



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 PM UTC

PDB ID : 6F90 / pdb_00006f90
Title : Structure of the family GH92 alpha-mannosidase BT3130 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 : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

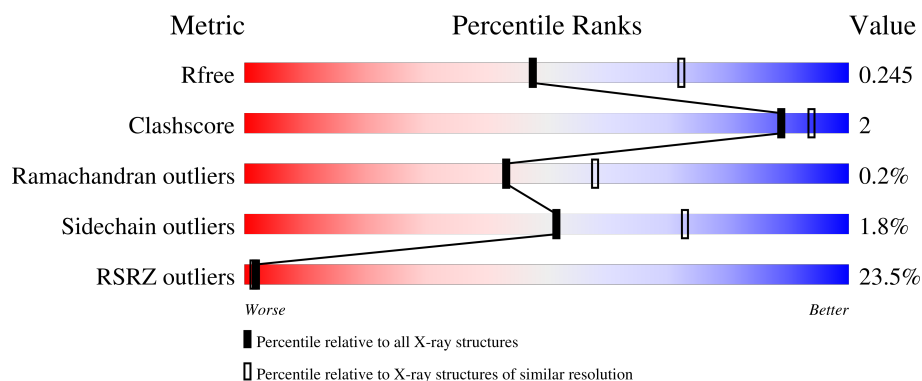
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	727	2% 94% • •
1	B	727	8% 91% 6% • •
1	C	727	58% 90% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17665 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 Alpha-1,2-mannosidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	1	0
			5651	3590	956	1078	27			
1	B	708	Total	C	N	O	S	0	0	0
			5523	3523	926	1047	27			
1	C	692	Total	C	N	O	S	0	3	0
			5260	3330	895	1011	24			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP A0A174L250
A	18	GLY	-	expression tag	UNP A0A174L250
A	736	LEU	-	expression tag	UNP A0A174L250
A	737	GLU	-	expression tag	UNP A0A174L250
A	738	HIS	-	expression tag	UNP A0A174L250
A	739	HIS	-	expression tag	UNP A0A174L250
A	740	HIS	-	expression tag	UNP A0A174L250
A	741	HIS	-	expression tag	UNP A0A174L250
A	742	HIS	-	expression tag	UNP A0A174L250
A	743	HIS	-	expression tag	UNP A0A174L250
B	17	MET	-	initiating methionine	UNP A0A174L250
B	18	GLY	-	expression tag	UNP A0A174L250
B	736	LEU	-	expression tag	UNP A0A174L250
B	737	GLU	-	expression tag	UNP A0A174L250
B	738	HIS	-	expression tag	UNP A0A174L250
B	739	HIS	-	expression tag	UNP A0A174L250
B	740	HIS	-	expression tag	UNP A0A174L250
B	741	HIS	-	expression tag	UNP A0A174L250
B	742	HIS	-	expression tag	UNP A0A174L250
B	743	HIS	-	expression tag	UNP A0A174L250
C	17	MET	-	initiating methionine	UNP A0A174L250
C	18	GLY	-	expression tag	UNP A0A174L250
C	736	LEU	-	expression tag	UNP A0A174L250

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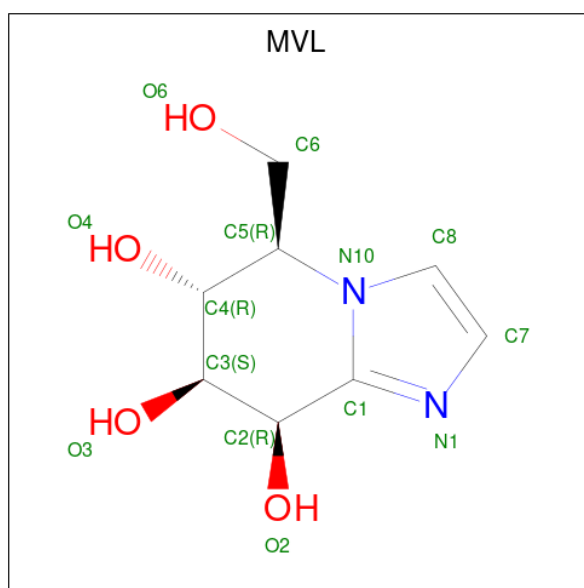
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Chain	Residue	Modelled	Actual	Comment	Reference
C	737	GLU	-	expression tag	UNP A0A174L250
C	738	HIS	-	expression tag	UNP A0A174L250
C	739	HIS	-	expression tag	UNP A0A174L250
C	740	HIS	-	expression tag	UNP A0A174L250
C	741	HIS	-	expression tag	UNP A0A174L250
C	742	HIS	-	expression tag	UNP A0A174L250
C	743	HIS	-	expression tag	UNP A0A174L250

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (CCD ID: MVL) (formula: C₈H₁₂N₂O₄) (labeled as "Ligand of Interest" by depositor).



