



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:18 pm BST

PDB ID : 6F92  
Title : Structure of the family GH92 alpha-mannosidase BT3965 from *Bacteroides thetaiotaomicron* in complex with Mannoimidazole (ManI)  
Authors : Thompson, A.J.; Spears, R.J.; Zhu, Y.; Suits, M.D.L.; Williams, S.J.; Gilbert, H.J.; Davies, G.J.  
Deposited on : 2017-12-13  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

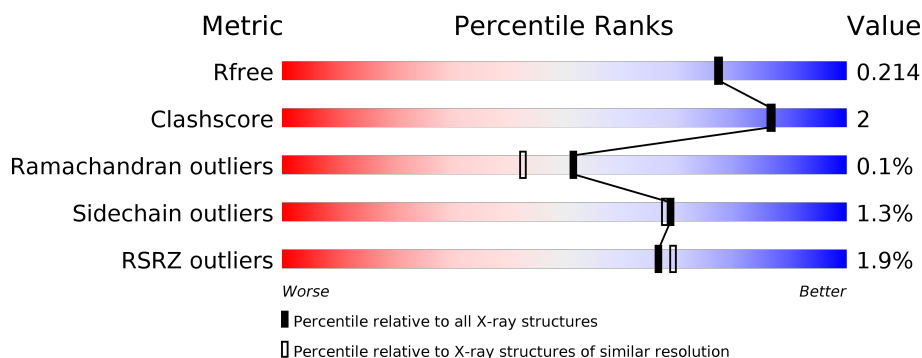
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	764	<div> <div>%</div> <div> </div> <div>92% 7% ..</div> </div>
1	B	764	<div> <div>2%</div> <div> </div> <div>94% 5% .</div> </div>
1	C	764	<div> <div>3%</div> <div> </div> <div>93% 6% .</div> </div>
1	D	764	<div> <div>2%</div> <div> </div> <div>93% 6% .</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26805 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 Putative alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	760	Total	C	N	O	S	0	24	0
			6234	3997	1029	1171	37			
1	B	749	Total	C	N	O	S	0	12	0
			6048	3871	992	1150	35			
1	C	747	Total	C	N	O	S	0	14	0
			5982	3831	979	1134	38			
1	D	760	Total	C	N	O	S	0	11	0
			6144	3930	1016	1162	36			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	757	LEU	-	expression tag	UNP A0A139JT15
A	758	GLU	-	expression tag	UNP A0A139JT15
A	759	HIS	-	expression tag	UNP A0A139JT15
A	760	HIS	-	expression tag	UNP A0A139JT15
A	761	HIS	-	expression tag	UNP A0A139JT15
A	762	HIS	-	expression tag	UNP A0A139JT15
A	763	HIS	-	expression tag	UNP A0A139JT15
A	764	HIS	-	expression tag	UNP A0A139JT15
B	757	LEU	-	expression tag	UNP A0A139JT15
B	758	GLU	-	expression tag	UNP A0A139JT15
B	759	HIS	-	expression tag	UNP A0A139JT15
B	760	HIS	-	expression tag	UNP A0A139JT15
B	761	HIS	-	expression tag	UNP A0A139JT15
B	762	HIS	-	expression tag	UNP A0A139JT15
B	763	HIS	-	expression tag	UNP A0A139JT15
B	764	HIS	-	expression tag	UNP A0A139JT15
C	757	LEU	-	expression tag	UNP A0A139JT15
C	758	GLU	-	expression tag	UNP A0A139JT15
C	759	HIS	-	expression tag	UNP A0A139JT15
C	760	HIS	-	expression tag	UNP A0A139JT15
C	761	HIS	-	expression tag	UNP A0A139JT15

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Chain	Residue	Modelled	Actual	Comment	Reference
C	762	HIS	-	expression tag	UNP A0A139JT15
C	763	HIS	-	expression tag	UNP A0A139JT15
C	764	HIS	-	expression tag	UNP A0A139JT15
D	757	LEU	-	expression tag	UNP A0A139JT15
D	758	GLU	-	expression tag	UNP A0A139JT15
D	759	HIS	-	expression tag	UNP A0A139JT15
D	760	HIS	-	expression tag	UNP A0A139JT15
D	761	HIS	-	expression tag	UNP A0A139JT15
D	762	HIS	-	expression tag	UNP A0A139JT15
D	763	HIS	-	expression tag	UNP A0A139JT15
D	764	HIS	-	expression tag	UNP A0A139JT15

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

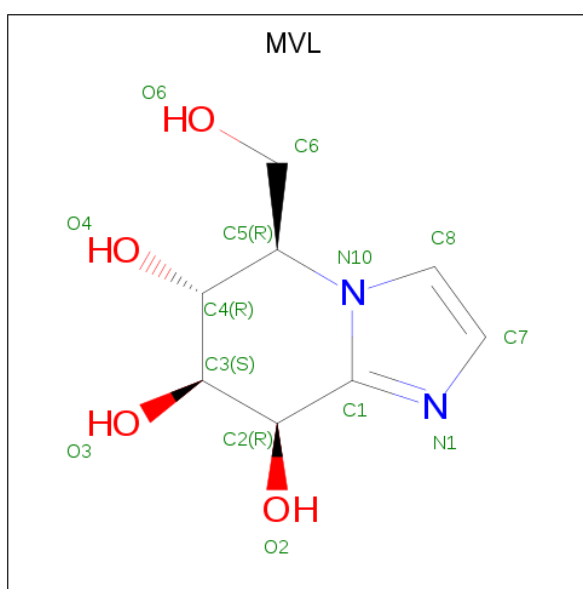
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: MVL) (formula: C<sub>8</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



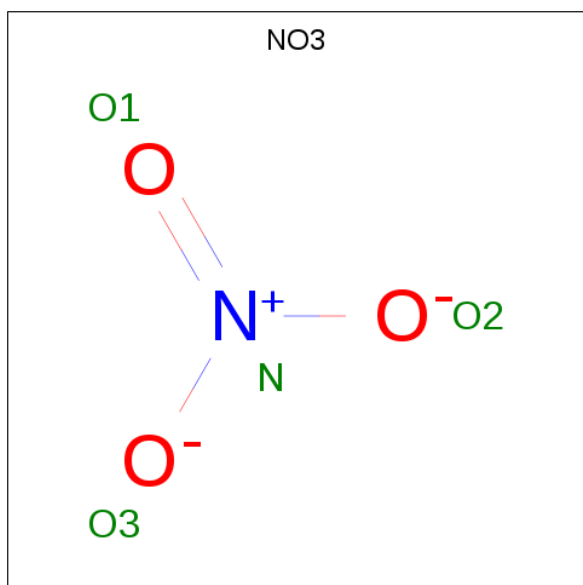
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	2	4		
5	B	1	Total	C	N	O	0	0
			14	8	2	4		
5	C	1	Total	C	N	O	0	0
			14	8	2	4		
5	D	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	N 1	O 3	0	0
7	D	1	Total 4	N 1	O 3	0	0

