



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2022 – 11:03 AM EDT

PDB ID : 7UBZ
Title : Chymotrypsin digested toxin/immunity complex for a T6SS lipase effector from *E. cloacae*
Authors : Cuthbert, B.J.; Jensen, S.J.; Goulding, C.W.; Hayes, C.S.
Deposited on : 2022-03-15
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 2.29
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) : 2.29

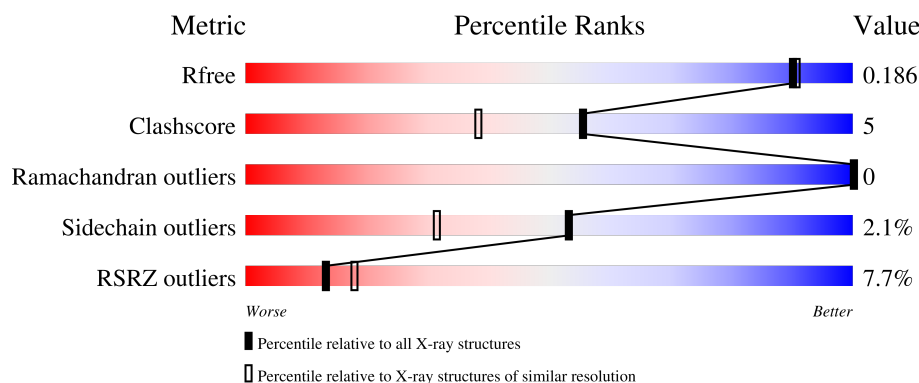
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	230	<div> <div>3%</div> <div>93%</div> <div>7%</div> </div>
1	C	230	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
2	B	313	<div> <div>7%</div> <div>53%</div> <div>8%</div> <div>39%</div> </div>
2	D	313	<div> <div>11%</div> <div>58%</div> <div>6%</div> <div>35%</div> </div>

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
3	GOL	D	903	-	X	-	-
5	MIE	D	901	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7837 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 Ankyrin repeat domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	2	0
			1796	1138	308	343	7			
1	C	230	Total	C	N	O	S	0	6	0
			1819	1152	313	347	7			

- Molecule 2 is a protein called T6SS lipase effector.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	4	0
			1462	913	263	282	4			
2	D	202	Total	C	N	O	S	0	9	0
			1557	969	285	299	4			

There are 24 discrepancies between the modelled and reference sequences:

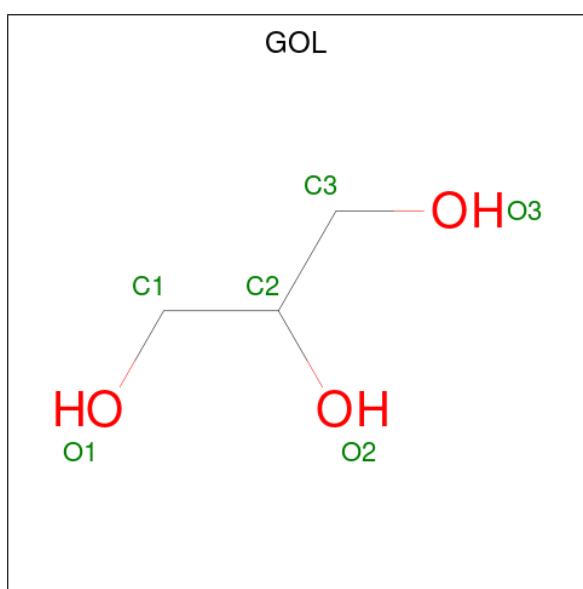
Chain	Residue	Modelled	Actual	Comment	Reference
B	160	MET	-	expression tag	UNP A0A0M7ENE2
B	161	ALA	-	expression tag	UNP A0A0M7ENE2
B	162	LYS	-	expression tag	UNP A0A0M7ENE2
B	163	SER	-	expression tag	UNP A0A0M7ENE2
B	164	HIS	-	expression tag	UNP A0A0M7ENE2
B	165	HIS	-	expression tag	UNP A0A0M7ENE2
B	166	HIS	-	expression tag	UNP A0A0M7ENE2
B	167	HIS	-	expression tag	UNP A0A0M7ENE2
B	168	HIS	-	expression tag	UNP A0A0M7ENE2
B	169	HIS	-	expression tag	UNP A0A0M7ENE2
B	170	THR	-	expression tag	UNP A0A0M7ENE2
B	171	SER	-	expression tag	UNP A0A0M7ENE2
D	160	MET	-	expression tag	UNP A0A0M7ENE2
D	161	ALA	-	expression tag	UNP A0A0M7ENE2
D	162	LYS	-	expression tag	UNP A0A0M7ENE2
D	163	SER	-	expression tag	UNP A0A0M7ENE2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	164	HIS	-	expression tag	UNP A0A0M7ENE2
D	165	HIS	-	expression tag	UNP A0A0M7ENE2
D	166	HIS	-	expression tag	UNP A0A0M7ENE2
D	167	HIS	-	expression tag	UNP A0A0M7ENE2
D	168	HIS	-	expression tag	UNP A0A0M7ENE2
D	169	HIS	-	expression tag	UNP A0A0M7ENE2
D	170	THR	-	expression tag	UNP A0A0M7ENE2
D	171	SER	-	expression tag	UNP A0A0M7ENE2

