG-CB	2.69	1.58	1.54
2	G	1656	FLC	CG-CB	2.68	1.58	1.54
4	D	1642	MO7	O15-MO5	2.67	1.73	1.68
4	J	1666	MO7	O15-MO5	2.66	1.73	1.68
4	I	1662	MO7	O15-MO5	2.62	1.73	1.68
4	A	1630	MO7	O11-MO3	2.53	1.72	1.68
4	G	1654	MO7	O12-MO4	-2.29	1.77	1.93
4	F	1650	MO7	O15-MO5	2.28	1.72	1.68
4	D	1642	MO7	O11-MO3	2.18	1.72	1.68

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

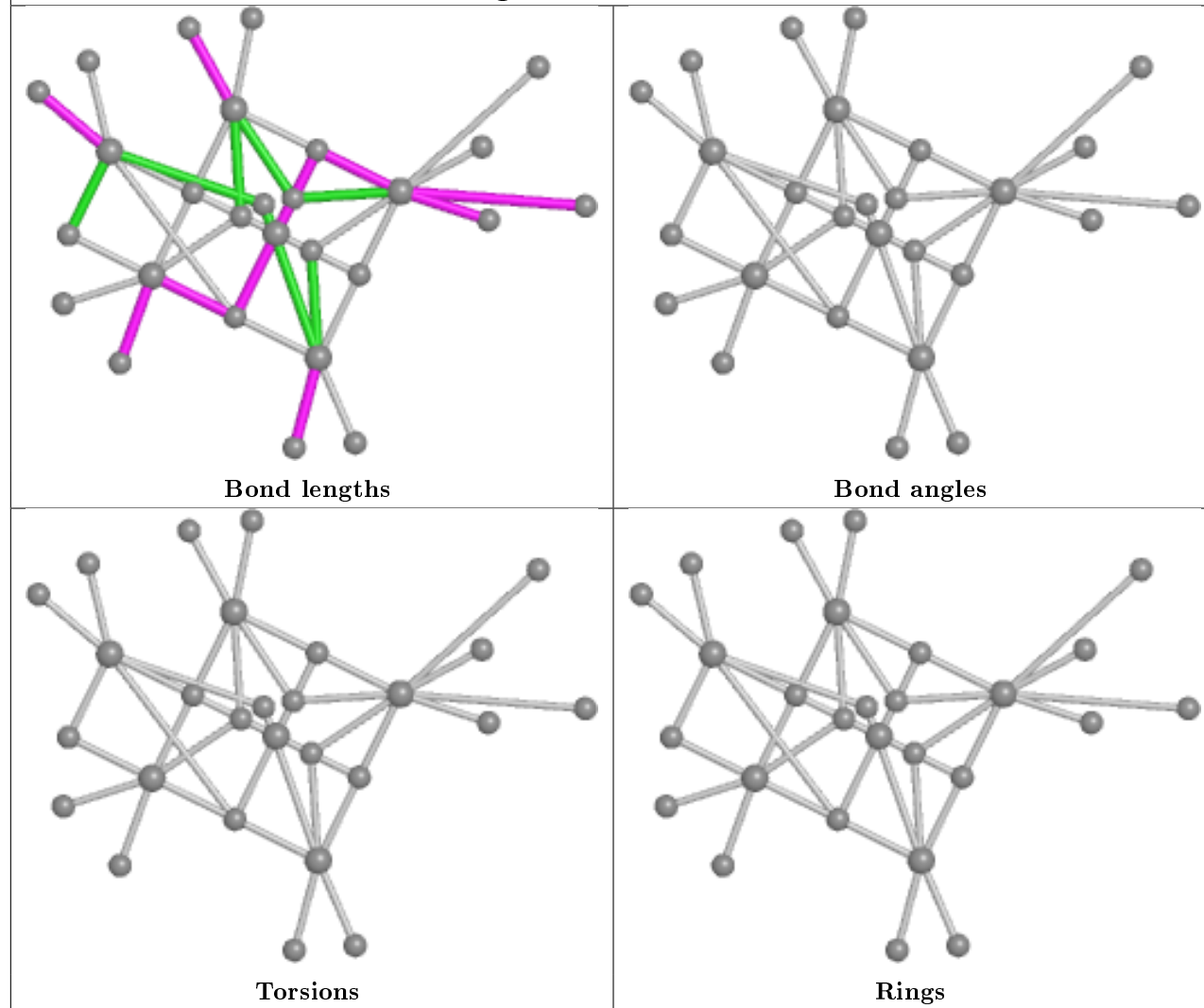
There are no ring outliers.

17 monomers are involved in 75 short contacts:

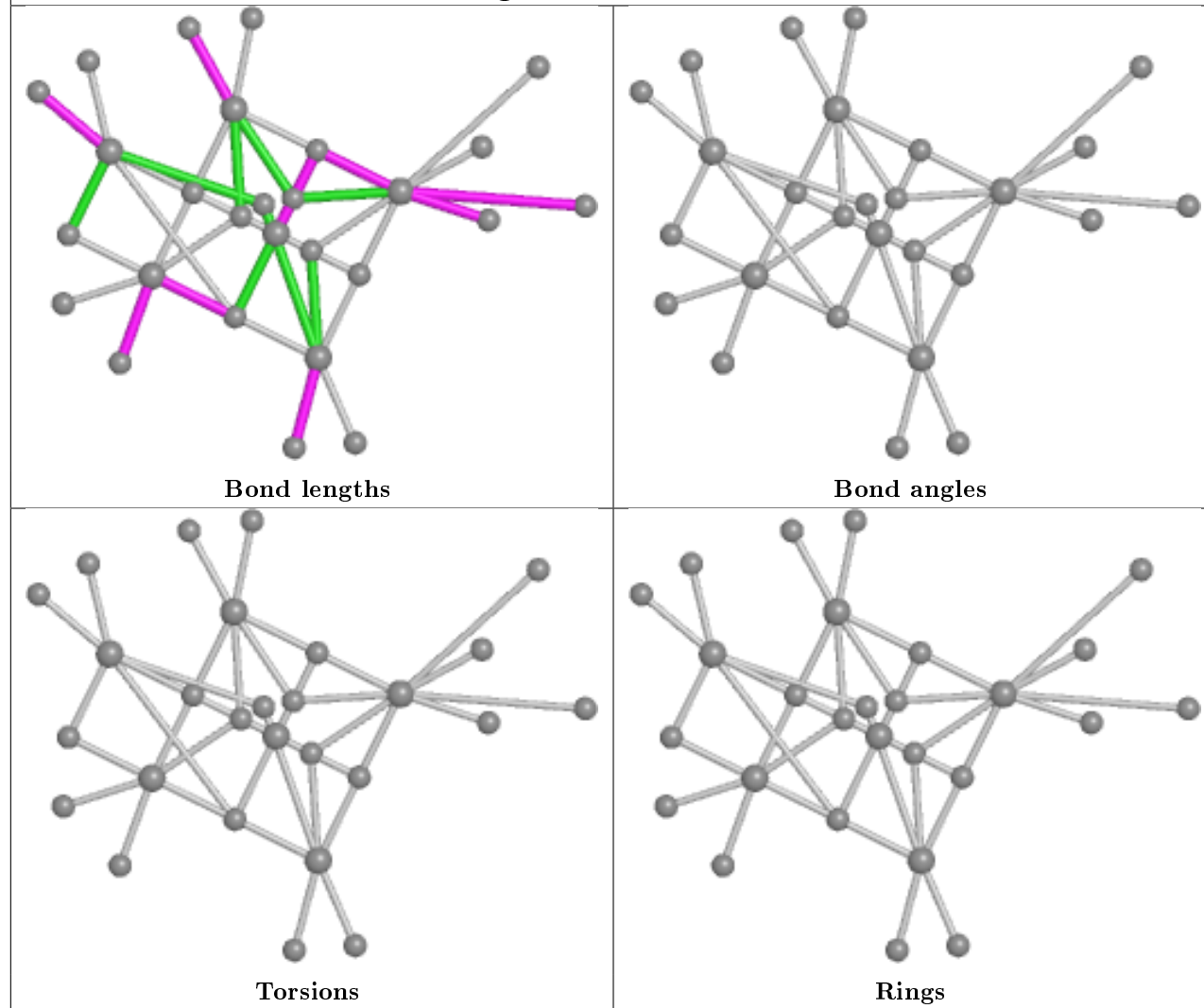
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1635	OMO	1	0
4	F	1650	MO7	7	0
5	A	1631	OMO	1	0
4	J	1666	MO7	7	0
5	C	1639	OMO	1	0
5	F	1651	OMO	1	0
4	E	1646	MO7	5	0
5	J	1667	OMO	2	0
4	I	1662	MO7	7	0
4	B	1634	MO7	7	0
4	D	1642	MO7	8	0
4	A	1630	MO7	6	0
4	C	1638	MO7	6	0
4	H	1658	MO7	7	0
4	G	1654	MO7	7	0
5	E	1647	OMO	1	0
5	I	1663	OMO	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.