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

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

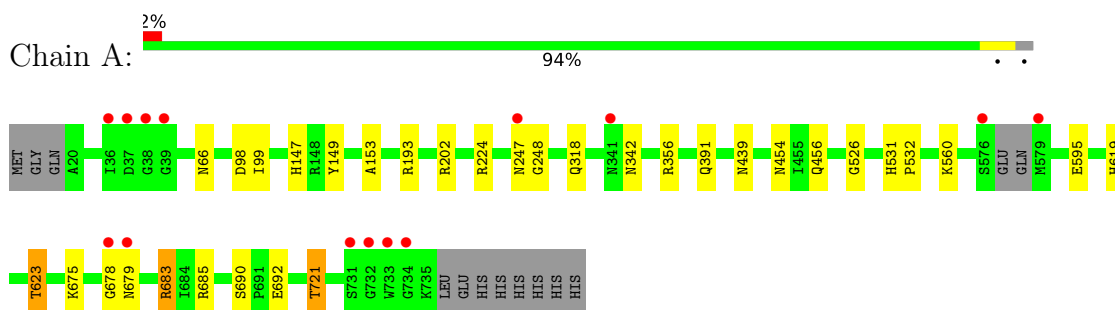
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	679	Total	O	0	0
			679	679		
4	B	323	Total	O	0	1
			324	324		
4	C	183	Total	O	0	0
			183	183		

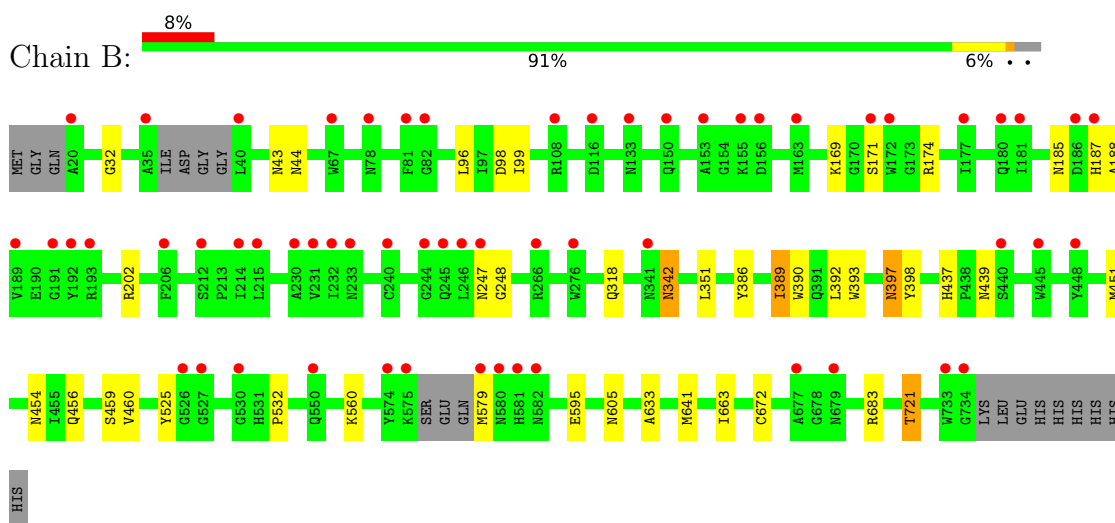
3 Residue-property plots

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.