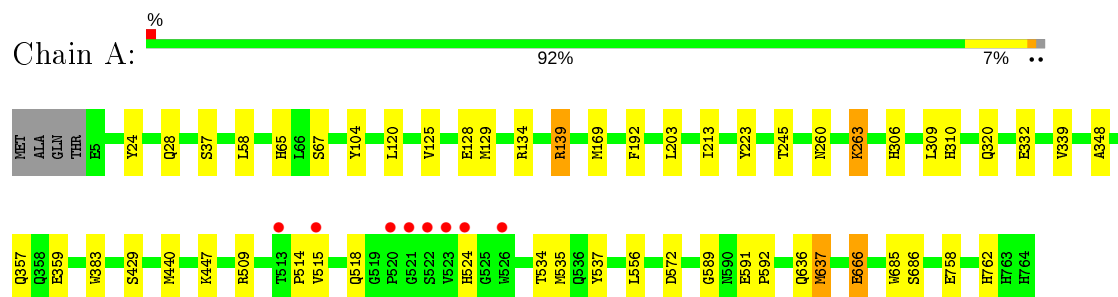
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	691	Total 691	O 691	0	0
8	B	529	Total 529	O 529	0	0
8	C	363	Total 363	O 363	0	0
8	D	722	Total 722	O 722	0	0

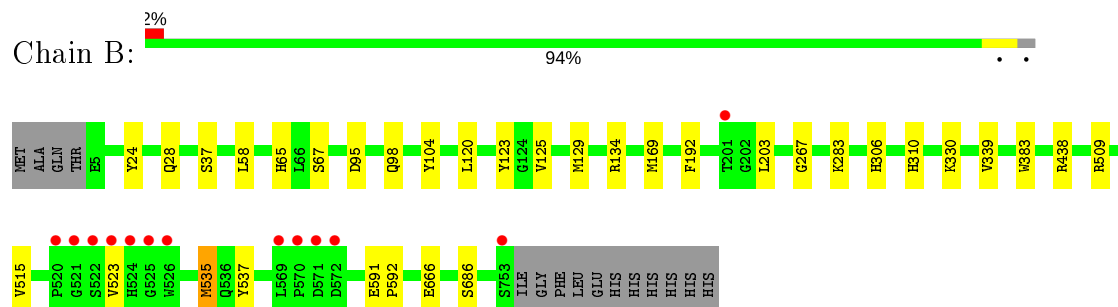
### 3 Residue-property plots [i](#)

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.

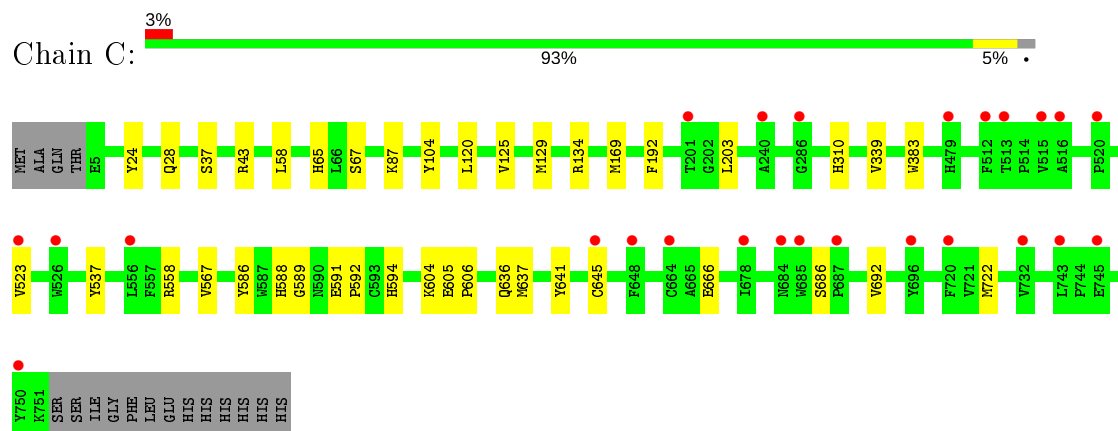
- Molecule 1: Putative alpha-1,2-mannosidase



- Molecule 1: Putative alpha-1,2-mannosidase

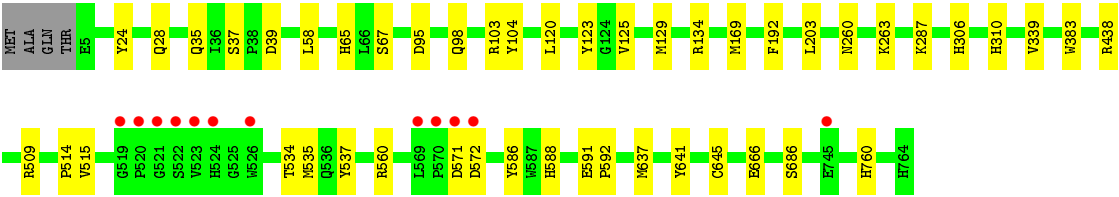
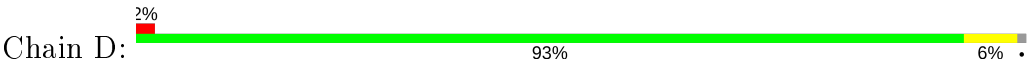


- Molecule 1: Putative alpha-1,2-mannosidase



- Molecule 1: Putative alpha-1,2-mannosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.51Å 186.90Å 95.05Å 90.00° 91.74° 90.00°	Depositor
Resolution (Å)	46.73 – 1.90 46.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.73-1.90) 96.0 (46.73-1.90)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.177 , 0.208 0.185 , 0.214	Depositor DCC
$R_{free}$ test set	10714 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, CA, EDO, MVL, NO3

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	0.57	0/6491	0.73	4/8804 (0.0%)
1	B	0.52	0/6259	0.72	4/8497 (0.0%)
1	C	0.51	0/6200	0.71	5/8431 (0.1%)
1	D	0.58	0/6359	0.74	6/8631 (0.1%)
All	All	0.55	0/25309	0.73	19/34363 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	571	ASP	N-CA-C	-6.82	92.59	111.00
1	D	509	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	637[A]	MET	CG-SD-CE	-6.35	90.04	100.20
1	A	637[B]	MET	CG-SD-CE	-6.35	90.04	100.20
1	B	134	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	134	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	134	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	558[A]	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	C	558[B]	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	D	103	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	438	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	134	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	509	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	C	558[A]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	558[B]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	283	LYS	CD-CE-NZ	5.09	123.40	111.70
1	D	509	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	438	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	509	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6234	0	5947	36	0
1	B	6048	0	5728	16	0
1	C	5982	0	5598	18	0
1	D	6144	0	5801	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	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
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	14	0	10	0	0
5	B	14	0	10	0	0
5	C	14	0	10	0	0
5	D	14	0	10	0	0
6	A	4	0	6	0	0
6	B	8	0	12	1	0
6	D	4	0	6	1	0
7	D	8	0	0	0	0
8	A	691	0	0	10	1
8	B	529	0	0	4	0
8	C	363	0	0	3	0
8	D	722	0	0	5	1
All	All	26805	0	23138	99	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 2.

