



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 10:51 AM EDT

PDB ID : 6O7R  
Title : Nitrogenase MoFeP mutant F99Y, S188A from *Azotobacter vinelandii* in the dithionite reduced state  
Authors : Rutledge, H.L.; Williamson, L.M.; Tezcan, F.A.  
Deposited on : 2019-03-08  
Resolution : 2.27 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

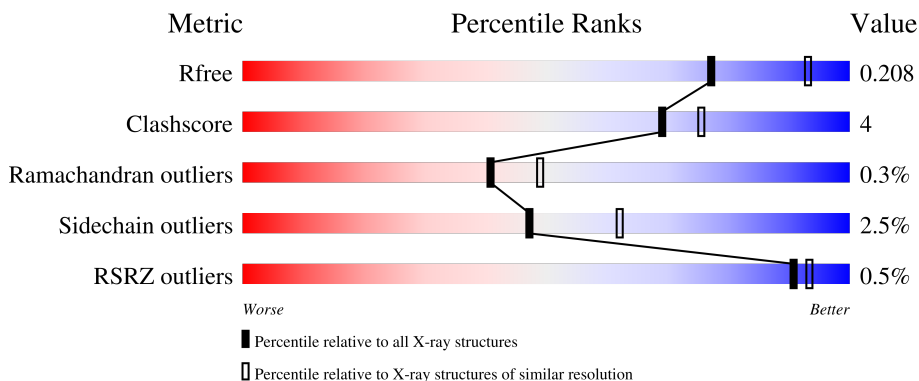
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	492	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 85%, grey 85%);"></div> <div style="margin-left: 10px;"> <p>85% 11% .</p> </div> </div>
1	C	492	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 87%, grey 87%);"></div> <div style="margin-left: 10px;"> <p>87% 10% ..</p> </div> </div>
2	B	523	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, green 91%, yellow 8%, grey 8%);"></div> <div style="margin-left: 10px;"> <p>91% 8% .</p> </div> </div>
2	D	523	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, green 91%, yellow 9%, grey 9%);"></div> <div style="margin-left: 10px;"> <p>91% 9%</p> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32662 atoms, of which 15402 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 Nitrogenase molybdenum-iron protein alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	476	7394	2389	3639	633	707	26	0	5	0
1	C	478	7399	2390	3642	639	703	25	0	0	0

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	522	8202	2657	4044	699	774	28	0	1	0
2	D	522	8232	2663	4065	701	775	28	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

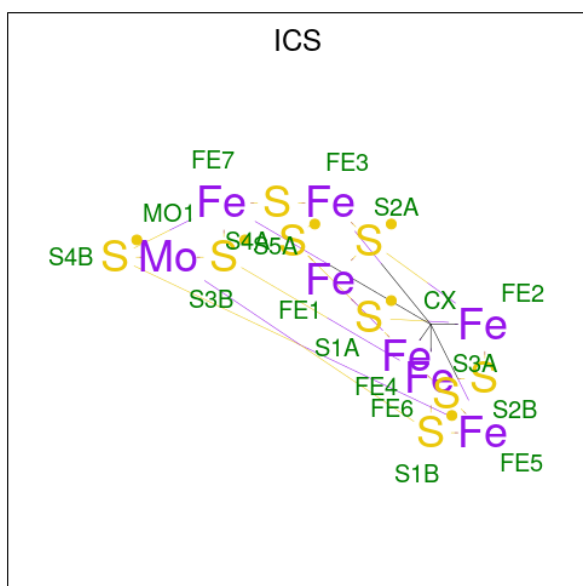
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	PHE	engineered mutation	UNP P07329
B	188	ALA	SER	engineered mutation	UNP P07329
D	99	TYR	PHE	engineered mutation	UNP P07329
D	188	ALA	SER	engineered mutation	UNP P07329

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	7	6	7		
3	C	1	Total	C	H	O	0	0
			20	7	6	7		

- Molecule 4 is iron-sulfur-molybdenum cluster with interstitial carbon (three-letter code: ICS) (formula:  $\text{CFe}_7\text{MoS}_9$ ).



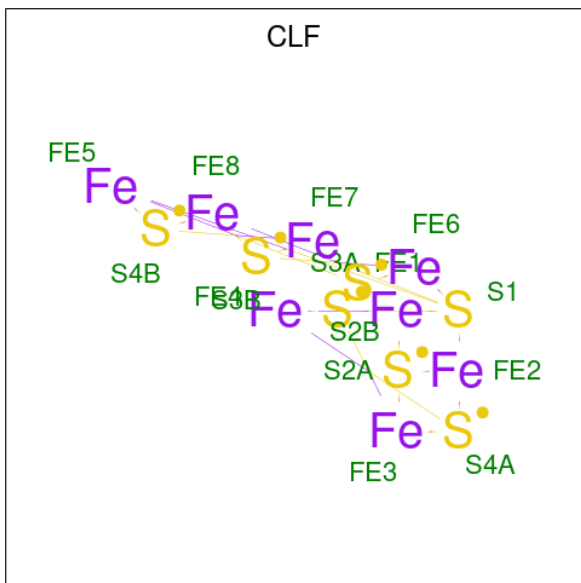
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	C	1	Total	C	Fe	Mo	S	0	0
			18	1	7	1	9		

- Molecule 5 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe<sub>8</sub>S<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Fe S	0	0
			15	8 7		
5	D	1	Total	Fe S	0	0
			15	8 7		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		
6	D	1	Total	Fe	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	0
			262	262		

Continued on next page...

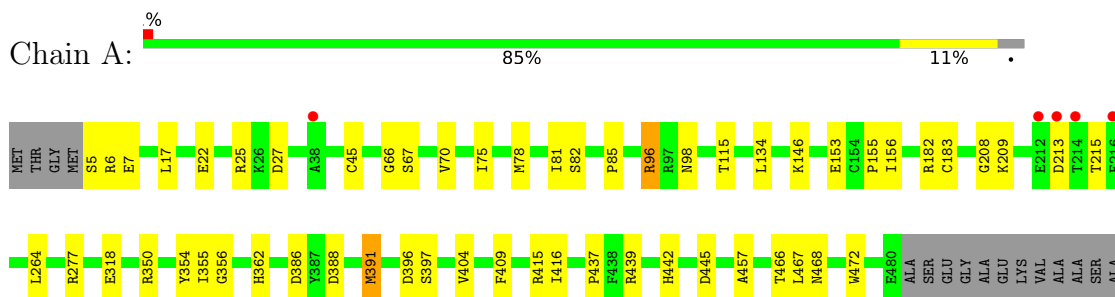
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	B	404	Total 404	O 404	0	0
7	C	289	Total 289	O 289	0	0
7	D	372	Total 372	O 372	0	0