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



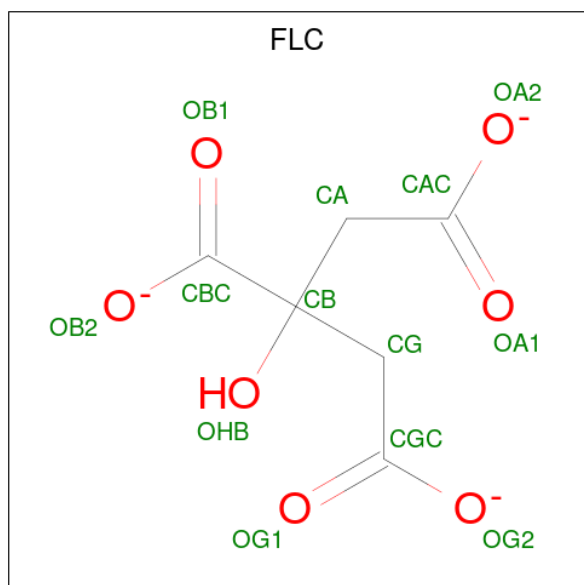
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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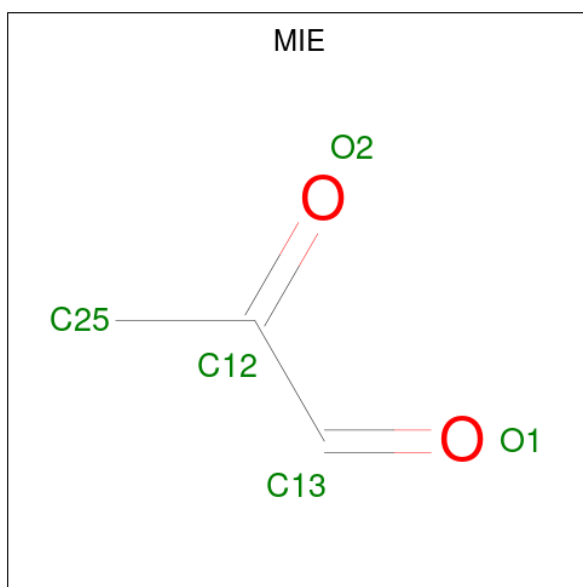
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	6	7		

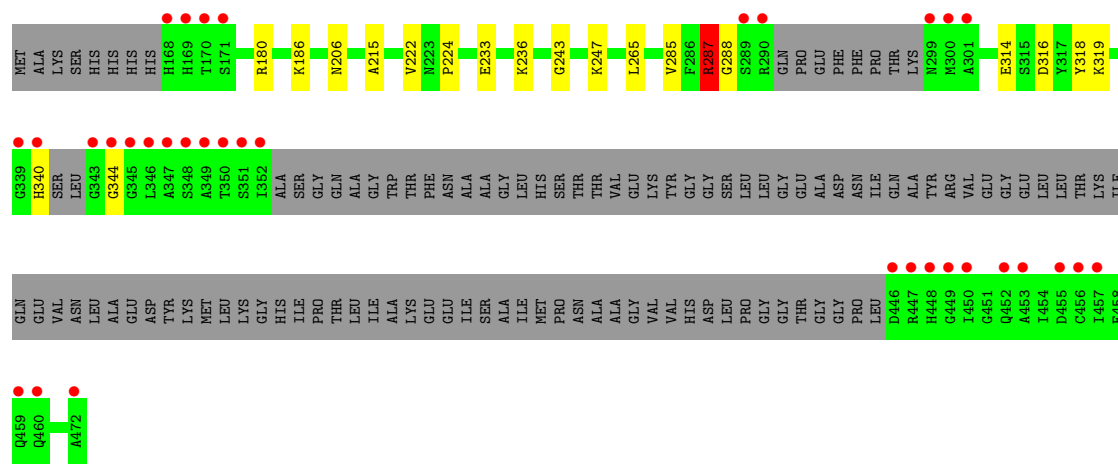
- Molecule 5 is methylglyoxal (three-letter code: MIE) (formula: $C_3H_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 3 3	0	0
5	D	1	Total C 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	394	Total O 394 394	0	0
6	C	393	Total O 393 393	0	0
6	B	173	Total O 173 173	0	0
6	D	170	Total O 170 170	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.17Å 120.49Å 122.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.76 – 1.75 38.88 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.76-1.75) 99.0 (38.88-1.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.1-4122	Depositor
R, R_{free}	0.164 , 0.188 0.161 , 0.186	Depositor DCC
R_{free} test set	13008 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, MIE, FLC