All (99) 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:A:139[A]:ARG:HH11	1:A:139[A]:ARG:HG2	0.88	1.04
1:A:139[A]:ARG:CG	1:A:139[A]:ARG:HH11	1.72	1.01
1:A:139[A]:ARG:NH1	1:A:139[A]:ARG:HG2	1.69	0.98
1:A:263:LYS:HE3	8:B:956:HOH:O	1.72	0.90
1:A:440:MET:HG2	8:A:1523:HOH:O	1.73	0.89
1:D:637[A]:MET:HE1	8:D:1071:HOH:O	1.75	0.86
1:D:35:GLN:HE21	1:D:65[A]:HIS:H	1.26	0.82
1:D:35:GLN:HE21	1:D:65[B]:HIS:H	1.27	0.82
1:A:556:LEU:HD12	8:A:1118:HOH:O	1.80	0.81
1:C:43:ARG:NH2	8:C:902:HOH:O	2.23	0.70
1:D:260:ASN:OD1	1:D:263:LYS:NZ	2.24	0.70
1:A:169[A]:MET:HE2	1:A:203:LEU:HD22	1.76	0.68
1:D:572:ASP:HB2	8:D:1180:HOH:O	1.95	0.67
1:C:169[A]:MET:HE2	1:C:203:LEU:HD22	1.77	0.67
1:A:169[A]:MET:CE	1:A:203:LEU:HD22	2.26	0.66
1:A:139[A]:ARG:NH1	1:A:139[A]:ARG:CG	2.41	0.65
1:C:169[A]:MET:CE	1:C:203:LEU:HD22	2.27	0.65
1:A:320:GLN:NE2	8:A:902:HOH:O	2.24	0.65
1:C:43:ARG:CZ	8:C:902:HOH:O	2.45	0.64
1:D:169[A]:MET:CE	1:D:203:LEU:HD22	2.28	0.64
1:D:39:ASP:OD1	1:D:65[B]:HIS:HE1	1.79	0.64
1:A:359:GLU:HG2	1:B:267:GLY:HA3	1.80	0.62
1:A:128:GLU:OE1	1:A:139[A]:ARG:NH1	2.32	0.62
1:B:169[A]:MET:CE	1:B:203:LEU:HD22	2.29	0.61
1:C:692:VAL:HA	1:C:722[B]:MET:HE1	1.81	0.61
1:D:169[A]:MET:HE2	1:D:203:LEU:HD22	1.82	0.61
1:A:332:GLU:CD	8:A:1046:HOH:O	2.41	0.59
1:C:589:GLY:HA2	1:C:637[A]:MET:HE1	1.84	0.59
1:A:260[A]:ASN:ND2	8:A:906:HOH:O	2.35	0.59
1:B:169[A]:MET:HE2	1:B:203:LEU:HD22	1.85	0.57
1:D:67:SER:H	1:D:310:HIS:CE1	2.23	0.57
1:A:589:GLY:HA2	1:A:637[A]:MET:HE1	1.85	0.56
1:A:67:SER:H	1:A:310:HIS:CE1	2.24	0.56
1:A:666[B]:GLU:HG3	1:A:685:TRP:HB3	1.86	0.56
1:C:67:SER:H	1:C:310:HIS:CE1	2.24	0.55
1:B:67:SER:H	1:B:310:HIS:CE1	2.24	0.55
1:C:594:HIS:HD2	1:C:636:GLN:HE21	1.55	0.53
1:D:39:ASP:OD1	1:D:65[B]:HIS:CE1	2.61	0.53
1:B:330[A]:LYS:HE2	8:B:1272:HOH:O	2.09	0.53
1:D:306[B]:HIS:HE1	8:D:1188:HOH:O	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306[B]:HIS:HE1	8:A:1029:HOH:O	1.92	0.51
1:A:429[B]:SER:OG	8:A:901:HOH:O	2.07	0.50
1:A:518:GLN:HG2	1:A:524:HIS:CD2	2.48	0.49
1:A:515:VAL:HG13	1:A:535[A]:MET:CE	2.43	0.48
1:D:560:ARG:NH1	6:D:805:EDO:O1	2.47	0.48
1:D:24:TYR:OH	1:D:28:GLN:NE2	2.46	0.48
1:A:120:LEU:HD12	1:A:125[A]:VAL:HG22	1.96	0.47
1:B:24:TYR:OH	1:B:28:GLN:NE2	2.47	0.47
1:C:24:TYR:OH	1:C:28:GLN:NE2	2.47	0.47
1:A:357:GLN:NE2	8:A:912:HOH:O	2.47	0.47
1:A:24:TYR:OH	1:A:28:GLN:NE2	2.47	0.47
1:C:588:HIS:O	1:C:594:HIS:HE1	1.98	0.46
1:B:120:LEU:HD12	1:B:125[A]:VAL:HG22	1.96	0.46
1:D:760:HIS:HE1	8:D:1489:HOH:O	1.98	0.46
6:B:805:EDO:H12	8:B:1222:HOH:O	2.16	0.46
1:A:139[A]:ARG:HD3	1:A:245:THR:HG22	1.97	0.45
1:D:515:VAL:HG13	1:D:535:MET:CE	2.47	0.45
1:D:120:LEU:HD12	1:D:125[A]:VAL:HG22	1.98	0.45
1:D:591:GLU:N	1:D:592:PRO:CD	2.80	0.45
1:A:348:ALA:H	1:A:636:GLN:HE22	1.66	0.44
1:B:306[B]:HIS:HE1	8:B:922:HOH:O	2.00	0.44
1:B:591:GLU:N	1:B:592:PRO:CD	2.80	0.44
1:B:58:LEU:HG	1:B:104:TYR:CD1	2.53	0.44
1:A:591:GLU:N	1:A:592:PRO:CD	2.81	0.43
1:C:120:LEU:HD12	1:C:125:VAL:HG22	1.98	0.43
1:A:447:LYS:NZ	8:A:927:HOH:O	2.52	0.43
1:C:604:LYS:C	1:C:606[B]:PRO:HD3	2.39	0.43
1:C:58:LEU:HG	1:C:104:TYR:CD1	2.53	0.43
1:A:213:ILE:HD11	8:A:1268:HOH:O	2.17	0.43
1:A:515:VAL:HG13	1:A:535[A]:MET:HE1	2.01	0.43
1:B:169[A]:MET:HE1	1:B:203:LEU:HD22	1.97	0.43
8:C:1041:HOH:O	1:D:287:LYS:HE3	2.19	0.42
1:D:58:LEU:HG	1:D:104:TYR:CD1	2.54	0.42
1:A:58:LEU:HG	1:A:104:TYR:CD1	2.55	0.42
1:D:123:TYR:HB3	1:D:125[A]:VAL:HG13	2.02	0.42
1:D:586:TYR:OH	1:D:588:HIS:HD2	2.03	0.42
1:A:37:SER:HB3	1:A:65:HIS:CE1	2.54	0.42
1:B:37:SER:HB3	1:B:65:HIS:CE1	2.55	0.42
1:C:591:GLU:N	1:C:592:PRO:CD	2.82	0.42
1:C:605:GLU:N	1:C:606[B]:PRO:HD3	2.34	0.42
1:D:169[A]:MET:HE1	1:D:203:LEU:HD22	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:GLU:O	1:A:762:HIS:CD2	2.73	0.42
1:C:37:SER:HB3	1:C:65:HIS:CE1	2.55	0.42
1:B:515:VAL:HG13	1:B:535:MET:CE	2.50	0.41
1:B:123:TYR:HB3	1:B:125[A]:VAL:HG13	2.02	0.41
1:D:637[A]:MET:HB3	1:D:637[A]:MET:HE3	1.76	0.41
1:D:37:SER:HB3	1:D:65[A]:HIS:CE1	2.55	0.41
1:B:95:ASP:O	1:B:98:GLN:HG2	2.20	0.41
1:D:306[B]:HIS:CD2	8:D:1063:HOH:O	2.74	0.41
1:D:641:TYR:CE2	1:D:645:CYS:SG	3.12	0.41
1:A:169[A]:MET:HE3	1:A:223:TYR:HD1	1.86	0.41
1:C:641:TYR:CE2	1:C:645:CYS:SG	3.14	0.41
1:B:203:LEU:HD23	1:B:203:LEU:C	2.42	0.40
1:A:514:PRO:HA	1:A:534:THR:HB	2.03	0.40
1:D:95:ASP:O	1:D:98:GLN:HG2	2.21	0.40
1:C:586:TYR:OH	1:C:588:HIS:HD2	2.04	0.40
1:A:309:LEU:O	1:A:310:HIS:HD2	2.05	0.40
1:D:514:PRO:HA	1:D:534:THR:HB	2.02	0.40
1:D:67:SER:H	1:D:310:HIS:HE1	1.68	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)
8:A:1126:HOH:O	8:D:947:HOH:O[2_546]	2.05	0.15