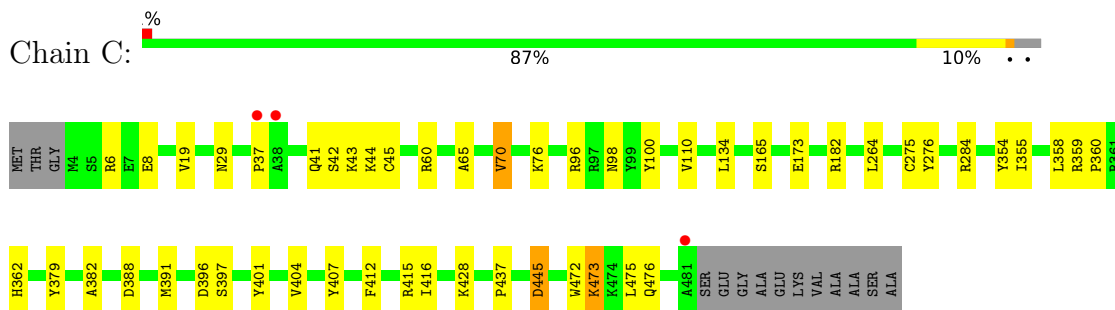
### 3 Residue-property plots [i](#)

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.

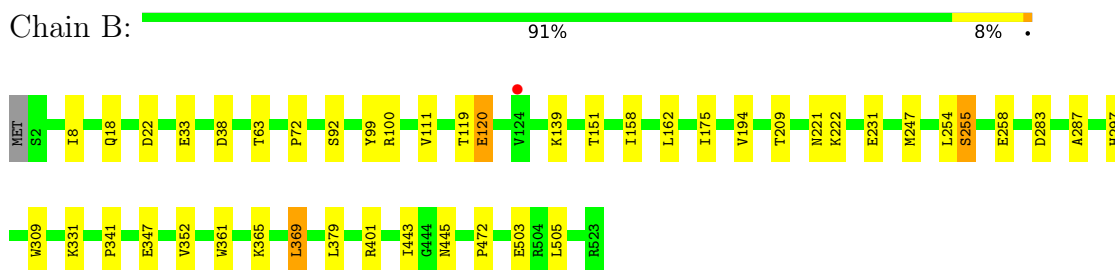
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



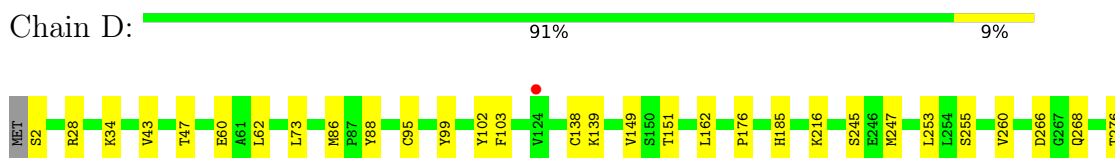
- Molecule 1: Nitrogenase molybdenum-iron protein alpha chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain



- Molecule 2: Nitrogenase molybdenum-iron protein beta chain







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.61Å 128.81Å 107.64Å 90.00° 109.07° 90.00°	Depositor
Resolution (Å)	47.31 – 2.27 79.84 – 2.27	Depositor EDS
% Data completeness (in resolution range)	90.5 (47.31-2.27) 90.6 (79.84-2.27)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.27Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.164 , 0.208 0.164 , 0.208	Depositor DCC
$R_{free}$ test set	8182 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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: HCA, CLF, ICS, FE

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	0.38	0/3858	0.50	0/5214
1	C	0.37	0/3845	0.49	0/5193
2	B	0.41	0/4267	0.49	0/5776
2	D	0.39	0/4279	0.48	0/5791
All	All	0.39	0/16249	0.49	0/21974

There are no bond length outliers.

There are no bond angle outliers.

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	3755	3639	3640	35	0
1	C	3757	3642	3642	28	0
2	B	4158	4044	4041	28	0
2	D	4167	4065	4064	30	0
3	A	14	6	6	3	0
3	C	14	6	6	0	0
4	A	18	0	0	2	0
4	C	18	0	0	1	0
5	B	15	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	15	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	262	0	0	6	0
7	B	404	0	0	6	0
7	C	289	0	0	4	1
7	D	372	0	0	11	1
All	All	17260	15402	15399	117	1

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

All (117) 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:6:ARG:NH2	1:C:396:ASP:OD1	2.20	0.75
2:D:317:ASN:ND2	7:D:704:HOH:O	2.20	0.72
1:A:22:GLU:OE2	1:A:25:ARG:NH1	2.22	0.70
2:B:331:LYS:NZ	7:B:706:HOH:O	2.24	0.70
2:D:60:GLU:OE2	7:D:701:HOH:O	2.12	0.68
2:B:283:ASP:OD2	7:B:701:HOH:O	2.14	0.66
2:D:255:SER:H	2:D:276[B]:THR:HG21	1.61	0.66
2:D:102:TYR:HB3	7:D:721:HOH:O	1.96	0.65
1:A:5:SER:O	1:A:7:GLU:N	2.30	0.64
2:B:352:VAL:HG11	1:C:475:LEU:HD12	1.80	0.64
2:B:38:ASP:OD2	7:B:702:HOH:O	2.16	0.61
2:D:260:VAL:O	7:D:702:HOH:O	2.16	0.60
2:D:434:VAL:HG22	2:D:464:VAL:HG21	1.82	0.60
1:A:146:LYS:NZ	2:B:33:GLU:O	2.29	0.59
2:D:453:ARG:HG3	2:D:454:ASP:N	2.18	0.59
1:C:19:VAL:HG21	1:C:407:TYR:OH	2.02	0.59
2:D:266:ASP:O	7:D:703:HOH:O	2.17	0.58
2:D:255:SER:N	2:D:276[B]:THR:HG21	2.19	0.58
2:B:209[A]:THR:HG21	2:B:309:TRP:NE1	2.18	0.57
2:B:231:GLU:OE1	7:B:703:HOH:O	2.18	0.56
1:A:75:ILE:HG21	1:A:78:MET:HE2	1.87	0.56
2:D:247:MET:HG2	2:D:341:PRO:HD3	1.86	0.56
2:B:100:ARG:HD2	2:B:111:VAL:O	2.07	0.55
1:A:468:ASN:O	7:A:601:HOH:O	2.18	0.54
1:A:442:HIS:HB3	3:A:501:HCA:O6	2.06	0.54
1:C:276:TYR:OH	1:C:284:ARG:NH2	2.40	0.54