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	0.62	0/1833	0.74	0/2484
1	C	0.59	0/1871	0.75	0/2535
2	B	0.69	3/1492 (0.2%)	0.84	3/2012 (0.1%)
2	D	0.51	0/1596	0.76	2/2148 (0.1%)
All	All	0.61	3/6792 (0.0%)	0.77	5/9179 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	ARG	CZ-NH2	10.07	1.46	1.33
2	B	180	ARG	NE-CZ	9.41	1.45	1.33
2	B	180	ARG	CZ-NH1	8.87	1.44	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	180	ARG	NE-CZ-NH1	10.24	125.42	120.30
2	B	180	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
2	B	180	ARG	NE-CZ-NH2	6.16	123.38	120.30
2	D	287[A]	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	287[B]	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	1796	0	1810	11	0
1	C	1819	0	1840	14	0
2	B	1462	0	1438	16	0
2	D	1557	0	1521	25	0
3	A	18	0	22	2	0
3	B	18	0	23	2	0
3	C	6	0	7	0	0
3	D	12	0	15	1	0
4	C	13	0	5	2	0
5	B	3	0	0	0	0
5	D	3	0	0	7	0
6	A	394	0	0	4	1
6	B	173	0	0	2	0
6	C	393	0	0	7	1
6	D	170	0	0	8	0
All	All	7837	0	6681	68	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 5.