## 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	782/764 (102%)	760 (97%)	21 (3%)	1 (0%)	51 43
1	B	759/764 (99%)	737 (97%)	21 (3%)	1 (0%)	51 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	759/764 (99%)	737 (97%)	21 (3%)	1 (0%)	51	43
1	D	769/764 (101%)	745 (97%)	23 (3%)	1 (0%)	51	43
All	All	3069/3056 (100%)	2979 (97%)	86 (3%)	4 (0%)	51	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	B	339	VAL
1	C	339	VAL
1	D	339	VAL

### 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	666/654 (102%)	654 (98%)	12 (2%)	59	55
1	B	640/654 (98%)	632 (99%)	8 (1%)	69	68
1	C	624/654 (95%)	615 (99%)	9 (1%)	67	65
1	D	649/654 (99%)	643 (99%)	6 (1%)	78	79
All	All	2579/2616 (99%)	2544 (99%)	35 (1%)	69	65

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	MET
1	A	139[A]	ARG
1	A	139[B]	ARG
1	A	192	PHE
1	A	263	LYS
1	A	383	TRP
1	A	537	TYR
1	A	572[A]	ASP

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Mol	Chain	Res	Type
1	A	572[B]	ASP
1	A	666[A]	GLU
1	A	666[B]	GLU
1	A	686	SER
1	B	129	MET
1	B	192	PHE
1	B	383	TRP
1	B	523	VAL
1	B	535	MET
1	B	537	TYR
1	B	666	GLU
1	B	686	SER
1	C	87	LYS
1	C	129	MET
1	C	192	PHE
1	C	383	TRP
1	C	523	VAL
1	C	537	TYR
1	C	567	VAL
1	C	666	GLU
1	C	686	SER
1	D	129	MET
1	D	192	PHE
1	D	383	TRP
1	D	537	TYR
1	D	666	GLU
1	D	686	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	310	HIS
1	A	357	GLN
1	A	524	HIS
1	A	636	GLN
1	A	644	ASN
1	A	759	HIS
1	A	762	HIS
1	A	763	HIS
1	B	28	GLN
1	B	310	HIS

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Mol	Chain	Res	Type
1	B	357	GLN
1	B	644	ASN
1	B	684	ASN
1	C	28	GLN
1	C	310	HIS
1	C	588	HIS
1	C	594	HIS
1	C	644	ASN
1	D	28	GLN
1	D	35	GLN
1	D	310	HIS
1	D	588	HIS
1	D	644	ASN
1	D	760	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 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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
6	EDO	D	805	-	3,3,3	0.22	0	2,2,2	0.29	0
6	EDO	A	805	-	3,3,3	0.32	0	2,2,2	0.47	0
6	EDO	B	805	-	3,3,3	0.28	0	2,2,2	0.93	0
7	NO3	D	806	-	1,3,3	0.07	0	0,3,3	0.00	-
6	EDO	B	806	-	3,3,3	0.36	0	2,2,2	0.77	0
5	MVL	A	804	3	13,15,15	0.98	2 (15%)	11,22,22	1.64	3 (27%)
7	NO3	D	807	-	1,3,3	0.65	0	0,3,3	0.00	-
5	MVL	D	804	3	13,15,15	1.18	2 (15%)	11,22,22	1.32	1 (9%)
5	MVL	B	804	3	13,15,15	0.87	0	11,22,22	1.67	2 (18%)
5	MVL	C	804	3	13,15,15	1.05	1 (7%)	11,22,22	1.93	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	D	805	-	-	0/1/1/1	-
6	EDO	A	805	-	-	1/1/1/1	-
6	EDO	B	805	-	-	0/1/1/1	-
6	EDO	B	806	-	-	0/1/1/1	-
5	MVL	A	804	3	-	0/2/22/22	0/1/2/2
5	MVL	D	804	3	-	0/2/22/22	0/1/2/2
5	MVL	B	804	3	-	0/2/22/22	0/1/2/2
5	MVL	C	804	3	-	0/2/22/22	0/1/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	804	MVL	C8-N10	-2.50	1.33	1.37
5	C	804	MVL	C8-N10	-2.35	1.33	1.37
5	D	804	MVL	C3-C2	2.34	1.57	1.52
5	A	804	MVL	C1-C2	-2.07	1.48	1.51
5	A	804	MVL	C8-N10	-2.01	1.34	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	MVL	C4-C3-C2	4.59	117.21	110.24
5	C	804	MVL	C4-C3-C2	4.13	116.51	110.24
5	A	804	MVL	C4-C3-C2	3.90	116.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	804	MVL	C4-C3-C2	3.41	115.42	110.24
5	C	804	MVL	O4-C4-C5	-2.79	104.82	109.77
5	C	804	MVL	C3-C4-C5	2.66	115.87	111.37
5	A	804	MVL	C3-C4-C5	2.64	115.83	111.37
5	B	804	MVL	C3-C4-C5	2.11	114.94	111.37
5	A	804	MVL	O4-C4-C5	-2.01	106.20	109.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