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLY:N	7:A:616:HOH:O	2.34	0.54
2:D:103:PHE:N	7:D:721:HOH:O	2.40	0.54
2:D:458:LYS:HG2	2:D:462:PHE:CD2	2.43	0.53
1:C:42:SER:OG	1:C:388:ASP:OD1	2.16	0.53
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.92	0.52
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.91	0.52
1:C:173:GLU:O	7:C:601:HOH:O	2.19	0.51
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.92	0.51
1:A:213[B]:ASP:OD2	1:A:215:THR:HG22	2.11	0.50
1:C:415:ARG:NE	7:C:627:HOH:O	2.45	0.50
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.47	0.49
7:A:615:HOH:O	2:D:360[A]:THR:HG21	2.12	0.49
2:D:95:CYS:HB3	2:D:99:TYR:CZ	2.48	0.49
1:C:8:GLU:HB3	1:C:415:ARG:NH2	2.28	0.48
1:A:96:ARG:NH2	4:A:502:ICS:S5A	2.87	0.48
2:B:445:ASN:HB2	2:B:472:PRO:O	2.13	0.48
1:C:428:LYS:NZ	1:C:445:ASP:OD1	2.43	0.48
2:B:254:LEU:O	2:B:255:SER:HB3	2.13	0.48
1:C:473:LYS:NZ	7:C:614:HOH:O	2.34	0.48
1:A:350:ARG:NH2	1:A:416:ILE:O	2.46	0.48
3:A:501:HCA:O2	3:A:501:HCA:O7	2.32	0.48
2:B:379:LEU:HD21	2:B:443:ILE:HG21	1.96	0.47
1:C:37:PRO:HG3	1:C:396:ASP:HB2	1.94	0.47
2:D:185:HIS:NE2	7:D:712:HOH:O	2.35	0.47
2:B:119:THR:HG22	2:B:120:GLU:N	2.29	0.47
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.15	0.47
1:C:134:LEU:HG	2:D:62:LEU:HD13	1.96	0.47
2:B:209[A]:THR:HG21	2:B:309:TRP:HE1	1.79	0.47
1:A:396:ASP:OD2	1:A:397:SER:N	2.48	0.47
1:A:442:HIS:CG	3:A:501:HCA:H52	2.50	0.46
2:D:431:ARG:O	2:D:434:VAL:HG12	2.16	0.46
1:A:388:ASP:O	1:A:391[A]:MET:HG3	2.16	0.46
2:D:2:SER:N	7:D:734:HOH:O	2.47	0.46
1:A:27:ASP:OD1	7:A:602:HOH:O	2.20	0.46
2:B:401:ARG:NH1	7:B:736:HOH:O	2.46	0.46
1:C:42:SER:C	1:C:44:LYS:H	2.18	0.46
2:B:194:VAL:HB	2:B:297:HIS:CG	2.50	0.45
2:B:72:PRO:HB2	2:B:99:TYR:CZ	2.51	0.45
1:A:318:GLU:H	1:A:318:GLU:CD	2.19	0.45
2:D:28:ARG:HG3	2:D:34:LYS:HD2	1.98	0.45
1:A:82:SER:HB3	1:A:153:GLU:OE2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLN:NE2	2:B:22:ASP:OD2	2.47	0.45
1:C:412:PHE:O	1:C:416:ILE:HG12	2.17	0.45
1:C:70:VAL:HA	1:C:96:ARG:NH2	2.32	0.44
2:D:268:GLN:NE2	7:D:713:HOH:O	2.36	0.44
2:B:119:THR:CG2	2:B:120:GLU:N	2.80	0.44
2:B:347:GLU:OE2	7:B:704:HOH:O	2.21	0.44
1:A:437:PRO:HB3	1:A:466:THR:HG22	2.00	0.44
2:D:86:MET:HG2	2:D:138:CYS:SG	2.58	0.44
1:A:85:PRO:HD3	1:A:155:PRO:HG2	1.98	0.44
1:A:442:HIS:HB2	7:A:686:HOH:O	2.17	0.44
2:B:254:LEU:O	2:B:255:SER:CB	2.65	0.44
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.53	0.43
1:A:67[B]:SER:OG	1:A:183:CYS:CB	2.66	0.43
2:B:369:LEU:HD13	2:B:379:LEU:HD23	1.99	0.43
2:D:253:LEU:O	2:D:276[A]:THR:CG2	2.67	0.43
1:A:437:PRO:HA	1:A:472:TRP:CZ2	2.54	0.43
1:C:76:LYS:HA	1:C:110:VAL:HG23	2.01	0.43
1:C:359:ARG:N	1:C:360:PRO:CD	2.81	0.43
1:A:81:ILE:HD12	1:A:134:LEU:HD21	2.00	0.43
2:D:43:VAL:O	2:D:47:THR:HG23	2.18	0.43
1:C:415:ARG:HH11	1:C:415:ARG:HG3	1.83	0.43
1:C:60:ARG:NH2	7:C:624:HOH:O	2.44	0.42
2:D:445:ASN:HB2	2:D:472:PRO:O	2.19	0.42
2:D:139:LYS:HZ3	2:D:176:PRO:HG2	1.83	0.42
1:A:67[B]:SER:HG	1:A:183:CYS:CB	2.32	0.42
1:A:356:GLY:HA3	4:A:502:ICS:S1B	2.60	0.42
2:B:247:MET:HG2	2:B:341:PRO:CD	2.50	0.42
1:C:96:ARG:NH1	4:C:502:ICS:S5A	2.93	0.42
1:A:457:ALA:HB1	2:B:8:ILE:HD12	2.02	0.42
1:C:275:CYS:HA	1:C:358:LEU:HD22	2.02	0.42
2:D:312:GLU:O	2:D:312:GLU:HG3	2.20	0.42
2:D:73:LEU:HD11	7:D:721:HOH:O	2.20	0.41
1:A:17:LEU:HB3	1:A:25:ARG:HG3	2.02	0.41
1:A:213[B]:ASP:CG	1:A:215:THR:HG22	2.40	0.41
1:C:396:ASP:O	1:C:397:SER:HB2	2.21	0.41
2:D:88:TYR:O	2:D:149:VAL:HA	2.20	0.41
1:A:415:ARG:NH1	7:A:643:HOH:O	2.53	0.41
1:C:415:ARG:O	1:C:415:ARG:HD2	2.20	0.41
1:A:213[B]:ASP:OD1	1:A:215:THR:HG22	2.20	0.41
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.56	0.41
1:A:277:ARG:HD2	1:A:386:ASP:OD2	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:TRP:O	2:B:365:LYS:HE3	2.21	0.41
1:C:437:PRO:HA	1:C:472:TRP:CZ2	2.56	0.41
1:A:66:GLY:O	1:A:70:VAL:HB	2.20	0.41
1:A:156:ILE:HG22	1:A:182:ARG:HH12	1.86	0.41
1:A:439:ARG:HD3	1:A:466:THR:OG1	2.21	0.41
1:C:65:ALA:O	1:C:70:VAL:HG13	2.21	0.41
1:C:379:TYR:CG	1:C:382:ALA:HB2	2.55	0.41
1:A:115:THR:HG23	2:B:63:THR:HB	2.04	0.40
2:D:245:SER:OG	7:D:705:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:871:HOH:O	7:D:957:HOH:O[2_655]	2.10	0.10