All (68) 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)
2:D:180[A]:ARG:HH22	5:D:901:MIE:C12	0.99	1.54
2:D:180[A]:ARG:NH1	5:D:901:MIE:C13	1.72	1.48
2:D:180[A]:ARG:NH2	5:D:901:MIE:C12	1.75	1.04
1:C:63:GLU:OE1	6:C:401:HOH:O	1.85	0.93
2:D:233[A]:GLU:OE2	6:D:1001:HOH:O	1.96	0.84
1:C:6[B]:ASP:OD2	1:C:18[B]:ARG:NH2	2.10	0.84
2:B:287[A]:ARG:HG2	2:B:287[A]:ARG:HH11	1.42	0.83
2:D:287[A]:ARG:HH11	2:D:287[A]:ARG:HG2	1.44	0.82
2:D:186:LYS:NZ	6:D:1002:HOH:O	2.13	0.82
1:C:18[B]:ARG:NH1	6:C:402:HOH:O	2.14	0.80
2:D:180[A]:ARG:NH1	5:D:901:MIE:C12	2.47	0.73
2:D:180[B]:ARG:HH21	2:D:206:ASN:HD21	1.39	0.70
2:D:180[A]:ARG:HH11	2:D:206:ASN:HD21	1.40	0.70
2:D:340:HIS:HA	2:D:344:GLY:HA2	1.73	0.69
4:C:301:FLC:OA2	4:C:301:FLC:OHB	2.11	0.67
2:D:180[A]:ARG:CZ	5:D:901:MIE:C13	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:GLU:OE2	6:B:601:HOH:O	2.15	0.64
1:A:3:LEU:HB2	3:A:301:GOL:H32	1.79	0.64
1:C:219[B]:GLN:HG2	6:C:478:HOH:O	1.98	0.64
2:D:243:GLY:O	2:D:247[B]:LYS:HE2	1.99	0.62
1:C:141:ASP:OD1	1:C:175[B]:ARG:NH2	2.34	0.61
1:A:30:LYS:NZ	6:A:401:HOH:O	2.33	0.61
3:B:503:GOL:H12	6:B:722:HOH:O	2.02	0.58
3:D:902:GOL:O2	6:D:1003:HOH:O	2.17	0.58
1:C:62:PRO:HD2	6:C:401:HOH:O	2.03	0.58
2:D:287[A]:ARG:HH11	2:D:287[A]:ARG:CG	2.15	0.57
2:B:257[B]:ASP:OD1	2:B:262:PRO:HA	2.04	0.57
2:D:247[A]:LYS:HE3	6:D:1015:HOH:O	2.05	0.56
2:D:236:LYS:HE2	6:D:1017:HOH:O	2.05	0.55
2:D:236:LYS:NZ	6:D:1005:HOH:O	2.28	0.54
1:A:170:LEU:O	1:A:174:GLU:HG3	2.06	0.54
2:B:180:ARG:NE	3:B:503:GOL:O2	2.26	0.53
2:B:324:LEU:O	2:B:328:LEU:HG	2.10	0.52
2:B:215:ALA:HA	2:B:285:VAL:HG11	1.91	0.51
1:A:164[B]:HIS:CE1	6:A:404:HOH:O	2.63	0.51
2:D:287[A]:ARG:NH1	2:D:288:GLY:O	2.44	0.50
1:C:174:GLU:OE1	6:C:403:HOH:O	2.19	0.50
2:D:319:LYS:HD2	6:D:1050:HOH:O	2.12	0.49
2:D:186:LYS:NZ	6:D:1009:HOH:O	2.43	0.49
2:D:180[A]:ARG:NH2	5:D:901:MIE:C25	2.69	0.48
1:A:1:MET:N	2:B:306:ASN:HD21	2.12	0.47
2:B:257[A]:ASP:OD1	2:B:320:ARG:HD2	2.13	0.47
2:D:314:GLU:HG2	2:D:316:ASP:OD1	2.14	0.47
1:A:107:ASN:HD22	3:A:302:GOL:H32	1.78	0.47
2:B:247:LYS:HE2	2:B:248:TYR:CZ	2.49	0.47
2:B:287[A]:ARG:HG2	2:B:287[A]:ARG:NH1	2.18	0.47
2:B:186:LYS:HB2	2:B:186:LYS:HE2	1.65	0.47
2:B:314:GLU:OE2	2:B:319:LYS:HD3	2.15	0.47
1:C:66:ASN:O	1:C:70:MET:HG2	2.14	0.46
1:A:226:PRO:HB3	6:A:507:HOH:O	2.15	0.46
1:A:39:LYS:NZ	6:A:413:HOH:O	2.49	0.45
2:B:219:TYR:HB3	2:B:447:ARG:HD2	1.99	0.45
1:C:214:LYS:HB3	1:C:214:LYS:HE3	1.62	0.45
1:C:61:THR:HB	6:C:401:HOH:O	2.16	0.45
2:B:240:ASN:HA	2:B:252:LYS:HD3	1.97	0.45
1:C:208:LYS:HA	4:C:301:FLC:OA2	2.17	0.45
2:B:465:ILE:O	2:B:469:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:SER:HB3	2:B:317:TYR:CD2	2.52	0.44
2:D:180[A]:ARG:CZ	5:D:901:MIE:C12	2.43	0.44
2:D:316:ASP:HB3	2:D:318:TYR:CD2	2.53	0.43
2:D:215:ALA:HA	2:D:285:VAL:HG11	2.00	0.43
1:A:112:PRO:HB2	1:A:144:ALA:HB2	2.00	0.42
1:C:209:LYS:HD3	1:C:209:LYS:HA	1.85	0.41
1:C:209:LYS:HE3	6:C:657:HOH:O	2.20	0.41
1:C:170:LEU:O	1:C:174:GLU:HG3	2.21	0.41
1:A:164[B]:HIS:O	1:A:164[B]:HIS:ND1	2.52	0.40
1:A:42:LYS:HA	1:A:42:LYS:HD2	1.83	0.40
2:D:222:VAL:O	2:D:224:PRO:HD3	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)
6:A:687:HOH:O	6:C:401:HOH:O[3_645]	2.02	0.18

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	230/230 (100%)	229 (100%)	1 (0%)	0	100	100
1	C	234/230 (102%)	233 (100%)	1 (0%)	0	100	100
2	B	189/313 (60%)	188 (100%)	1 (0%)	0	100	100
2	D	203/313 (65%)	201 (99%)	2 (1%)	0	100	100
All	All	856/1086 (79%)	851 (99%)	5 (1%)	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	195/195 (100%)	190 (97%)	5 (3%)	46	23
1	C	199/195 (102%)	195 (98%)	4 (2%)	55	34
2	B	148/245 (60%)	144 (97%)	4 (3%)	44	22
2	D	155/245 (63%)	152 (98%)	3 (2%)	57	37
All	All	697/880 (79%)	681 (98%)	16 (2%)	53	28