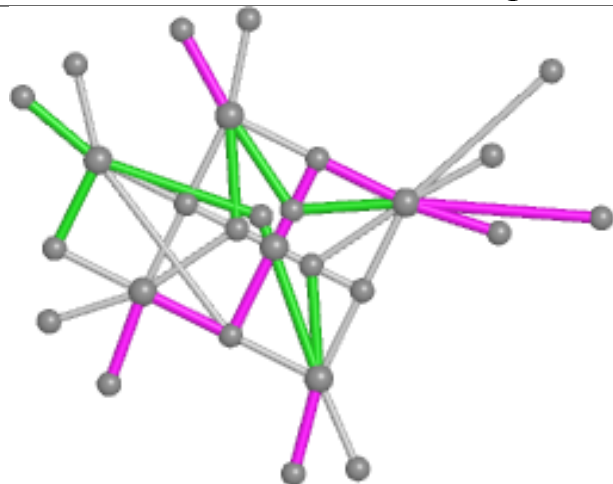
## Ligand MO7 F 1650



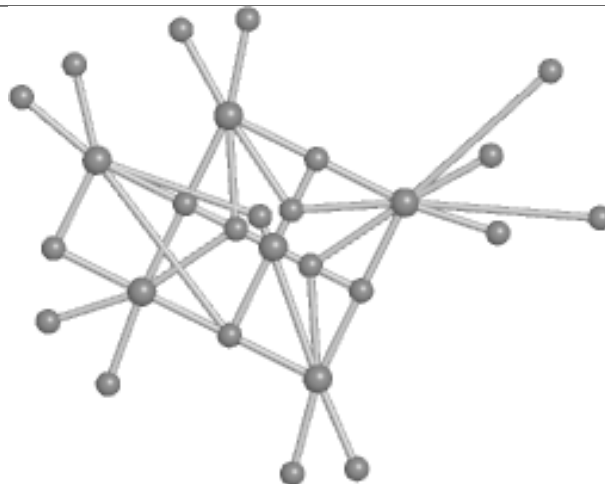
## Ligand MO7 J 1666



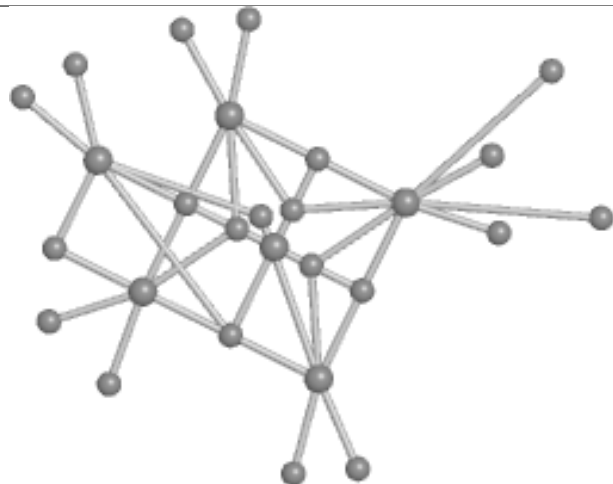
## Ligand MO7 E 1646



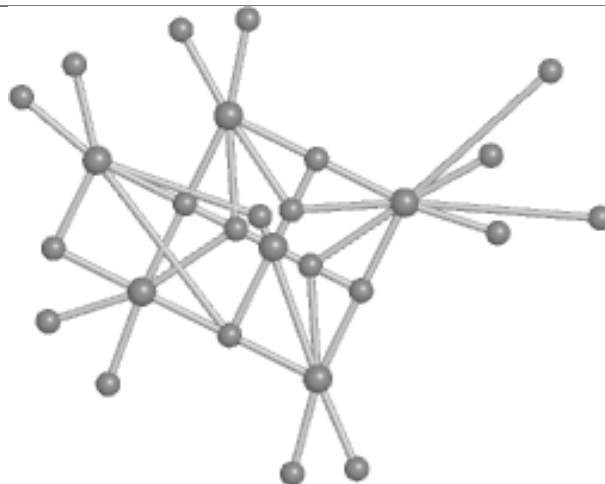
Bond lengths



Bond angles

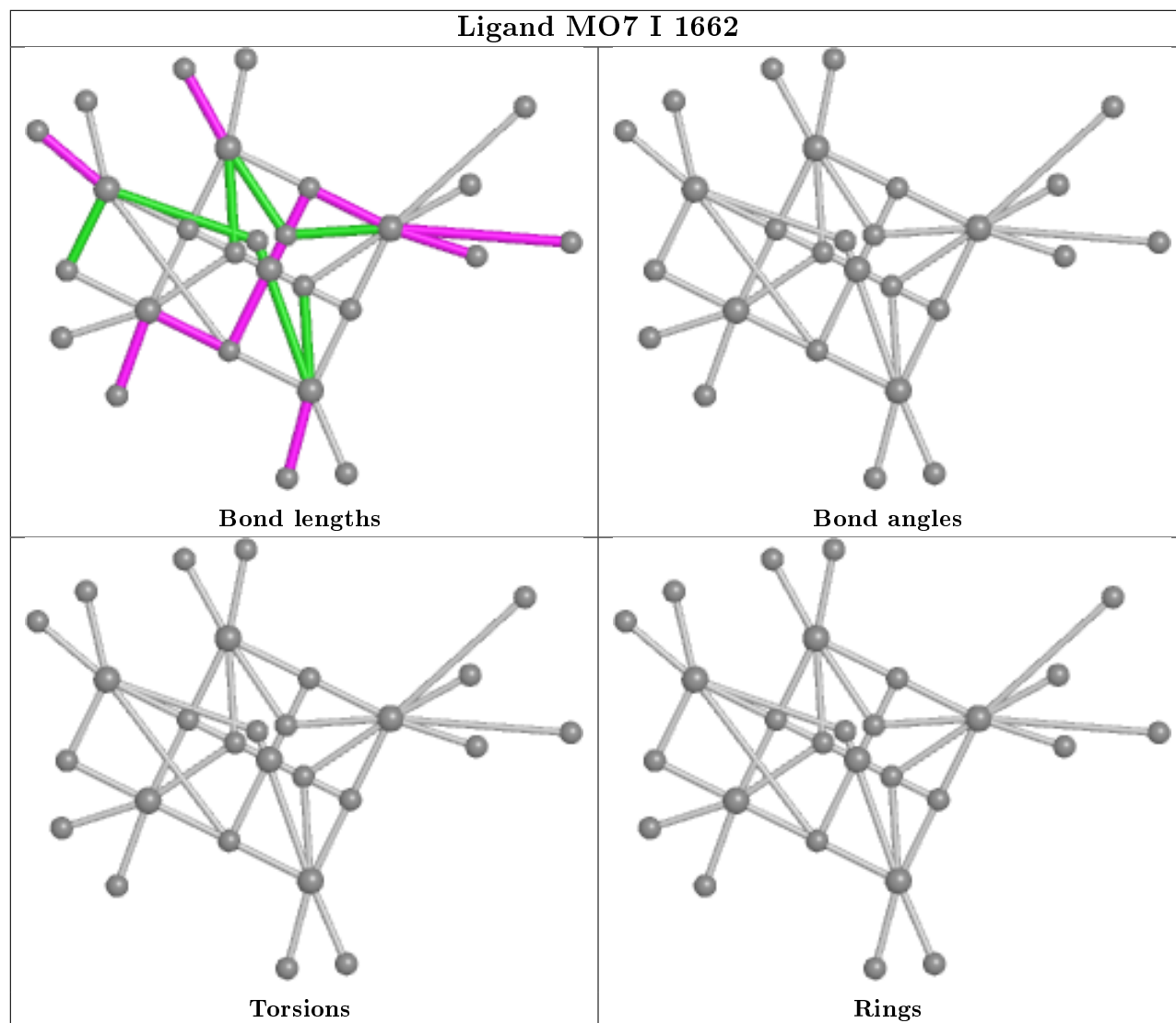


Torsions

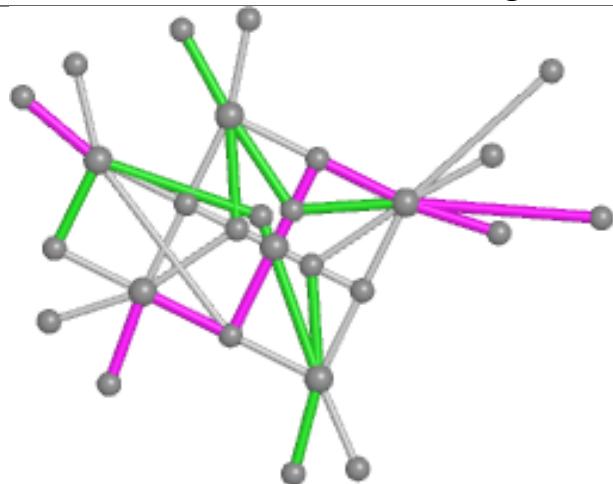


Rings

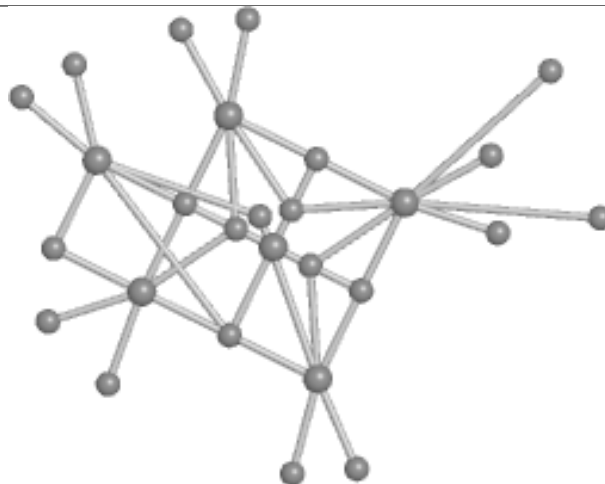




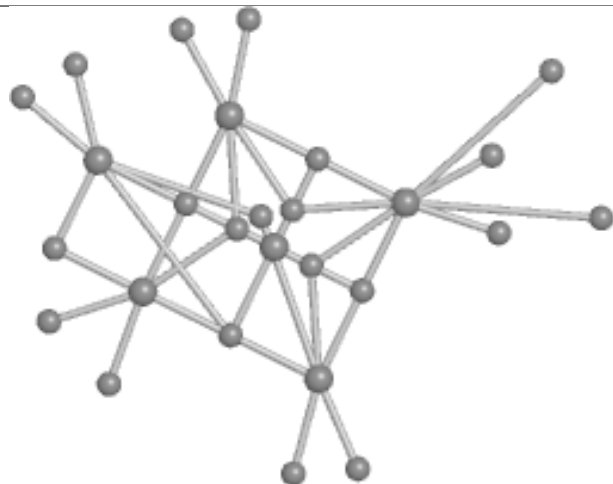
## Ligand MO7 B 1634



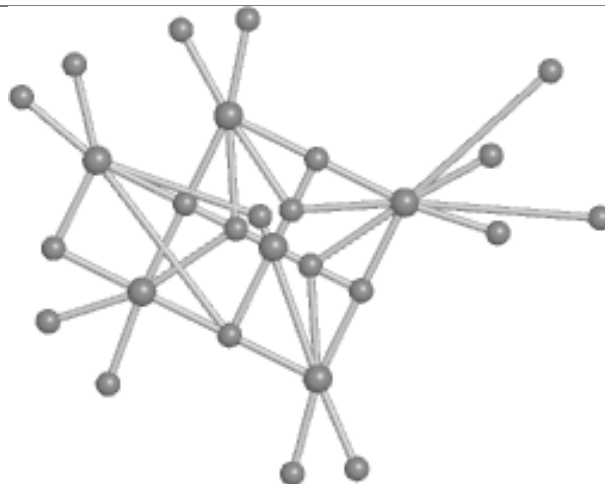
Bond lengths



Bond angles

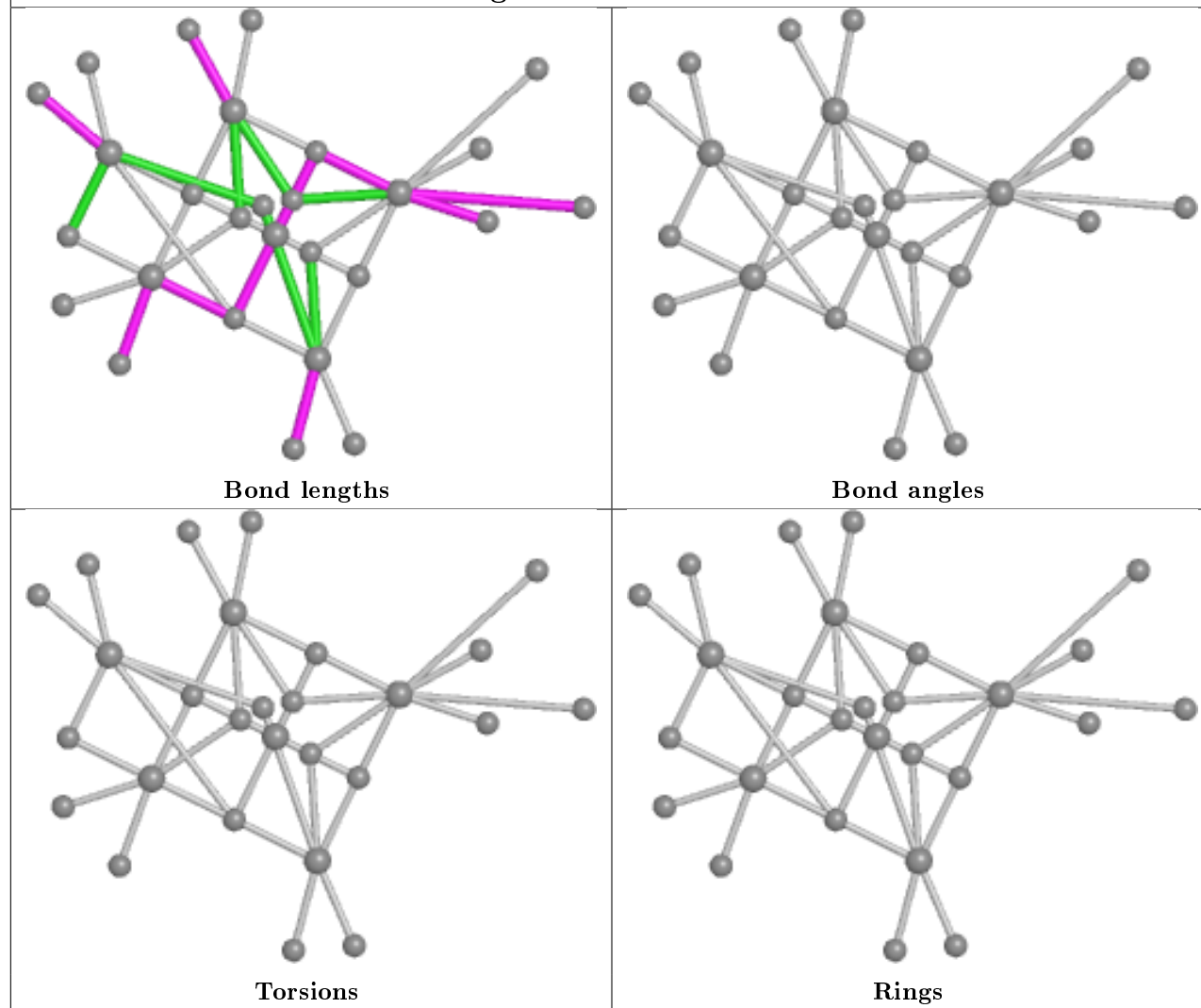


Torsions

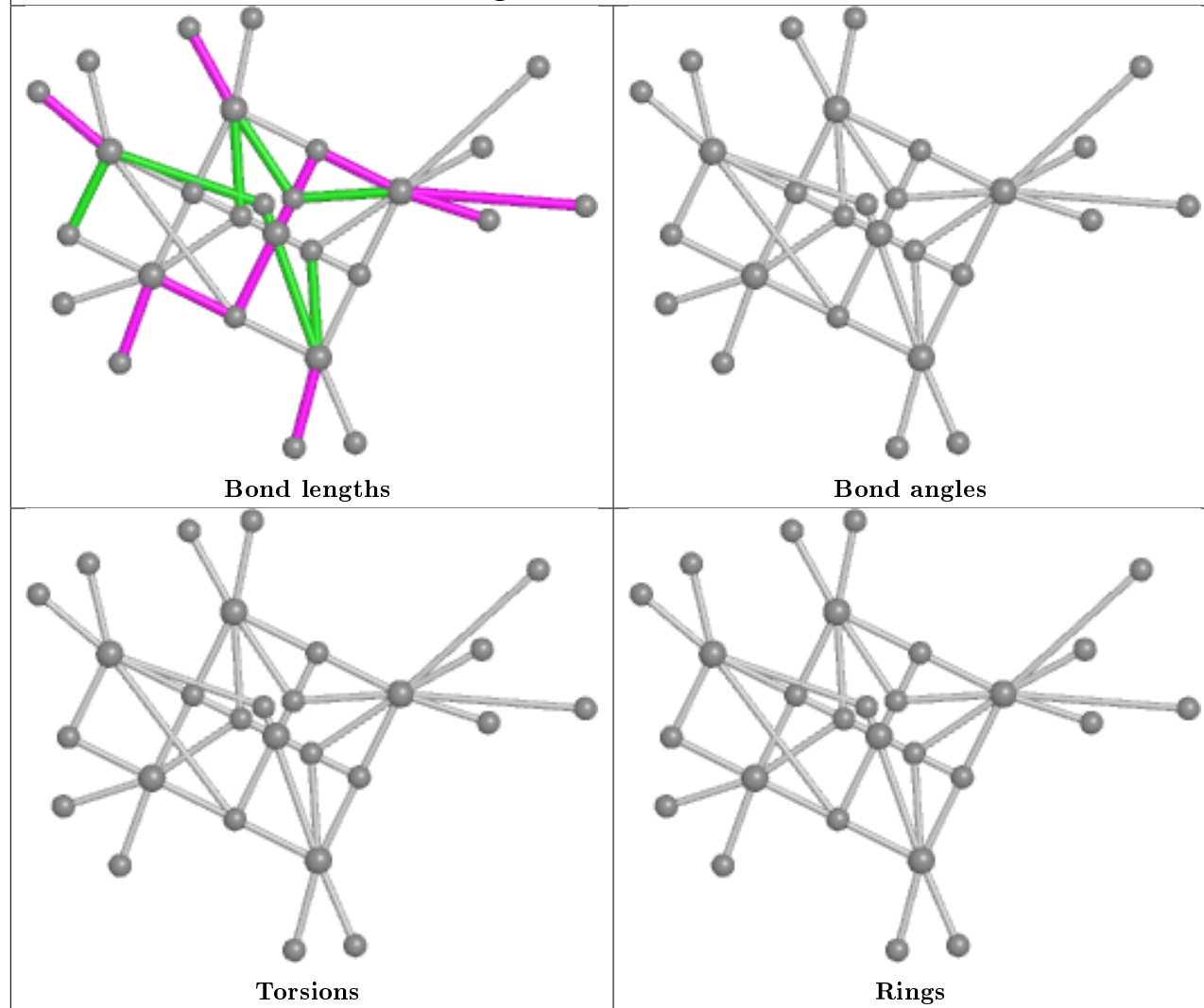


Rings

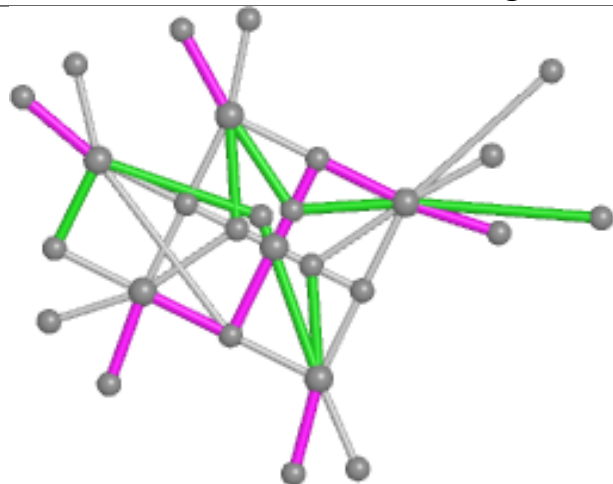
## Ligand MO7 D 1642



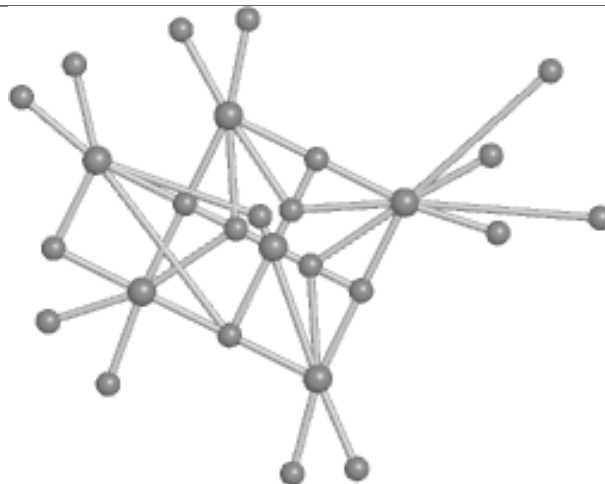
## Ligand MO7 A 1630



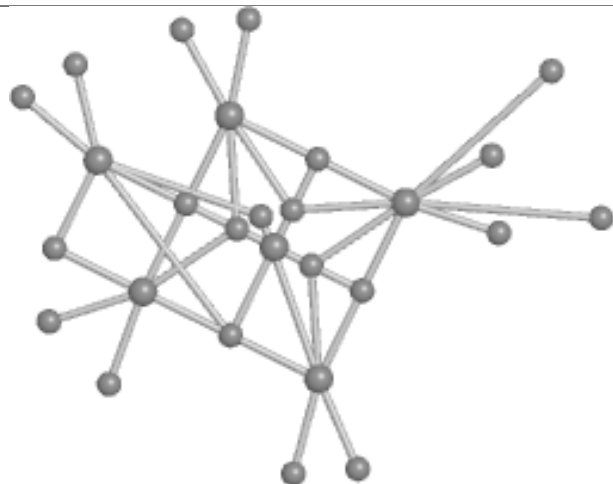
## Ligand MO7 C 1638



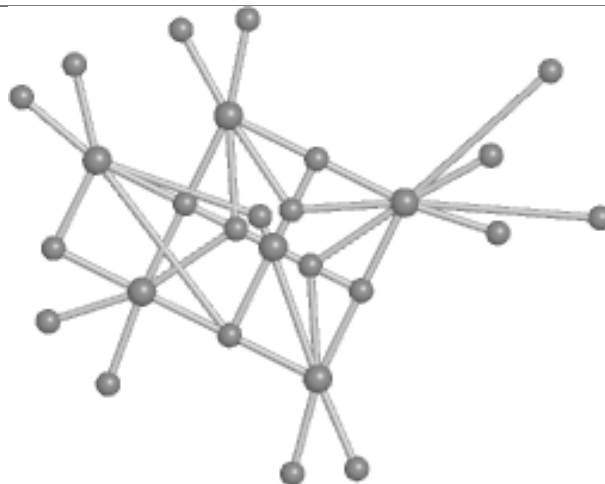
Bond lengths



Bond angles

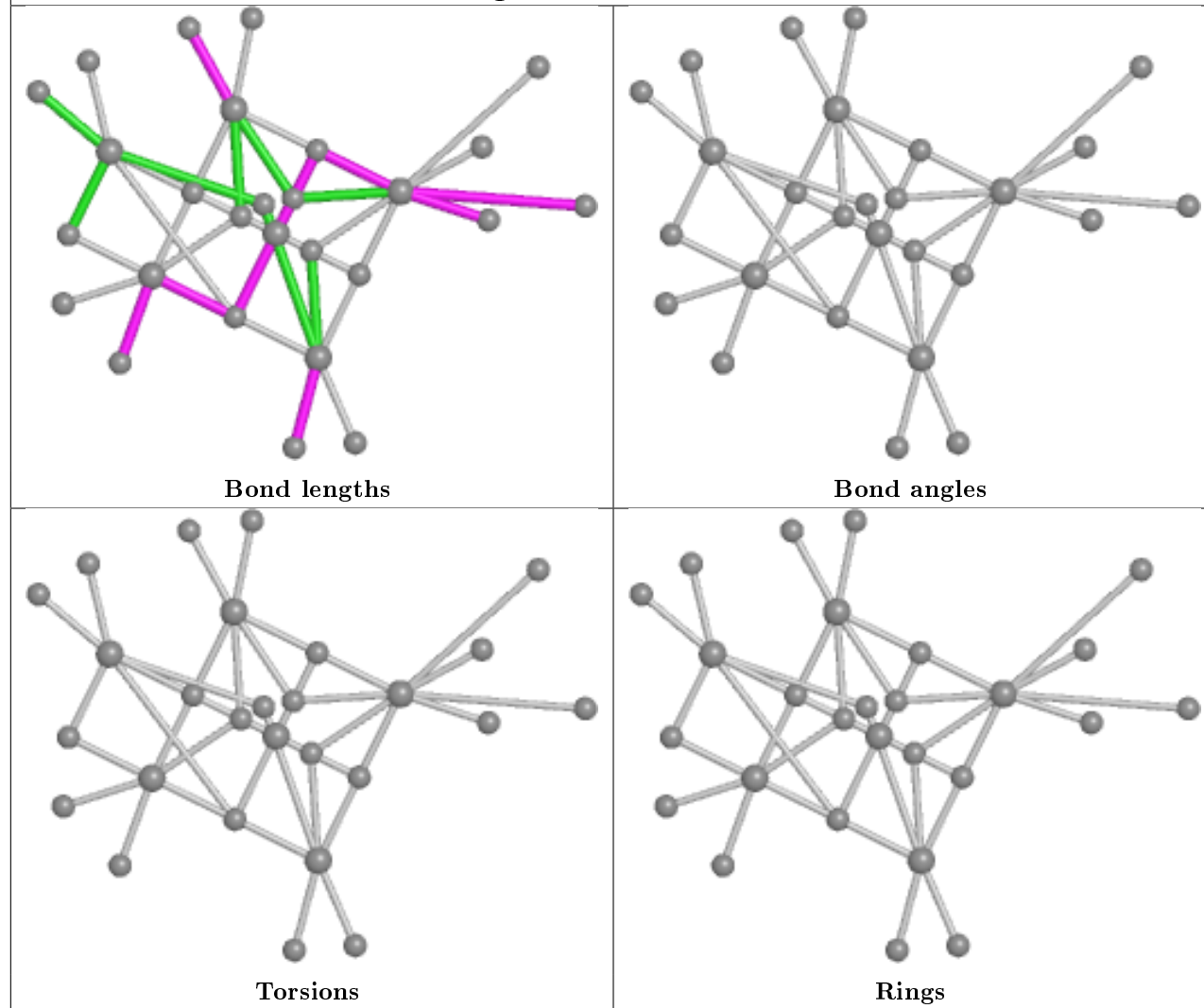


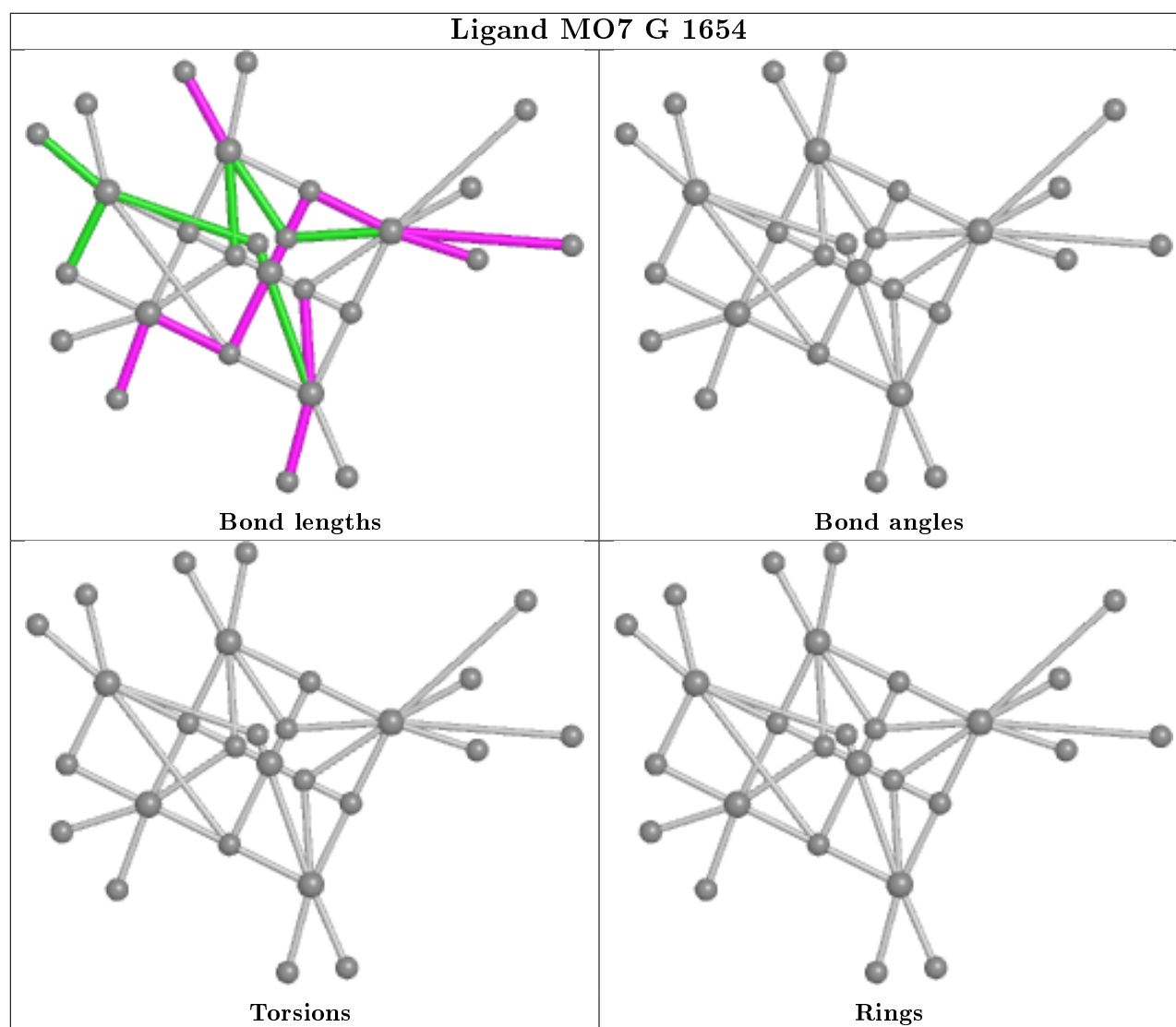