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/492 (97%)	459 (96%)	18 (4%)	2 (0%)	34	40
1	C	476/492 (97%)	454 (95%)	20 (4%)	2 (0%)	34	40
2	B	521/523 (100%)	503 (96%)	17 (3%)	1 (0%)	47	57
2	D	522/523 (100%)	509 (98%)	13 (2%)	0	100	100
All	All	1998/2030 (98%)	1925 (96%)	68 (3%)	5 (0%)	41	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	255	SER
1	C	43	LYS
1	A	355	ILE
1	C	355	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/415 (96%)	387 (97%)	11 (3%)	43	57
1	C	394/415 (95%)	380 (96%)	14 (4%)	35	47
2	B	447/454 (98%)	437 (98%)	10 (2%)	52	66
2	D	450/454 (99%)	442 (98%)	8 (2%)	59	72
All	All	1689/1738 (97%)	1646 (98%)	43 (2%)	47	62

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	CYS
1	A	96	ARG
1	A	98	ASN
1	A	209	LYS
1	A	264	LEU
1	A	362	HIS
1	A	391[A]	MET
1	A	391[B]	MET
1	A	409	PHE
1	A	445	ASP
1	A	467	LEU
2	B	92	SER
2	B	120	GLU
2	B	139	LYS
2	B	158	ILE
2	B	175	ILE
2	B	222	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	258	GLU
2	B	369	LEU
2	B	503	GLU
2	B	505	LEU
1	C	29	ASN
1	C	41	GLN
1	C	45	CYS
1	C	70	VAL
1	C	98	ASN
1	C	165	SER
1	C	182	ARG
1	C	264	LEU
1	C	362	HIS
1	C	391	MET
1	C	401	TYR
1	C	445	ASP
1	C	473	LYS
1	C	476	GLN
2	D	216	LYS
2	D	279	GLU
2	D	315	LYS
2	D	379	LEU
2	D	434	VAL
2	D	453	ARG
2	D	505	LEU
2	D	512	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	HCA	A	501	-	13,13,13	1.01	0	14,18,18	1.87	1 (7%)
5	CLF	D	601	1,2	0,24,24	-	-	-	-	-
4	ICS	A	502	1	18,30,30	2.50	9 (50%)	-	-	-
5	CLF	B	601	1,2	0,24,24	-	-	-	-	-
3	HCA	C	501	-	13,13,13	0.89	0	14,18,18	1.12	1 (7%)
4	ICS	C	502	1	18,30,30	2.41	10 (55%)	-	-	-

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
5	CLF	D	601	1,2	-	-	0/12/10/10
3	HCA	C	501	-	-	0/17/17/17	-
5	CLF	B	601	1,2	-	-	0/12/10/10
3	HCA	A	501	-	-	13/17/17/17	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S3B-FE6	-5.16	2.19	2.32
4	C	502	ICS	S4B-FE7	-4.72	2.20	2.32
4	A	502	ICS	S4B-FE7	-4.25	2.21	2.32
4	A	502	ICS	S1B-FE6	-3.72	2.23	2.32
4	C	502	ICS	S2A-FE2	-3.42	2.23	2.32
4	C	502	ICS	S3B-FE7	-3.42	2.23	2.32
4	C	502	ICS	S1B-FE6	-3.31	2.24	2.32
4	A	502	ICS	S1B-FE5	-3.03	2.24	2.32
4	C	502	ICS	S3B-FE6	-2.90	2.25	2.32

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	ICS	S2A-FE2	-2.74	2.25	2.32
4	C	502	ICS	S4B-FE5	-2.68	2.25	2.32
4	A	502	ICS	S3B-FE7	-2.66	2.25	2.32
4	C	502	ICS	S1B-FE5	-2.41	2.26	2.32
4	C	502	ICS	S1A-FE2	-2.40	2.26	2.32
4	C	502	ICS	S1A-FE4	-2.40	2.26	2.32
4	A	502	ICS	S4A-FE3	-2.19	2.26	2.32
4	C	502	ICS	S2B-FE6	-2.18	2.19	2.24
4	A	502	ICS	S4A-FE4	-2.10	2.27	2.32
4	A	502	ICS	S3A-FE5	2.07	2.29	2.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HCA	O6-C7-C3	4.98	121.70	113.05
3	C	501	HCA	O6-C7-C3	2.85	117.99	113.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HCA	C2-C3-C4-C5
3	A	501	HCA	O7-C3-C4-C5
3	A	501	HCA	C7-C3-C4-C5
3	A	501	HCA	O7-C3-C7-O5
3	A	501	HCA	O7-C3-C7-O6
3	A	501	HCA	C2-C3-C7-O5
3	A	501	HCA	C2-C3-C7-O6
3	A	501	HCA	C4-C3-C7-O5
3	A	501	HCA	C4-C3-C7-O6
3	A	501	HCA	O1-C1-C2-C3
3	A	501	HCA	O2-C1-C2-C3
3	A	501	HCA	C1-C2-C3-C4
3	A	501	HCA	C1-C2-C3-C7

There are no ring outliers.

3 monomers are involved in 6 short contacts:

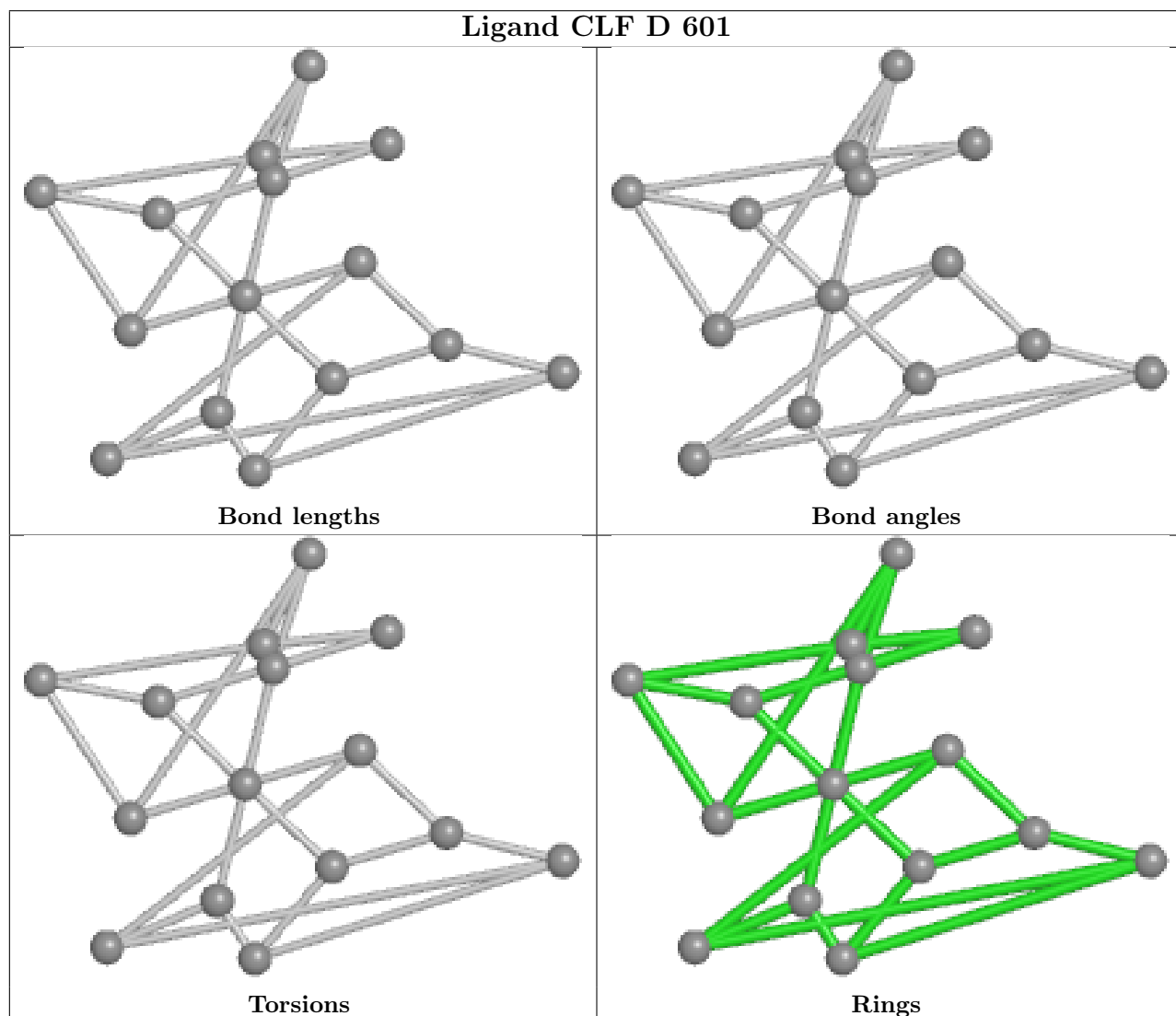
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HCA	3	0
4	A	502	ICS	2	0

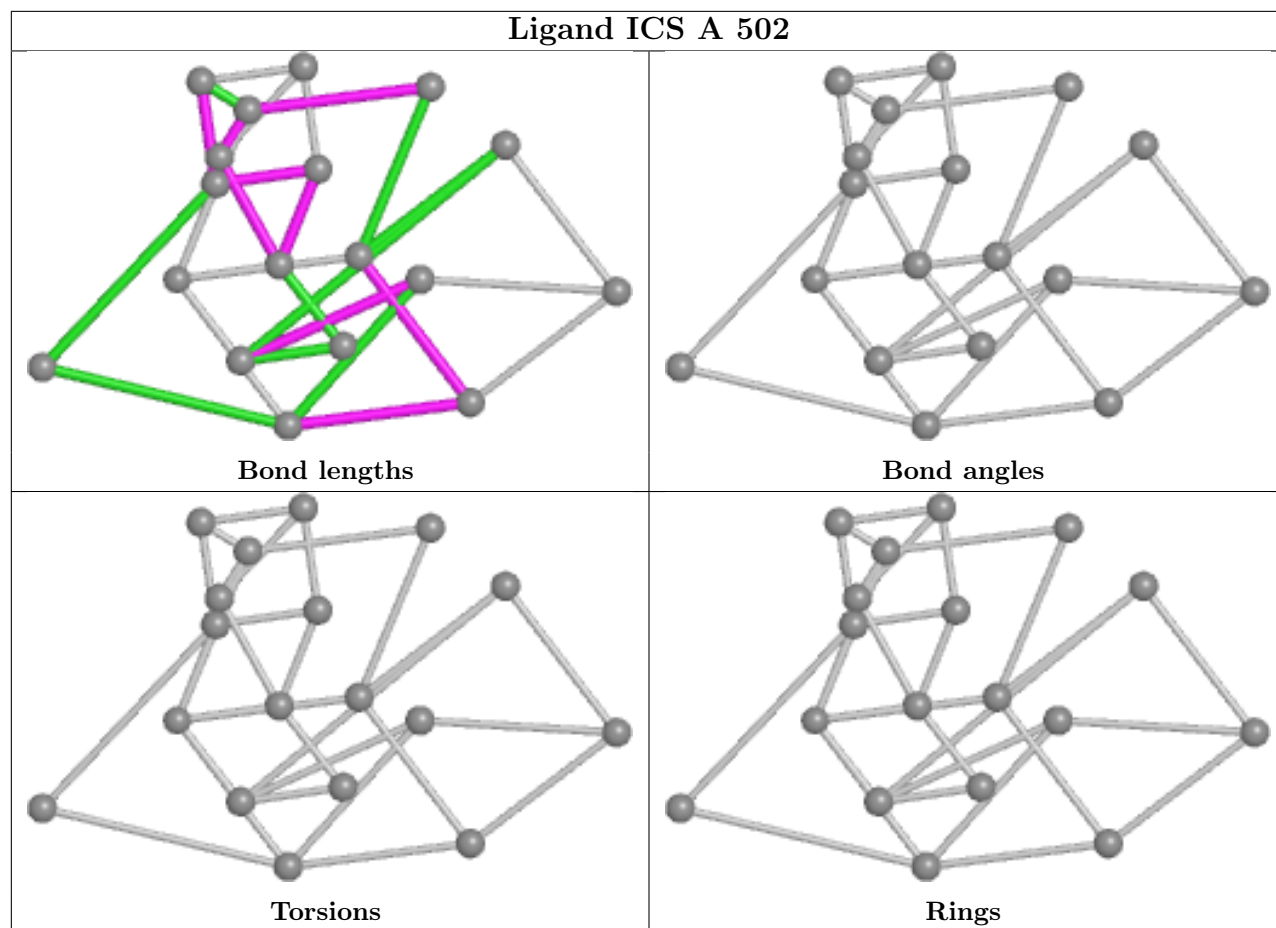
Continued on next page...