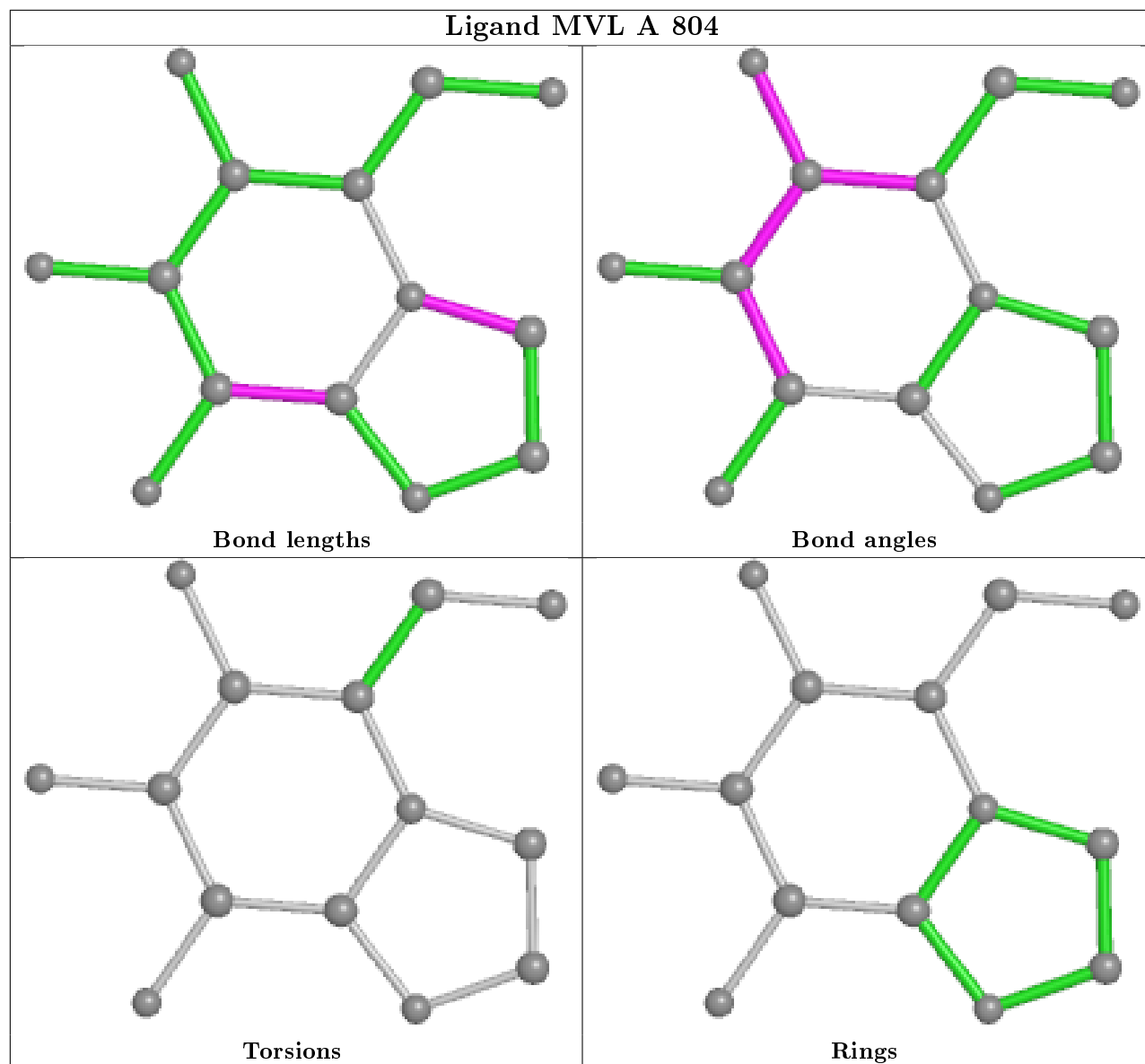
Mol	Chain	Res	Type	Atoms
6	A	805	EDO	O1-C1-C2-O2

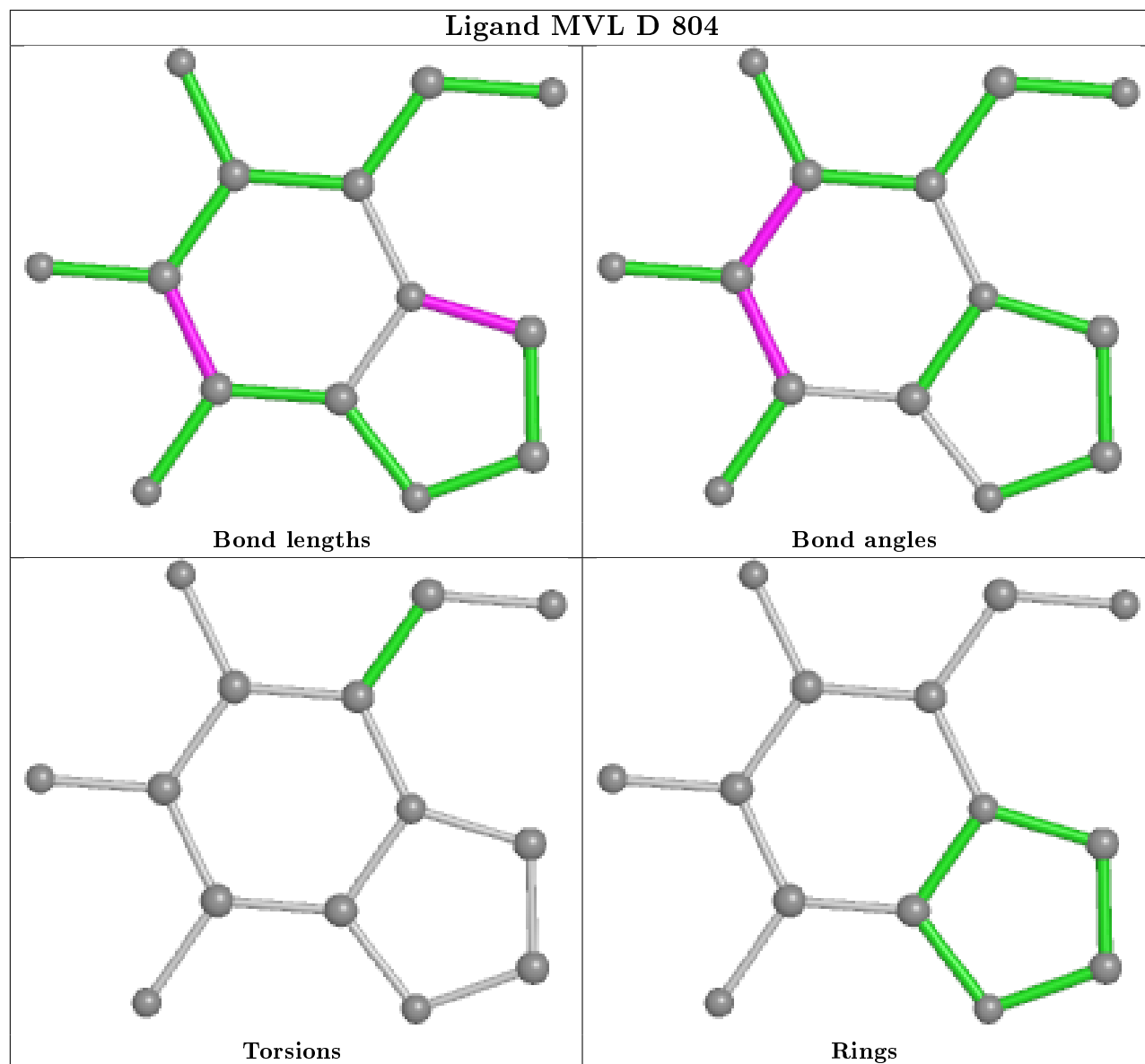
There are no ring outliers.