Torsions



Rings

## Ligand MO7 H 1658





## 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	131/131 (100%)	-0.06	2 (1%) 73 73	16, 23, 34, 44	0
1	B	131/131 (100%)	0.09	5 (3%) 40 37	17, 23, 37, 45	0
1	C	131/131 (100%)	0.04	1 (0%) 86 86	16, 23, 35, 42	0
1	D	131/131 (100%)	0.10	3 (2%) 60 59	15, 22, 32, 46	0
1	E	131/131 (100%)	0.27	9 (6%) 16 15	18, 25, 36, 47	0
1	F	131/131 (100%)	-0.17	1 (0%) 86 86	15, 23, 35, 42	0
1	G	131/131 (100%)	0.51	10 (7%) 13 12	19, 27, 42, 44	0
1	H	131/131 (100%)	0.34	4 (3%) 49 46	18, 28, 41, 48	0
1	I	131/131 (100%)	0.31	9 (6%) 16 15	19, 28, 42, 46	0
1	J	131/131 (100%)	0.17	6 (4%) 32 29	19, 28, 41, 45	0
All	All	1310/1310 (100%)	0.16	50 (3%) 40 37	15, 25, 40, 48	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	HIS	3.8
1	A	5	GLU	3.8
1	G	39	ALA	3.7
1	H	35	LYS	3.5
1	J	134	HIS	3.4
1	E	73	ASP	3.2
1	I	130	GLU	3.1
1	J	28	GLU	3.1
1	J	133	GLU	3.1
1	I	33	VAL	3.1
1	I	116	THR	3.0
1	G	72	PRO	3.0