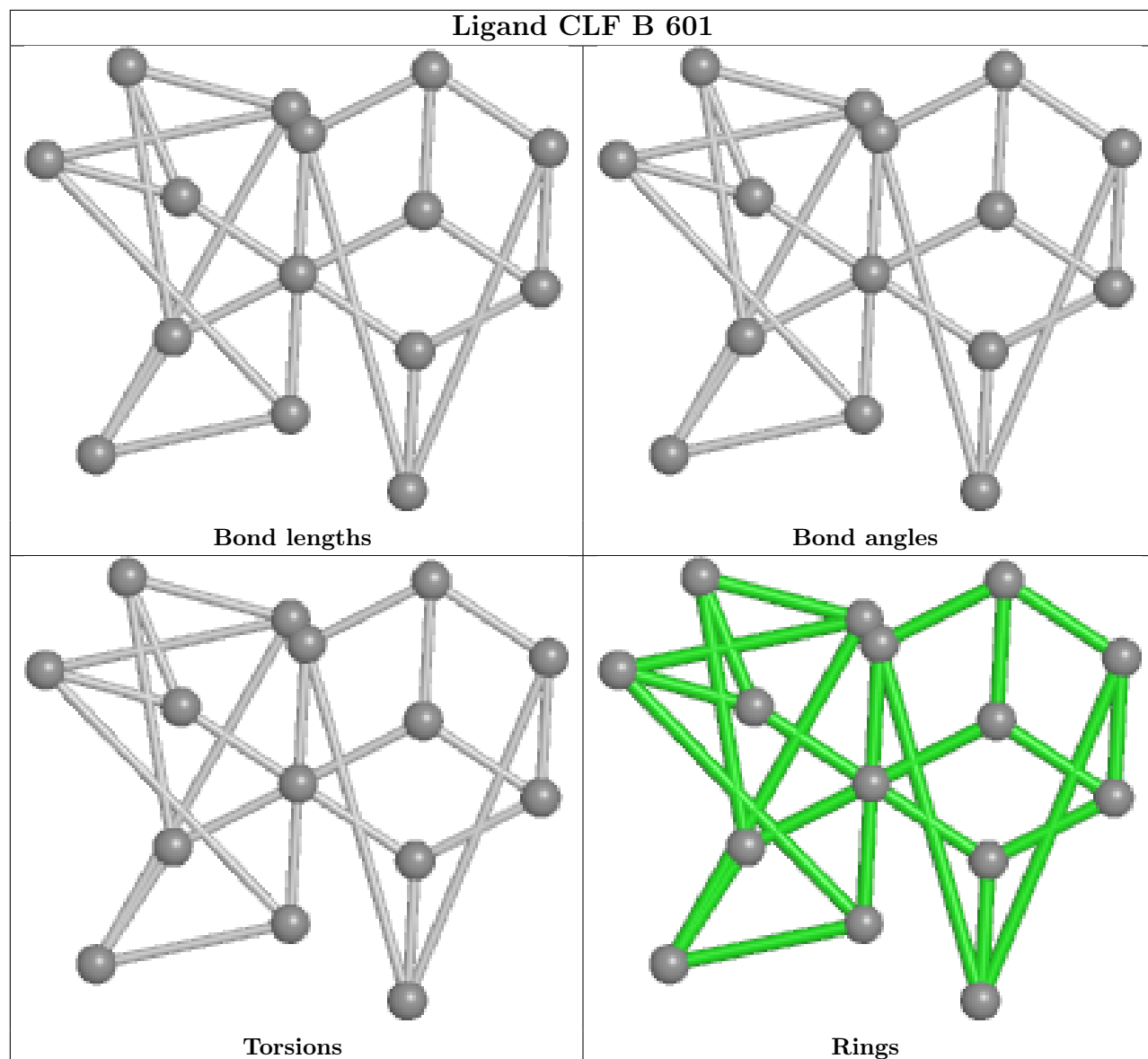
*Continued from previous page...*

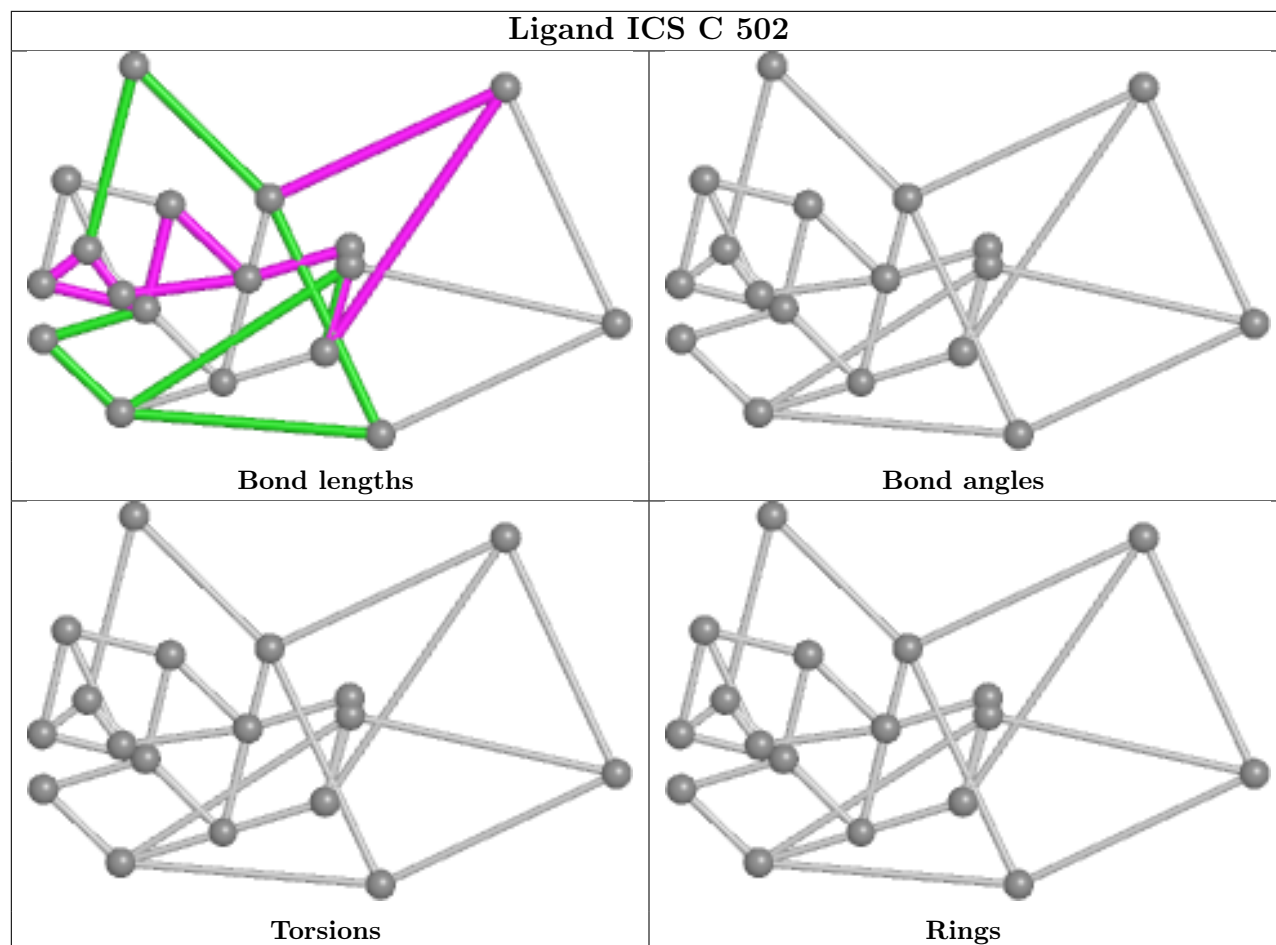
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	ICS	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	476/492 (96%)	-0.18	5 (1%) 80 84	17, 24, 38, 53	0
1	C	478/492 (97%)	-0.16	3 (0%) 89 91	18, 25, 40, 59	0
2	B	522/523 (99%)	-0.27	1 (0%) 95 96	14, 22, 30, 44	0
2	D	522/523 (99%)	-0.24	1 (0%) 95 96	15, 23, 32, 45	0
All	All	1998/2030 (98%)	-0.21	10 (0%) 91 93	14, 23, 35, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	THR	6.3
1	C	481	ALA	4.6
1	A	212	GLU	4.4
2	D	124	VAL	3.1
1	C	38	ALA	3.1
1	A	38	ALA	2.3
1	C	37	PRO	2.2
1	A	213[A]	ASP	2.2
1	A	216	PHE	2.2
2	B	124	VAL	2.1