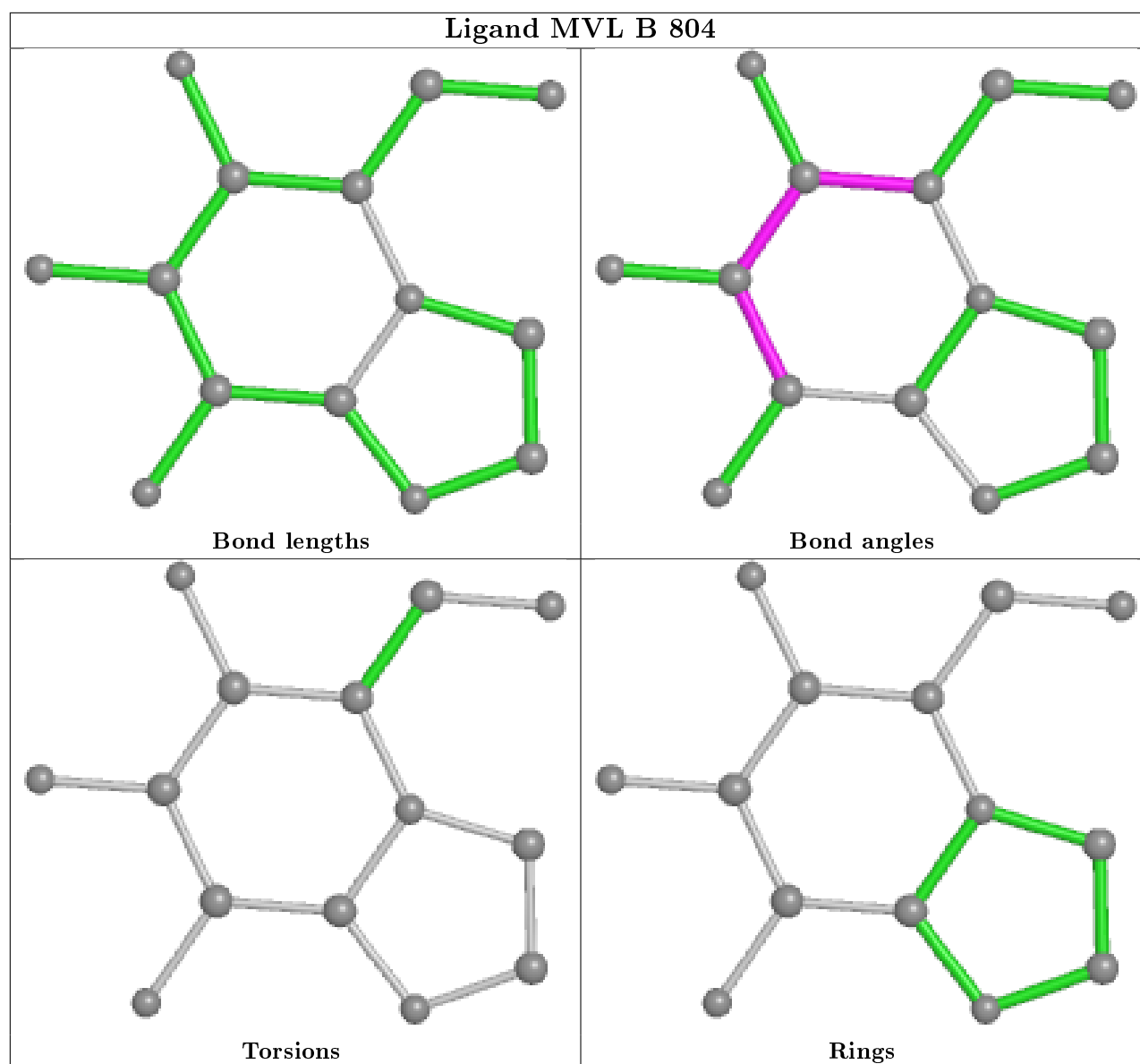
2 monomers are involved in 2 short contacts:

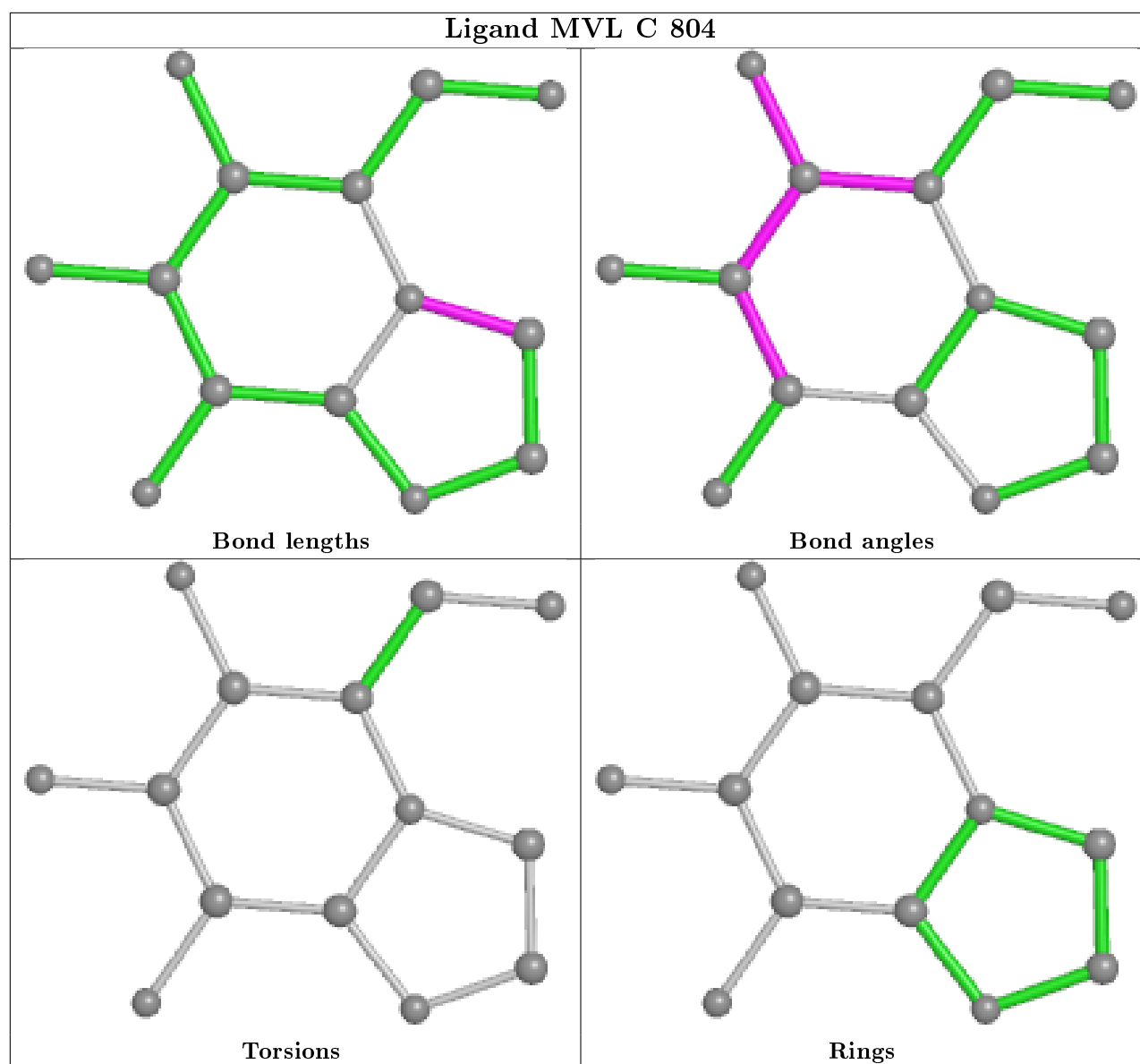
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	805	EDO	1	0
6	B	805	EDO	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	760/764 (99%)	-0.27	8 (1%) 80 82	8, 16, 30, 61	0
1	B	749/764 (98%)	-0.14	13 (1%) 70 72	14, 23, 39, 73	0
1	C	747/764 (97%)	0.42	25 (3%) 46 49	17, 33, 50, 65	0
1	D	760/764 (99%)	-0.32	12 (1%) 72 74	9, 16, 30, 77	0
All	All	3016/3056 (98%)	-0.08	58 (1%) 66 69	8, 21, 44, 77	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	520	PRO	6.9
1	D	526	TRP	5.3
1	D	521	GLY	4.7
1	B	523	VAL	4.7
1	B	521	GLY	4.5
1	D	519	GLY	4.3
1	D	522	SER	4.2
1	D	523	VAL	4.2
1	B	526	TRP	3.5
1	C	526	TRP	3.3
1	B	524	HIS	3.3
1	A	526	TRP	3.3
1	D	572	ASP	3.3
1	D	571	ASP	3.2
1	B	571	ASP	3.1
1	D	524	HIS	3.1
1	C	520	PRO	3.0
1	C	523	VAL	3.0
1	A	523	VAL	3.0
1	C	513	THR	2.9
1	C	516	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	515	VAL	2.8
1	B	520	PRO	2.7
1	A	513	THR	2.6
1	C	515	VAL	2.6
1	C	745	GLU	2.6
1	B	572	ASP	2.5
1	B	522	SER	2.5
1	B	525	GLY	2.5
1	C	512	PHE	2.5
1	C	664	CYS	2.4
1	C	685	TRP	2.4
1	A	524	HIS	2.4
1	C	479	HIS	2.4
1	B	570	PRO	2.4
1	C	645	CYS	2.4
1	D	745	GLU	2.3
1	B	569	LEU	2.3
1	D	569	LEU	2.3
1	C	743	LEU	2.3
1	C	687	PRO	2.2
1	C	240	ALA	2.2
1	C	684	ASN	2.2
1	C	696	TYR	2.2
1	C	201	THR	2.2
1	C	648	PHE	2.2
1	C	732	VAL	2.2
1	C	556	LEU	2.2
1	A	521	GLY	2.2
1	C	678	ILE	2.1
1	B	201	THR	2.1
1	C	286	GLY	2.1
1	D	570	PRO	2.1
1	A	520	PRO	2.1
1	C	750	TYR	2.1
1	B	753	SER	2.1
1	C	720	PHE	2.1
1	A	522	SER	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 ⓘ