1	G	43	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	130	GLU	2.9
1	G	97	VAL	2.8
1	E	5	GLU	2.8
1	H	31	GLU	2.8
1	H	76	GLY	2.7
1	D	5	GLU	2.6
1	E	95	VAL	2.6
1	I	39	ALA	2.5
1	E	72	PRO	2.5
1	G	73	ASP	2.5
1	A	134	HIS	2.4
1	B	31	GLU	2.4
1	E	97	VAL	2.4
1	I	38	LEU	2.4
1	I	5	GLU	2.4
1	I	73	ASP	2.4
1	E	75	ILE	2.3
1	G	38	LEU	2.3
1	B	5	GLU	2.3
1	H	73	ASP	2.3
1	B	35	LYS	2.3
1	G	35	LYS	2.3
1	G	5	GLU	2.3
1	I	28	GLU	2.3
1	C	133	GLU	2.2
1	G	106[A]	LEU	2.2
1	I	31	GLU	2.2
1	E	89	ILE	2.2
1	E	35	LYS	2.2
1	D	134	HIS	2.1
1	E	134	HIS	2.1
1	D	133	GLU	2.1
1	G	71	ASN	2.1
1	F	5	GLU	2.1
1	J	39	ALA	2.1
1	B	130	GLU	2.0
1	J	5	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	FLC	J	1668	13/13	0.90	0.11	20,24,27,28	0
2	FLC	I	1664	13/13	0.95	0.07	22,24,25,25	0
2	FLC	F	1652	13/13	0.96	0.07	17,19,20,21	0
2	FLC	G	1656	13/13	0.96	0.08	24,25,27,28	0
2	FLC	H	1660	13/13	0.96	0.07	22,22,24,24	0
2	FLC	E	1648	13/13	0.97	0.06	20,22,24,25	0
2	FLC	C	1640	13/13	0.97	0.07	16,17,19,20	0
2	FLC	B	1636	13/13	0.97	0.07	18,19,21,23	0