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	116	ASP
1	A	131	LYS
1	A	152	LEU
1	A	163	PHE
1	C	159	ASP
1	C	163	PHE
1	C	199	ARG
1	C	214	LYS
2	B	287[A]	ARG
2	B	287[B]	ARG
2	B	315	SER
2	B	334	LYS
2	D	265	LEU
2	D	287[A]	ARG
2	D	287[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	22	ASN
1	C	220	HIS
2	B	306	ASN

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Mol	Chain	Res	Type
2	D	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	GOL	A	302	-	5,5,5	2.29	2 (40%)	5,5,5	1.32	1 (20%)
3	GOL	B	501	-	5,5,5	1.19	0	5,5,5	0.82	0
3	GOL	D	903	-	5,5,5	1.74	2 (40%)	5,5,5	0.85	0
3	GOL	B	504	-	5,5,5	1.10	0	5,5,5	0.87	0
4	FLC	C	301	-	12,12,12	1.27	2 (16%)	17,17,17	1.80	4 (23%)
5	MIE	D	901	2	2,2,4	0.30	0	0,1,4	-	-
3	GOL	D	902	-	5,5,5	1.03	0	5,5,5	0.80	0
3	GOL	C	302	-	5,5,5	0.96	0	5,5,5	1.81	2 (40%)
5	MIE	B	502	2	2,2,4	0.25	0	0,1,4	-	-
3	GOL	A	301	-	5,5,5	1.02	0	5,5,5	0.73	0
3	GOL	A	303	-	5,5,5	1.27	1 (20%)	5,5,5	0.81	0
3	GOL	B	503	-	5,5,5	1.81	1 (20%)	5,5,5	1.04	1 (20%)

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
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	B	501	-	-	4/4/4/4	-
3	GOL	D	903	-	-	4/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
4	FLC	C	301	-	-	6/16/16/16	-
3	GOL	D	902	-	-	4/4/4/4	-
3	GOL	C	302	-	-	3/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	GOL	O2-C2	-4.37	1.30	1.43
3	B	503	GOL	O2-C2	-3.23	1.33	1.43
4	C	301	FLC	OA2-CAC	-2.88	1.21	1.30
3	D	903	GOL	C3-C2	2.70	1.62	1.51
4	C	301	FLC	OA1-CAC	2.60	1.30	1.22
3	A	302	GOL	O1-C1	-2.33	1.32	1.42
3	D	903	GOL	O2-C2	-2.23	1.36	1.43
3	A	303	GOL	C3-C2	2.02	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	FLC	OHB-CB-CA	-4.64	98.55	109.40
4	C	301	FLC	CB-CA-CAC	-3.23	105.99	113.81
4	C	301	FLC	CA-CB-CBC	3.00	116.56	110.11
3	C	302	GOL	C3-C2-C1	-2.72	101.12	111.70
3	C	302	GOL	O2-C2-C3	2.63	120.72	109.12
4	C	301	FLC	OA2-CAC-CA	2.21	121.45	114.35
3	B	503	GOL	C3-C2-C1	-2.08	103.61	111.70
3	A	302	GOL	O1-C1-C2	-2.08	100.22	110.20

There are no chirality outliers.

All (29) torsion outliers are listed below:

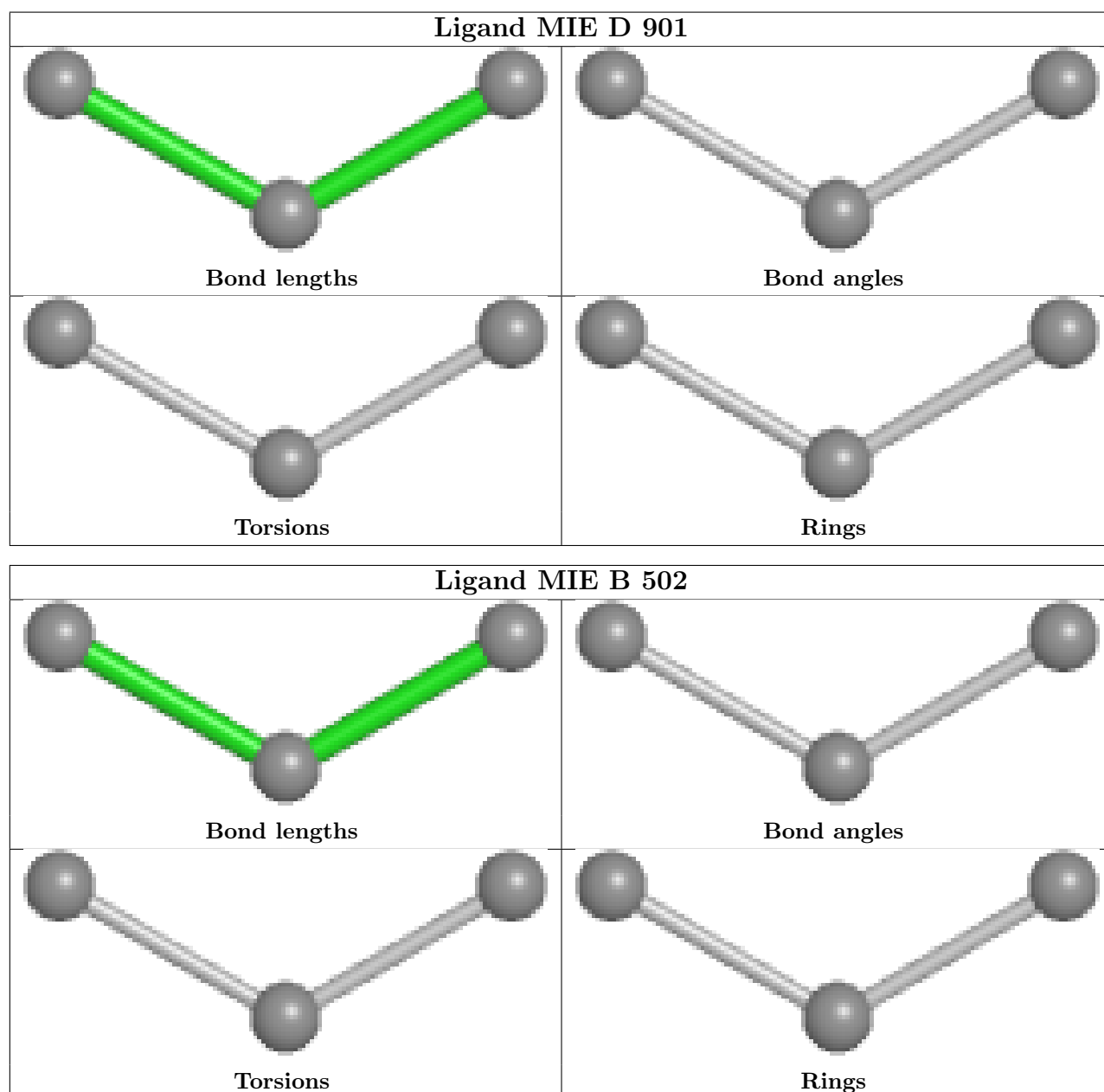
Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-C3
3	B	501	GOL	O1-C1-C2-C3
3	B	501	GOL	C1-C2-C3-O3
3	B	501	GOL	O2-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
3	D	902	GOL	C1-C2-C3-O3
3	D	903	GOL	O1-C1-C2-C3
3	B	503	GOL	O2-C2-C3-O3
3	A	301	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	B	504	GOL	C1-C2-C3-O3
3	D	902	GOL	O1-C1-C2-C3
3	D	903	GOL	C1-C2-C3-O3
3	B	501	GOL	O1-C1-C2-O2
3	D	902	GOL	O1-C1-C2-O2
3	D	902	GOL	O2-C2-C3-O3
4	C	301	FLC	OHB-CB-CG-CGC
3	C	302	GOL	O2-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
3	D	903	GOL	O2-C2-C3-O3
3	D	903	GOL	O1-C1-C2-O2
4	C	301	FLC	CAC-CA-CB-CBC
4	C	301	FLC	CA-CB-CBC-OB2
4	C	301	FLC	CB-CA-CAC-OA2
4	C	301	FLC	CB-CA-CAC-OA1
3	C	302	GOL	O1-C1-C2-C3
4	C	301	FLC	CAC-CA-CB-CG
3	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	GOL	1	0
4	C	301	FLC	2	0
5	D	901	MIE	7	0
3	D	902	GOL	1	0
3	A	301	GOL	1	0
3	B	503	GOL	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/230 (100%)	0.16	8 (3%) 44 50	19, 24, 39, 77	0
1	C	230/230 (100%)	0.08	2 (0%) 84 89	18, 24, 38, 75	0
2	B	191/313 (61%)	0.60	22 (11%) 4 6	21, 34, 61, 79	0
2	D	202/313 (64%)	0.87	34 (16%) 1 2	21, 35, 74, 90	0
All	All	853/1086 (78%)	0.41	66 (7%) 13 18	18, 28, 61, 90	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	346	LEU	10.1
2	B	301	ALA	8.7
2	D	340	HIS	8.6
2	D	301	ALA	8.1
2	B	170	THR	7.9
2	D	448	HIS	6.9
2	D	289	SER	6.9
2	D	344	GLY	6.8
1	A	1	MET	6.7
2	D	300	MET	6.3
2	D	446	ASP	6.2
2	D	290	ARG	6.1
2	D	450	ILE	6.0
2	D	347	ALA	5.9
2	B	456	CYS	5.9
2	D	352	ILE	5.9
2	B	450	ILE	5.6
2	B	300	MET	5.6
2	D	339	GLY	5.6
2	D	345	GLY	5.5
2	D	351	SER	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	168	HIS	5.4
2	B	289	SER	5.2
2	B	448	HIS	5.1
1	A	230	LYS	5.0
2	B	169	HIS	5.0
2	D	456	CYS	4.6
2	D	348	SER	4.5
2	B	453	ALA	4.5
2	B	299	ASN	4.4
2	D	343	GLY	4.2
2	D	459	GLN	4.2
2	B	290	ARG	4.1
1	C	1	MET	4.1
2	D	350	THR	4.0
2	B	452	GLN	4.0
2	B	449	GLY	3.9
2	D	447	ARG	3.9
2	B	171	SER	3.8
2	D	299	ASN	3.8
2	D	449	GLY	3.7
2	D	349	ALA	3.7
2	D	453	ALA	3.7
2	B	472	ALA	3.7
2	B	459	GLN	3.7
2	B	339	GLY	3.6
2	D	171	SER	3.6
2	D	472	ALA	3.5
2	B	446	ASP	3.4
2	D	170	THR	3.3
2	D	169	HIS	3.2
2	D	455	ASP	3.1
1	A	2	ASP	3.0
2	D	452	GLN	3.0
2	D	168	HIS	2.9
2	B	288	GLY	2.8
2	B	447	ARG	2.8
2	D	457	ILE	2.6
1	A	3	LEU	2.6
1	A	4	LYS	2.5
2	D	460	GLN	2.5
1	A	6	ASP	2.3
2	B	314	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	42	LYS	2.2
1	A	10[A]	SER	2.0
1	C	230	LYS	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](#)