### 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](#)

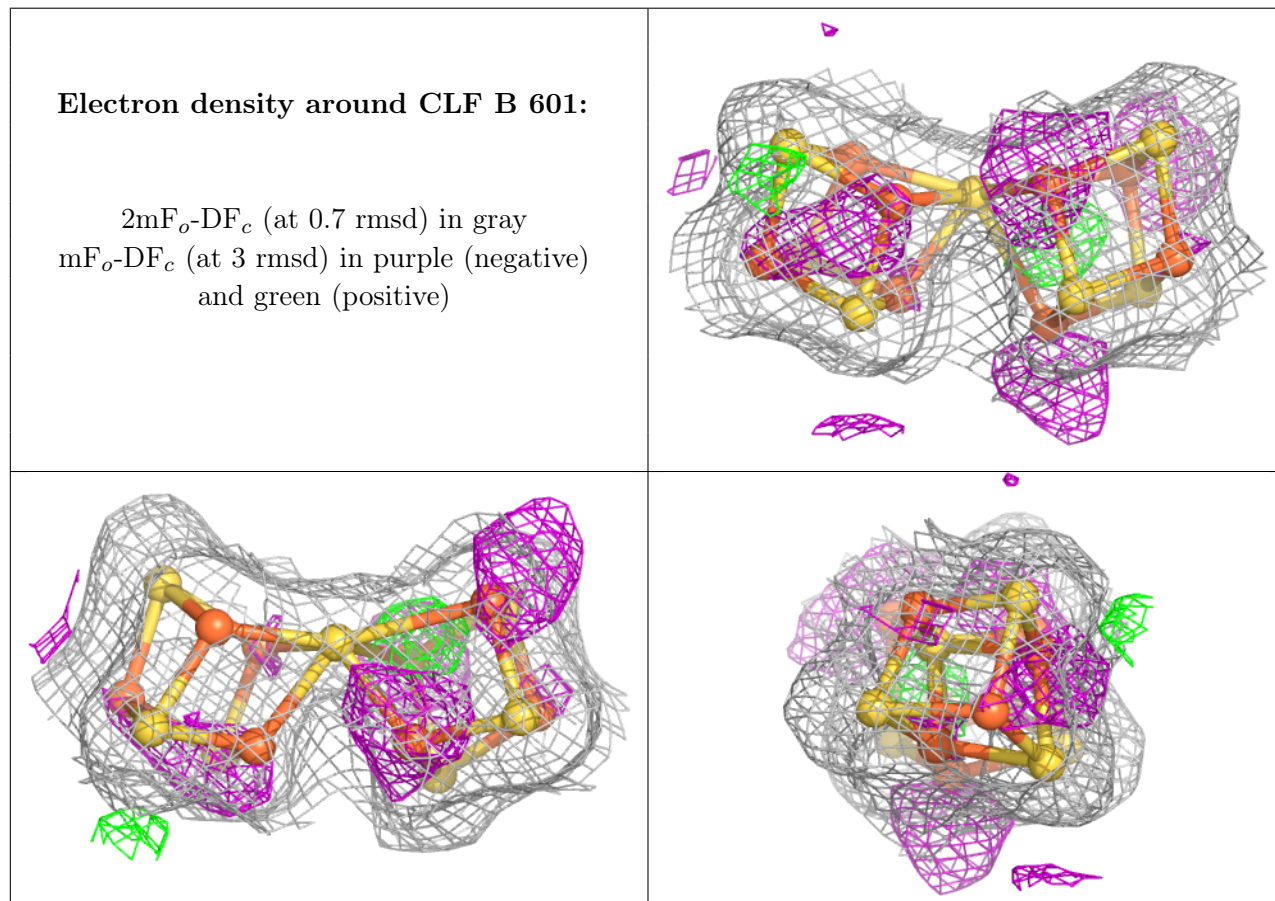
There are no monosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
5	CLF	B	601	15/15	0.92	0.07	18,26,36,37	0
5	CLF	D	601	15/15	0.92	0.08	20,28,37,39	0
4	ICS	A	502	18/18	0.96	0.08	16,19,29,31	0
4	ICS	C	502	18/18	0.96	0.09	14,19,29,29	0
6	FE	B	602	1/1	0.96	0.06	23,23,23,23	1
6	FE	D	602	1/1	0.96	0.06	24,24,24,24	1
3	HCA	A	501	14/14	0.97	0.13	17,21,23,23	0
3	HCA	C	501	14/14	0.97	0.12	17,20,22,22	0