3	NA	J	1669	1/1	0.98	0.10	23,23,23,23	0
2	FLC	D	1644	13/13	0.98	0.09	15,17,18,19	0
2	FLC	A	1632	13/13	0.98	0.07	16,18,20,20	0
5	OMO	J	1667	4/4	0.99	0.07	20,21,22,22	0
4	MO7	I	1662	31/31	0.99	0.07	19,23,26,27	0
4	MO7	B	1634	31/31	0.99	0.07	18,21,27,28	0
3	NA	G	1657	1/1	0.99	0.04	23,23,23,23	0
3	NA	D	1645	1/1	0.99	0.09	17,17,17,17	0
4	MO7	E	1646	31/31	0.99	0.07	19,23,25,28	0
4	MO7	F	1650	31/31	0.99	0.08	17,20,23,25	0
3	NA	F	1653	1/1	0.99	0.04	19,19,19,19	0
4	MO7	C	1638	31/31	0.99	0.07	17,19,24,25	0
3	NA	A	1633	1/1	0.99	0.04	19,19,19,19	0
4	MO7	H	1658	31/31	0.99	0.07	21,25,27,30	0
3	NA	C	1641	1/1	0.99	0.06	17,17,17,17	0
3	NA	H	1661	1/1	0.99	0.06	23,23,23,23	0
3	NA	I	1665	1/1	0.99	0.06	24,24,24,24	0
4	MO7	G	1654	31/31	0.99	0.07	18,24,27,29	0
4	MO7	J	1666	31/31	0.99	0.07	19,23,26,28	0
5	OMO	I	1663	4/4	0.99	0.06	20,22,23,25	0
3	NA	B	1637	1/1	0.99	0.06	18,18,18,18	0
5	OMO	B	1635	4/4	1.00	0.07	18,19,20,21	0
5	OMO	D	1643	4/4	1.00	0.07	18,18,18,20	0
4	MO7	D	1642	31/31	1.00	0.07	19,23,27,28	0