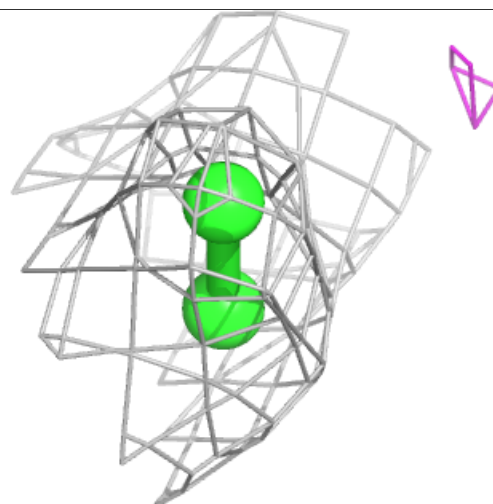
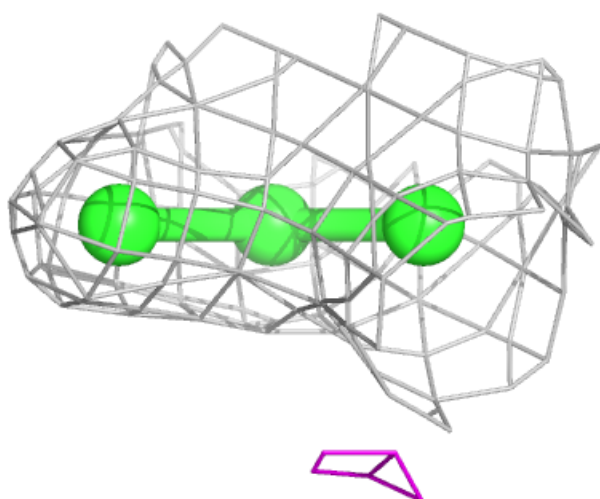
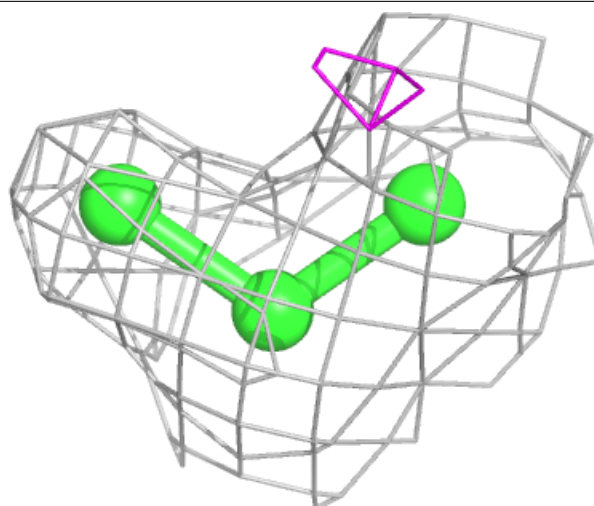
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	902	6/6	0.67	0.20	63,70,78,94	0
3	GOL	A	303	6/6	0.71	0.29	50,58,94,95	0
3	GOL	B	504	6/6	0.75	0.38	59,69,77,79	0
3	GOL	B	503	6/6	0.79	0.28	36,50,77,86	0
3	GOL	B	501	6/6	0.80	0.16	54,64,64,76	0
4	FLC	C	301	13/13	0.80	0.38	25,49,61,68	13
3	GOL	D	903	6/6	0.82	0.17	31,45,58,60	0
3	GOL	A	301	6/6	0.87	0.18	51,63,66,81	6
3	GOL	C	302	6/6	0.89	0.16	48,52,55,60	0
3	GOL	A	302	6/6	0.93	0.23	22,27,48,55	6
5	MIE	D	901	3/5	0.96	0.07	31,31,33,35	3
5	MIE	B	502	3/5	0.98	0.07	38,38,41,41	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.