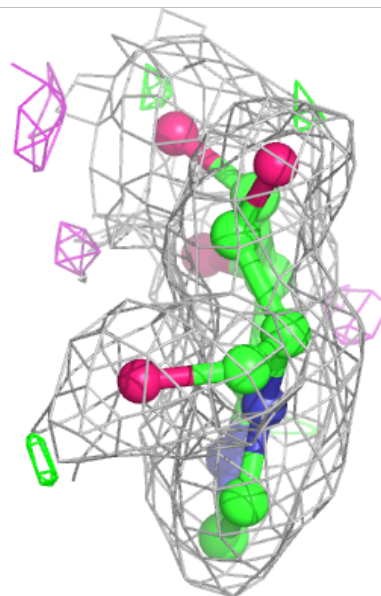
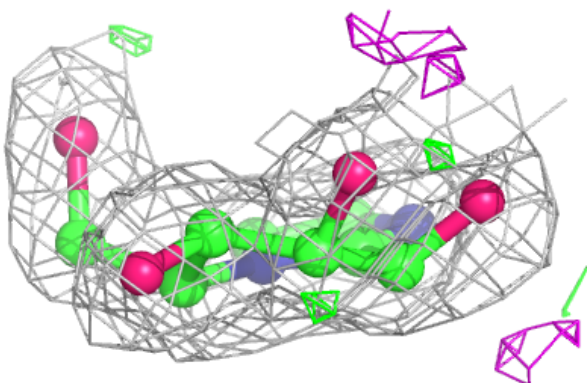
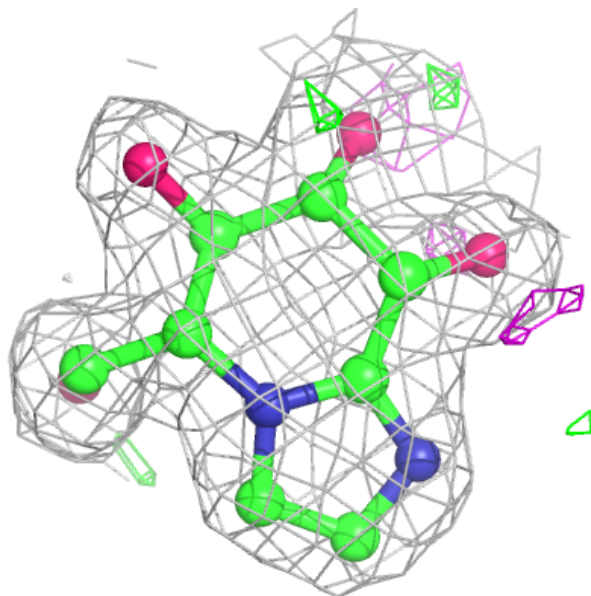
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	EDO	B	805	4/4	0.87	0.20	30,31,35,38	0
6	EDO	D	805	4/4	0.89	0.20	32,34,36,41	0
6	EDO	B	806	4/4	0.91	0.13	40,41,41,43	0
5	MVL	C	804	14/14	0.92	0.12	25,28,29,30	0
6	EDO	A	805	4/4	0.94	0.13	28,31,31,34	0
2	NA	A	801	1/1	0.94	0.15	19,19,19,19	0
2	NA	C	801	1/1	0.95	0.21	32,32,32,32	0
5	MVL	B	804	14/14	0.95	0.11	17,21,22,23	0
2	NA	B	801	1/1	0.95	0.06	23,23,23,23	0
3	CA	C	802	1/1	0.96	0.06	27,27,27,27	0
4	CL	C	803	1/1	0.96	0.08	34,34,34,34	0
5	MVL	D	804	14/14	0.96	0.11	13,14,16,18	0
5	MVL	A	804	14/14	0.96	0.12	12,15,17,18	0
7	NO3	D	807	4/4	0.97	0.10	24,27,27,29	0
7	NO3	D	806	4/4	0.97	0.10	25,25,26,27	0
3	CA	D	802	1/1	0.99	0.03	16,16,16,16	0
2	NA	D	801	1/1	0.99	0.06	16,16,16,16	0
4	CL	D	803	1/1	0.99	0.04	15,15,15,15	0
3	CA	B	802	1/1	0.99	0.04	20,20,20,20	0
4	CL	B	803	1/1	0.99	0.04	21,21,21,21	0
3	CA	A	802	1/1	1.00	0.03	15,15,15,15	0
4	CL	A	803	1/1	1.00	0.07	14,14,14,14	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.