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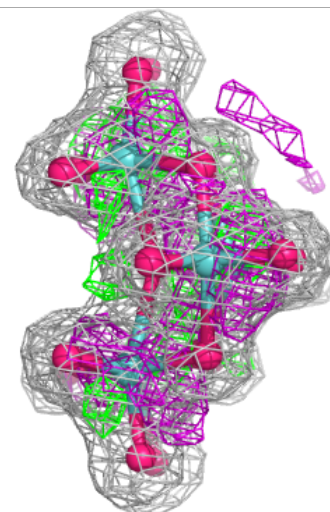
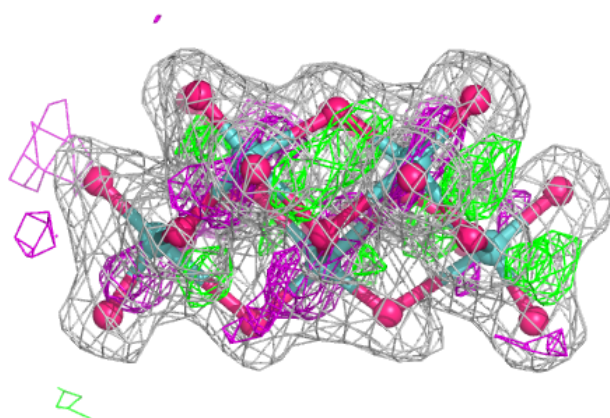
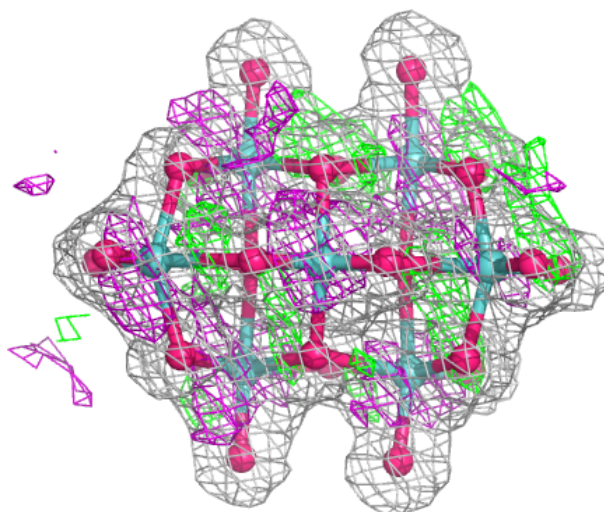
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OMO	G	1655	4/4	1.00	0.07	22,24,24,24	0
4	MO7	A	1630	31/31	1.00	0.07	19,23,27,29	0
5	OMO	A	1631	4/4	1.00	0.07	17,18,18,19	0
5	OMO	E	1647	4/4	1.00	0.06	21,22,24,24	0
5	OMO	C	1639	4/4	1.00	0.07	16,17,18,19	0
5	OMO	H	1659	4/4	1.00	0.06	22,23,23,25	0
3	NA	E	1649	1/1	1.00	0.06	21,21,21,21	0
5	OMO	F	1651	4/4	1.00	0.05	18,18,19,20	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.

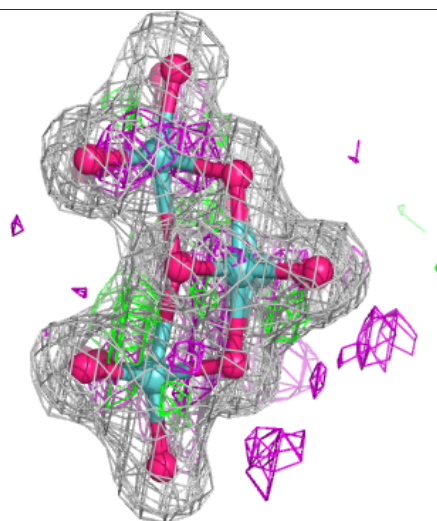
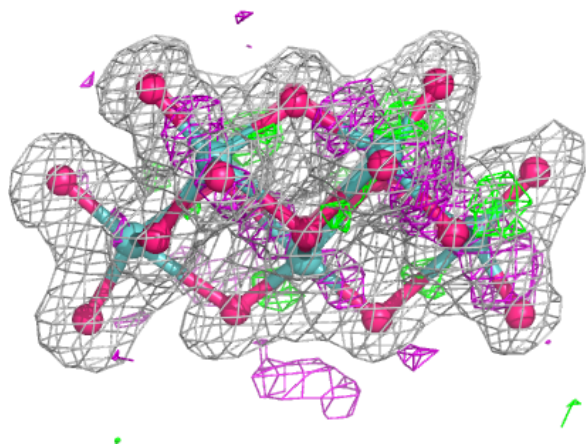
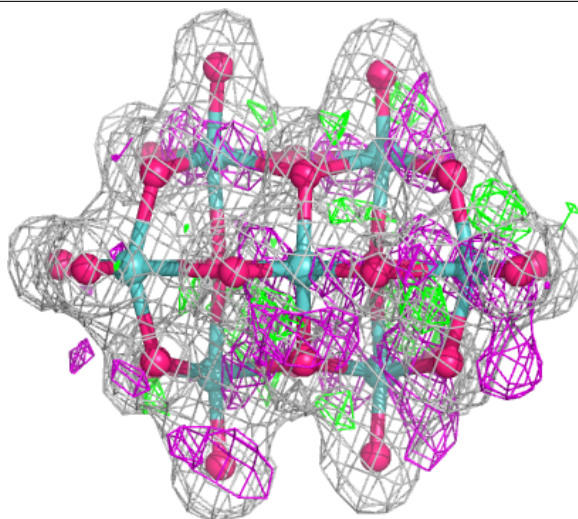
**Electron density around MO7 I 1662:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



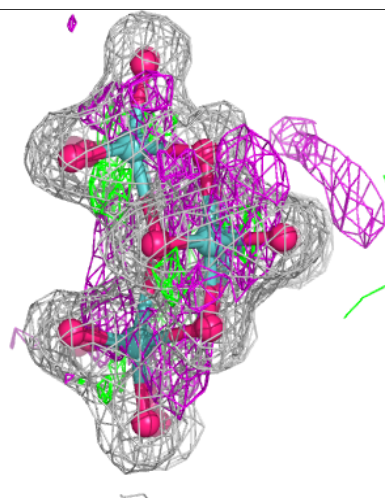
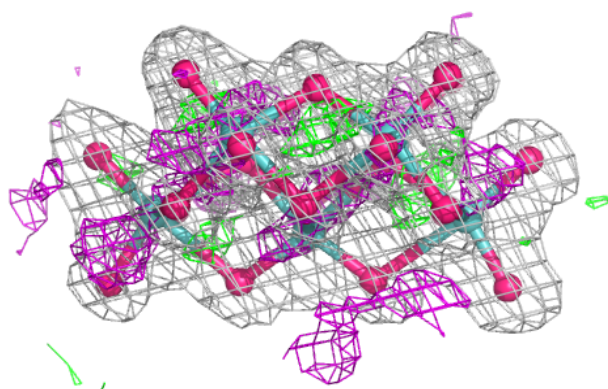
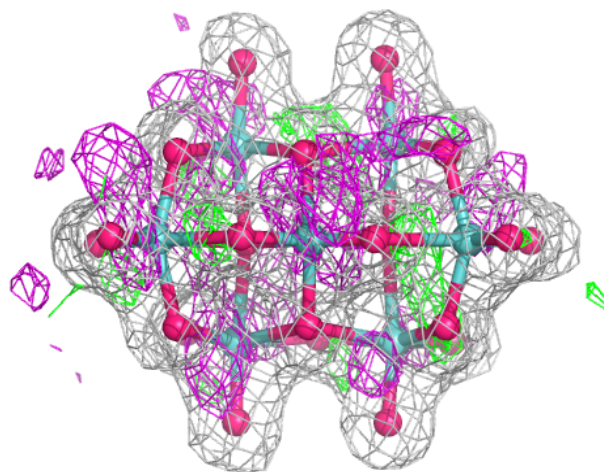
**Electron density around MO7 B 1634:**