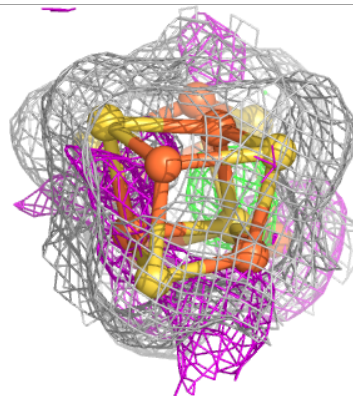
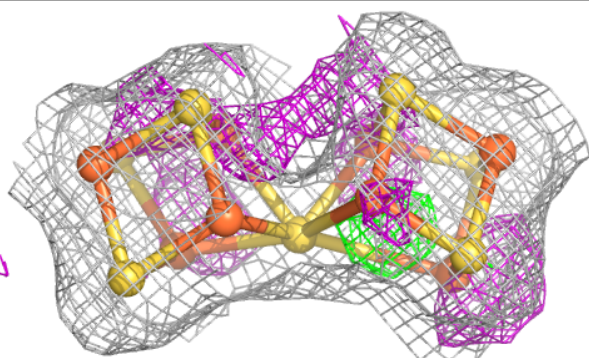
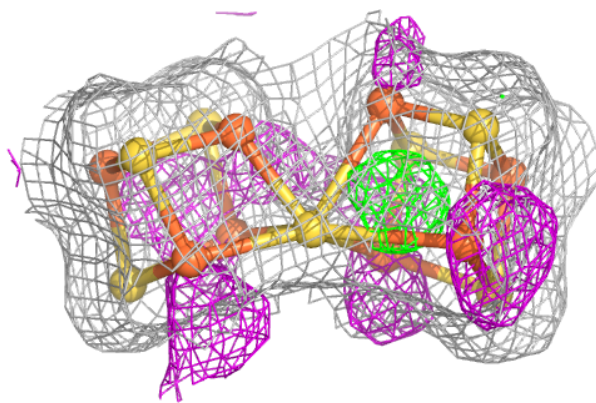
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





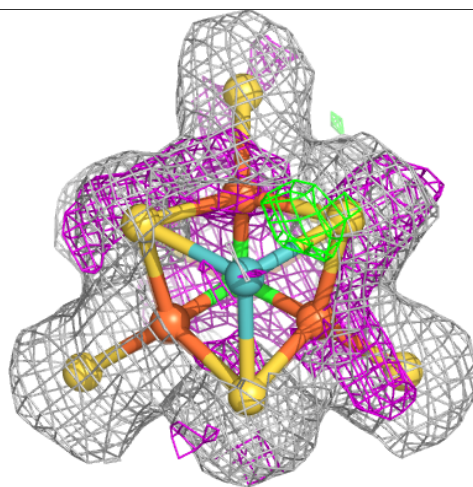
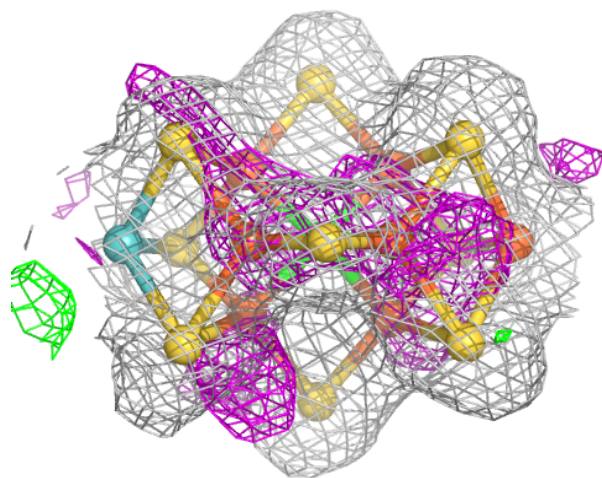
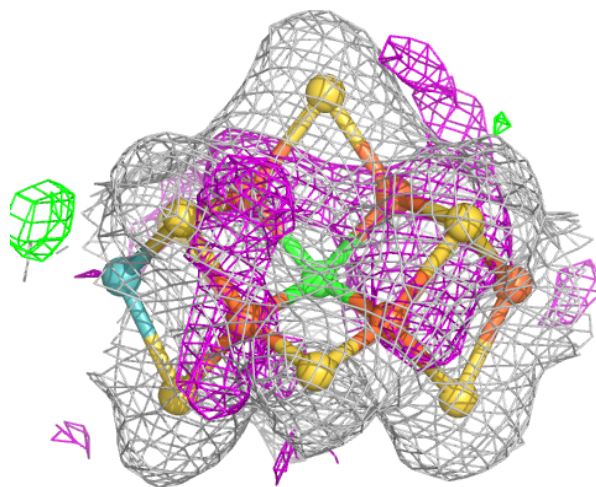
**Electron density around CLF D 601:**

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



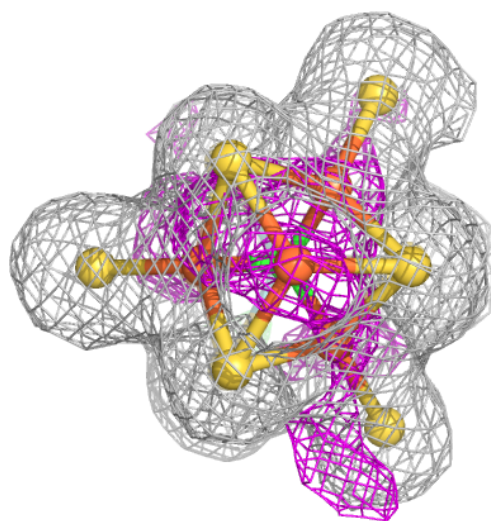
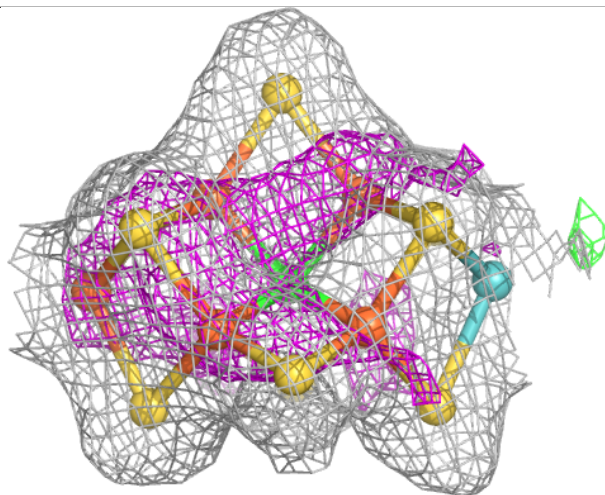
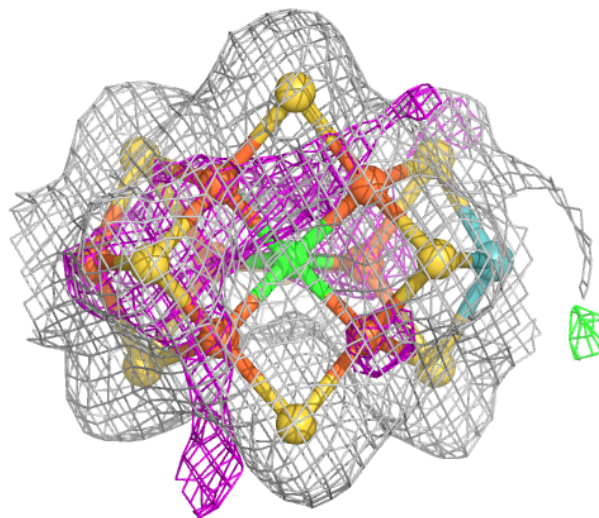
**Electron density around ICS A 502:**

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



**Electron density around ICS C 502:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.