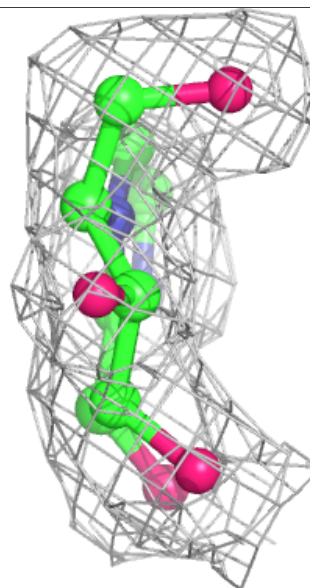
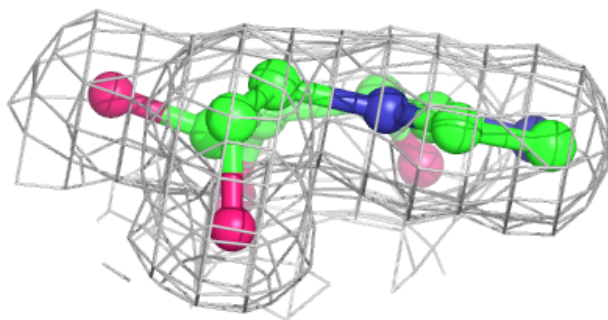
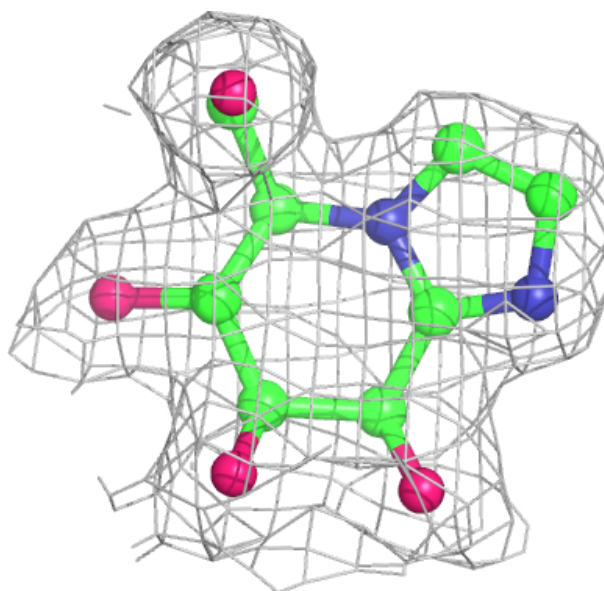
**Electron density around MVL C 804:**

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



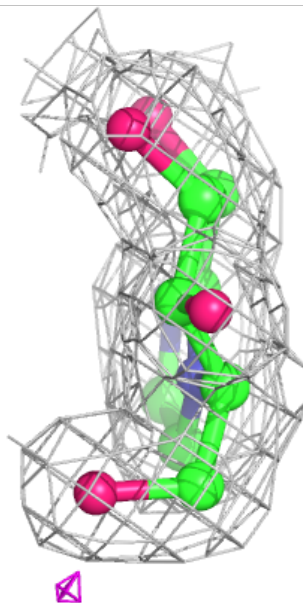
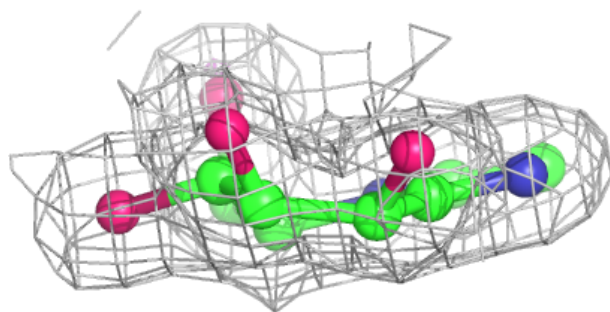
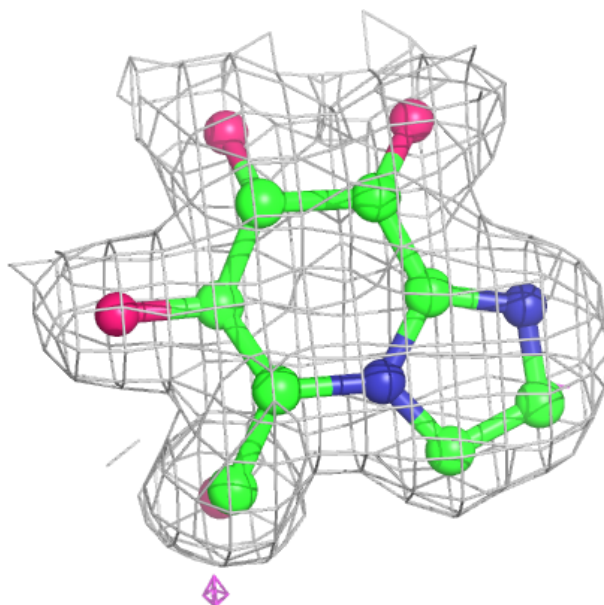
**Electron density around MVL B 804:**

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



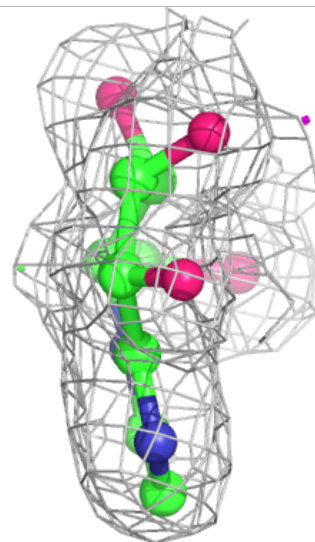
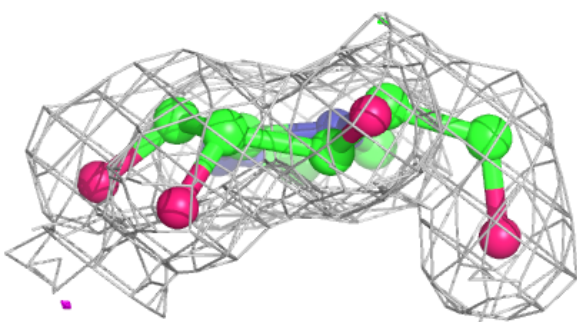
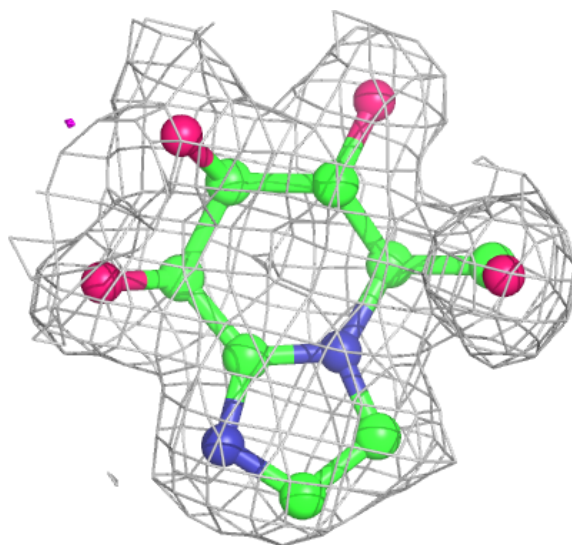
**Electron density around MVL D 804:**

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



**Electron density around MVL A 804:**

$2mF_o-DF_c$  (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.