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



**Electron density around MO7 E 1646:**

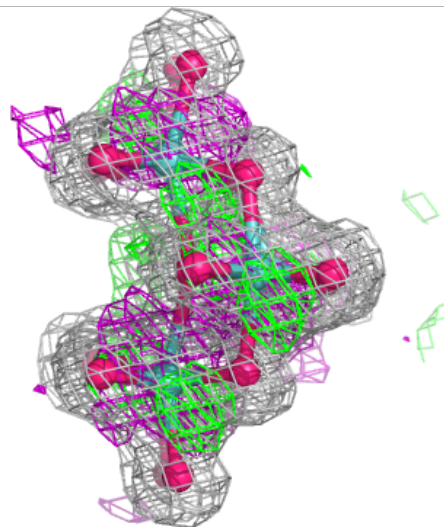
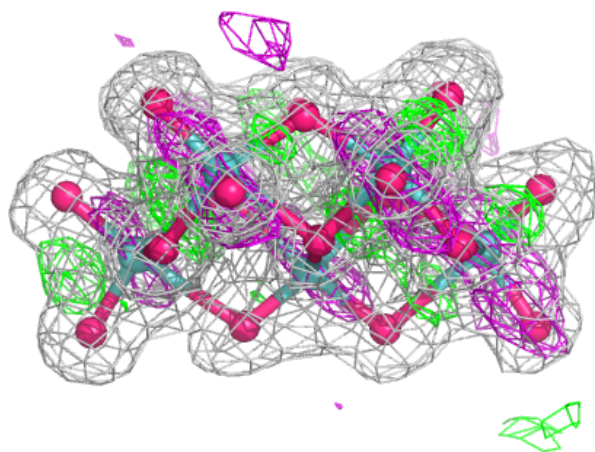
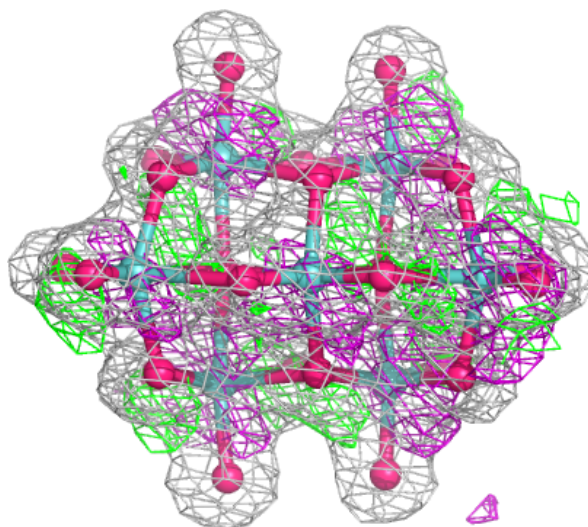
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





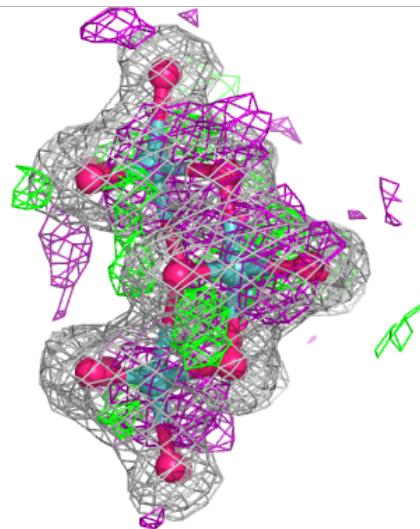
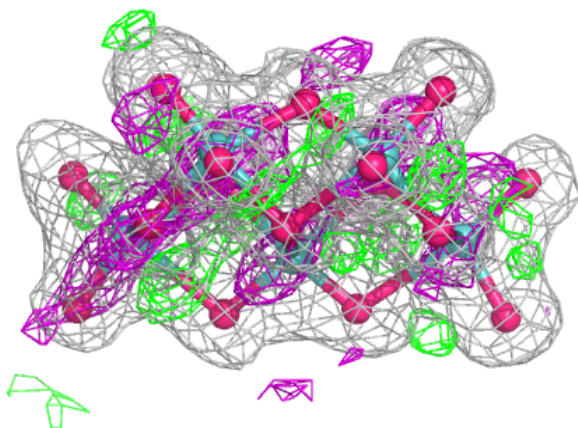
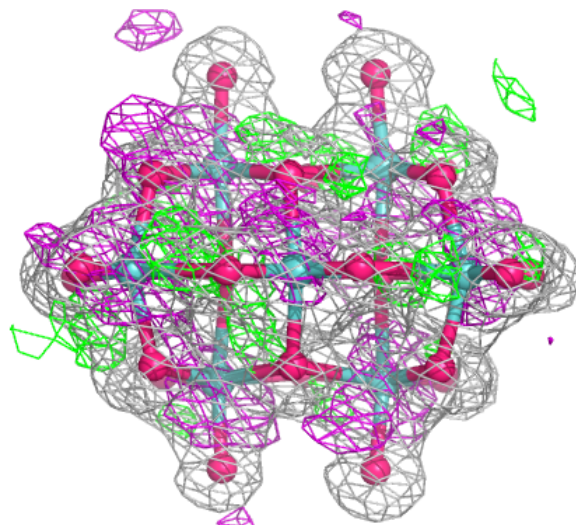
**Electron density around MO7 F 1650:**

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



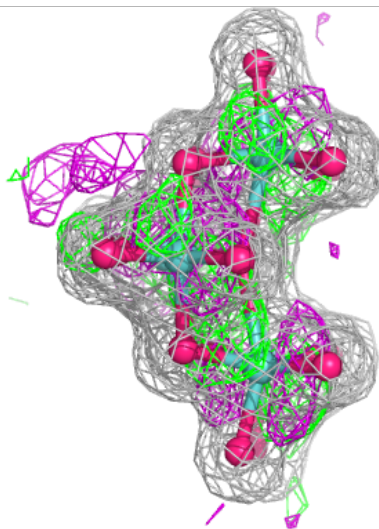
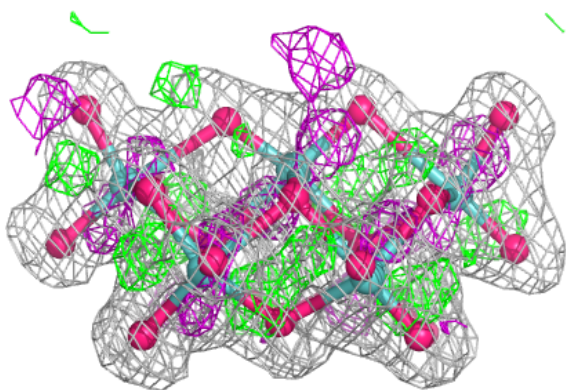
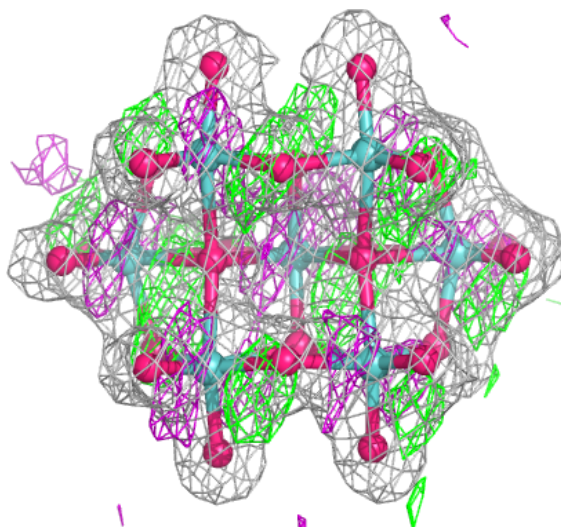
**Electron density around MO7 C 1638:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MO7 H 1658:**

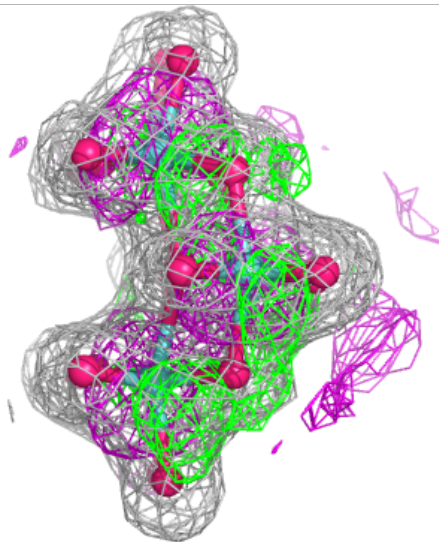
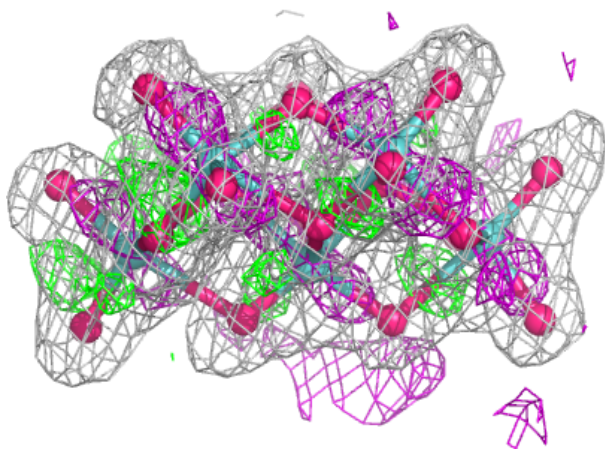
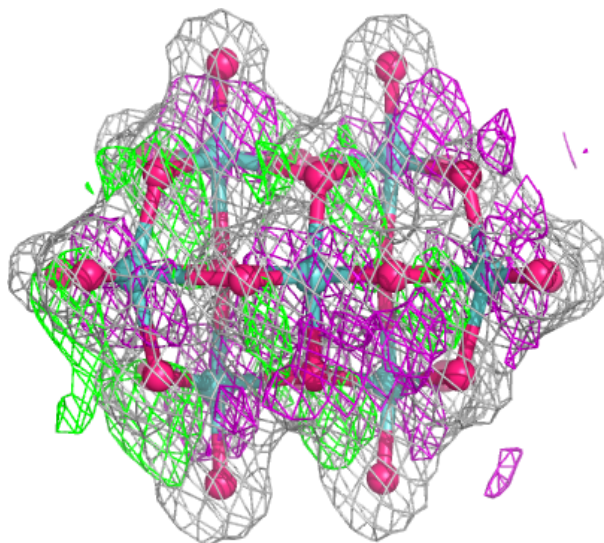
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