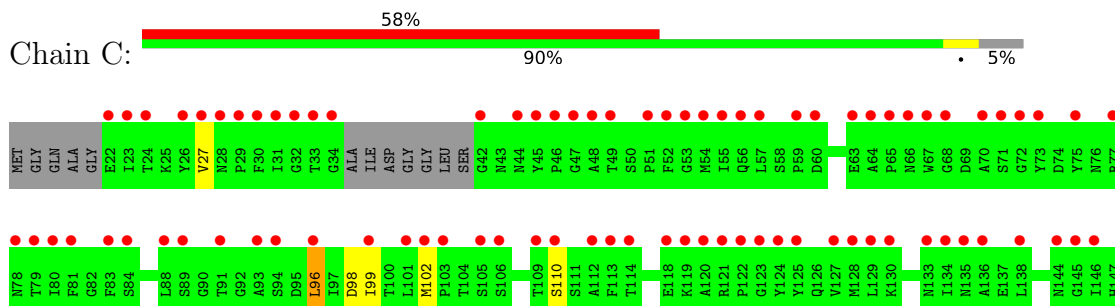
- Molecule 1: Alpha-1,2-mannosidase, putative



- Molecule 1: Alpha-1,2-mannosidase, putative



- Molecule 1: Alpha-1,2-mannosidase, putative





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	273.67Å 273.67Å 189.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.38 – 2.40 49.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.38-2.40) 99.3 (49.38-2.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.207 , 0.242 0.211 , 0.245	Depositor DCC
R_{free} test set	7949 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17665	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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

5.1 Standard geometry

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

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	0.63	0/5819	0.79	3/7913 (0.0%)
1	B	0.61	0/5687	0.81	2/7749 (0.0%)
1	C	0.67	0/5420	0.88	3/7398 (0.0%)
All	All	0.64	0/16926	0.82	8/23060 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	LYS	CA-C-N	11.64	131.75	119.76
1	C	249	LYS	C-N-CA	11.64	131.75	119.76
1	A	356	ARG	N-CA-C	6.45	118.11	111.14
1	C	459	SER	N-CA-C	6.00	117.83	111.28
1	A	690	SER	N-CA-C	5.66	113.11	108.07
1	B	351	LEU	N-CA-C	5.64	118.20	111.71
1	A	678	GLY	N-CA-C	-5.54	102.18	112.37
1	B	389	ILE	N-CA-C	-5.04	106.88	111.67