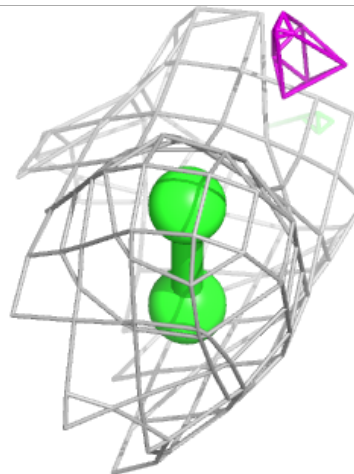
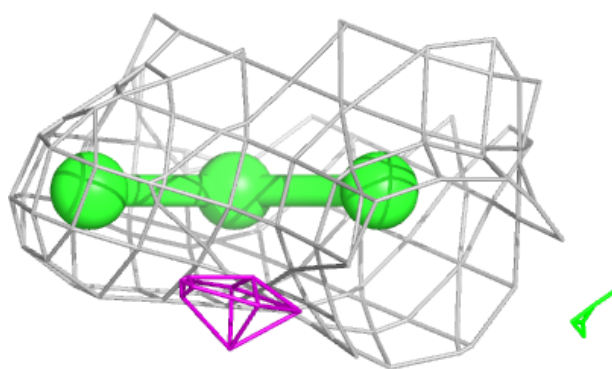
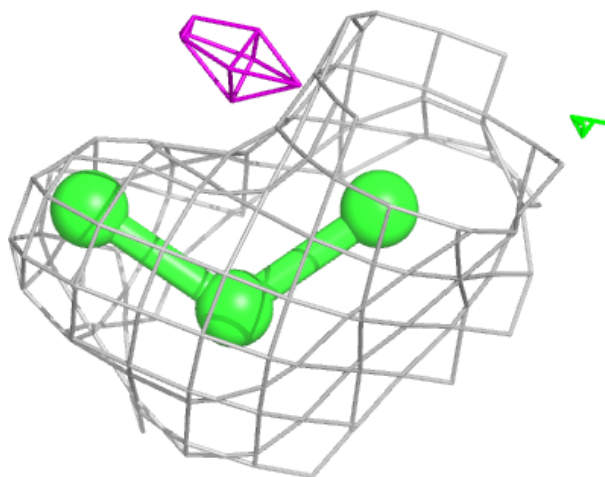
Electron density around MIE D 901:

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



Electron density around MIE B 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.