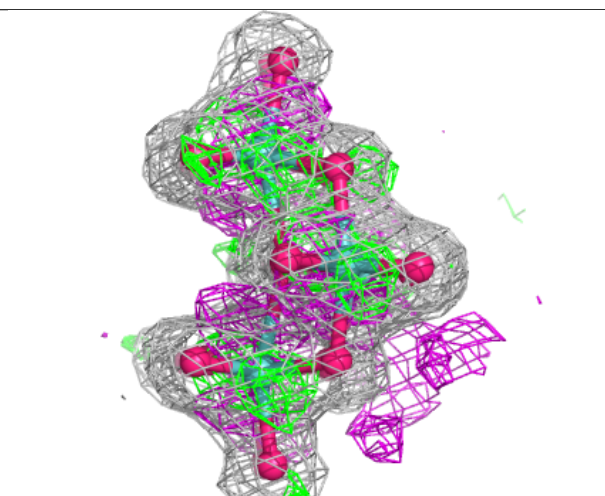
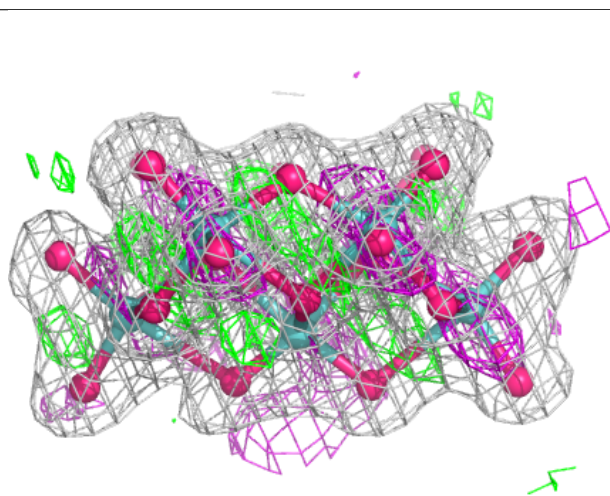
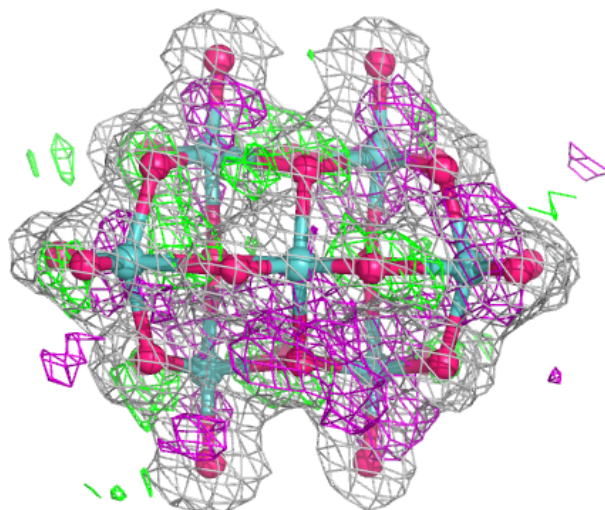
**Electron density around MO7 G 1654:**

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



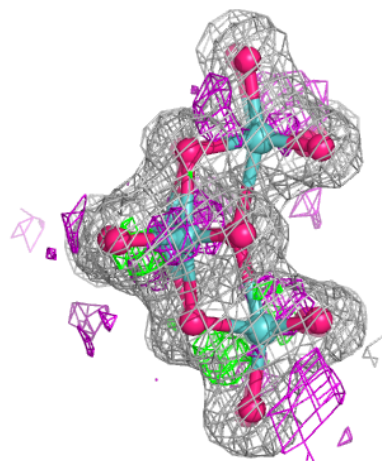
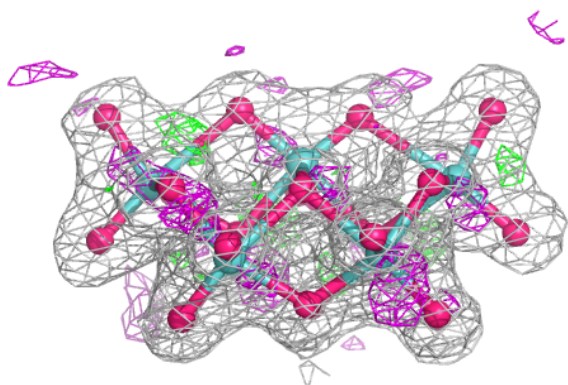
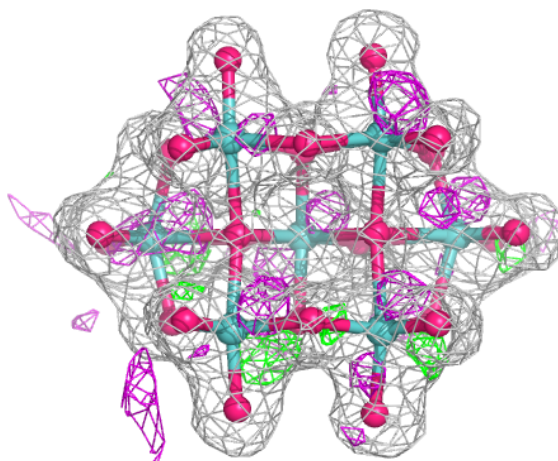
**Electron density around MO7 J 1666:**

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



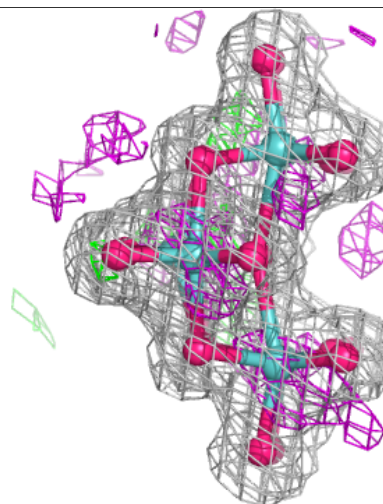
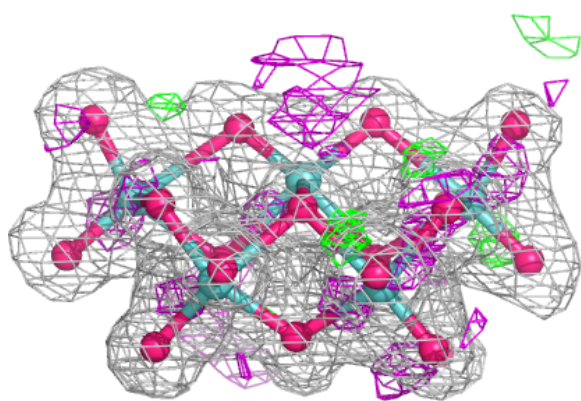
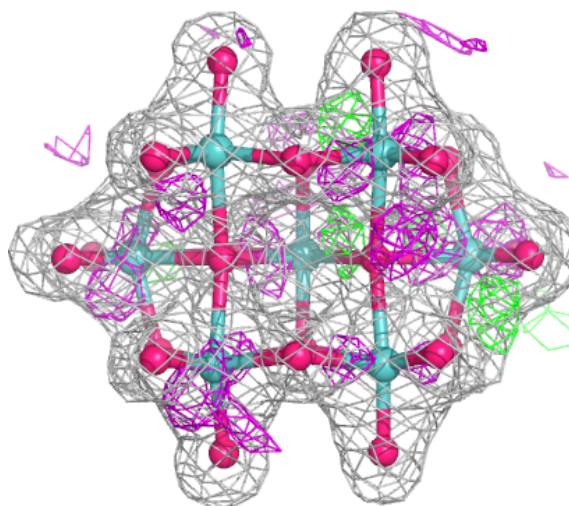
**Electron density around MO7 D 1642:**

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



**Electron density around MO7 A 1630:**

$2mF_o-DF_c$  (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.