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	5651	0	5238	15	0
1	B	5523	0	5060	24	0
1	C	5260	0	4637	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	14	0	10	0	0
3	B	14	0	10	0	0
3	C	14	0	10	0	0
4	A	679	0	0	5	1
4	B	324	0	0	5	0
4	C	183	0	0	1	0
All	All	17665	0	14965	60	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 (60) 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:175[B]:ARG:HH11	1:C:175[B]:ARG:HG3	0.97	1.07
1:C:175[B]:ARG:HG3	1:C:175[B]:ARG:NH1	1.77	0.86
1:C:553:MET:CE	1:C:559:THR:HG22	2.08	0.84
1:C:175[B]:ARG:HH11	1:C:175[B]:ARG:CG	1.88	0.83
1:C:553:MET:HE1	1:C:559:THR:HG22	1.65	0.78
1:B:672:CYS:SG	4:B:1169:HOH:O	2.41	0.77
1:C:552:LEU:O	1:C:556:THR:OG1	2.03	0.75
1:B:386:TYR:HH	1:B:398:TYR:HH	1.37	0.69
1:A:619:HIS:O	1:A:623:THR:HB	1.96	0.65
1:A:439:ASN:HD22	1:A:456:GLN:HE22	1.46	0.64
1:C:98:ASP:OD2	1:C:202:ARG:NH2	2.34	0.60
1:B:342:ASN:HD22	1:B:342:ASN:H	1.50	0.59
1:B:386:TYR:OH	1:B:398:TYR:OH	2.18	0.58
1:B:98:ASP:OD2	1:B:202:ARG:NH2	2.36	0.58
1:C:202:ARG:HD3	4:C:903:HOH:O	2.04	0.58
1:C:553:MET:HE2	1:C:559:THR:HG22	1.87	0.57
1:B:633:ALA:HB3	1:B:641:MET:HE1	1.92	0.51
1:B:672:CYS:HB3	4:B:1169:HOH:O	2.09	0.51
1:B:32:GLY:HA3	1:B:44:ASN:HD22	1.74	0.51
1:A:98:ASP:OD2	1:A:202:ARG:NH2	2.39	0.51
1:A:692:GLU:CB	4:A:1400:HOH:O	2.60	0.50
1:C:98:ASP:CG	1:C:202:ARG:HH22	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1110:HOH:O	1:B:721:THR:HG21	2.12	0.49
1:C:437:HIS:HB2	1:C:438:PRO:CD	2.43	0.48
1:A:202:ARG:HD3	4:A:1080:HOH:O	2.13	0.48
1:A:683:ARG:HG2	1:A:685:ARG:NH1	2.28	0.48
1:B:185:ASN:OD1	1:B:188:ALA:N	2.47	0.48
1:A:224:ARG:NH2	4:A:904:HOH:O	2.45	0.47
1:B:185:ASN:OD1	1:B:187:HIS:N	2.45	0.47
1:A:247:ASN:HA	1:A:248:GLY:HA2	1.58	0.47
1:B:439:ASN:HD22	1:B:456:GLN:HE22	1.63	0.47
1:B:672:CYS:CB	4:B:1169:HOH:O	2.63	0.47
1:C:440:SER:HB3	1:C:442:PHE:CZ	2.52	0.45
1:C:96:LEU:HD11	1:C:392:LEU:HD11	1.99	0.45
1:A:98:ASP:CG	1:A:202:ARG:HH22	2.24	0.45
1:A:153:ALA:HA	1:A:247:ASN:CB	2.47	0.45
1:C:633:ALA:HB3	1:C:641:MET:HE1	1.99	0.44
1:B:460:VAL:HG23	1:B:532:PRO:HB2	1.98	0.44
1:A:679:ASN:CB	4:A:1411:HOH:O	2.65	0.44
1:B:43:ASN:HD22	1:B:43:ASN:HA	1.66	0.43
1:A:721:THR:HG21	4:B:952:HOH:O	2.18	0.43
1:B:389:ILE:HD11	1:B:437:HIS:CE1	2.54	0.42
1:A:526:GLY:HA3	1:A:531:HIS:CD2	2.55	0.42
1:B:171:SER:N	4:B:901:HOH:O	2.52	0.42
1:B:525:TYR:CD1	1:B:579:MET:HA	2.54	0.42
1:C:311:ALA:O	1:C:642:SER:HB3	2.19	0.42
1:C:96:LEU:CD1	1:C:392:LEU:HD11	2.49	0.42
1:A:147:HIS:HD2	1:A:149:TYR:OH	2.02	0.42
1:B:397:ASN:C	1:B:397:ASN:HD22	2.27	0.42
1:B:451:MET:O	1:B:459:SER:HB2	2.20	0.42
1:C:389:ILE:HD11	1:C:437:HIS:CE1	2.55	0.42
1:A:531:HIS:CG	1:A:532:PRO:HD2	2.56	0.41
1:C:27:VAL:HG13	1:C:310:THR:HA	2.02	0.41
1:B:169:LYS:HA	1:B:174:ARG:HB3	2.02	0.41
1:B:392:LEU:O	1:B:393:TRP:C	2.64	0.41
1:C:102:MET:HE2	1:C:110:SER:HA	2.03	0.41
1:B:247:ASN:HA	1:B:248:GLY:HA2	1.80	0.41
1:C:256:ALA:O	1:C:257:LEU:HD12	2.20	0.41
1:C:318:GLN:HA	1:C:319:PRO:C	2.46	0.41
1:B:605:ASN:HD22	1:B:663:ILE:CG2	2.33	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)
4:A:1172:HOH:O	4:A:1172:HOH:O[10_664]	2.08	0.12

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	711/727 (98%)	686 (96%)	24 (3%)	1 (0%)	48	64
1	B	702/727 (97%)	663 (94%)	38 (5%)	1 (0%)	48	64
1	C	689/727 (95%)	653 (95%)	34 (5%)	2 (0%)	36	50
All	All	2102/2181 (96%)	2002 (95%)	96 (5%)	4 (0%)	43	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	LEU
1	A	99	ILE
1	B	99	ILE
1	C	99	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	585/618 (95%)	573 (98%)	12 (2%)	47	69
1	B	560/618 (91%)	550 (98%)	10 (2%)	51	73
1	C	505/618 (82%)	497 (98%)	8 (2%)	55	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1650/1854 (89%)	1620 (98%)	30 (2%)	51 73

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	193	ARG
1	A	318	GLN
1	A	342	ASN
1	A	391	GLN
1	A	454	ASN
1	A	560	LYS
1	A	595	GLU
1	A	623	THR
1	A	675	LYS
1	A	683	ARG
1	A	721	THR
1	B	96	LEU
1	B	318	GLN
1	B	342	ASN
1	B	390	TRP
1	B	397	ASN
1	B	454	ASN
1	B	560	LYS
1	B	595	GLU
1	B	683	ARG
1	B	721	THR
1	C	193	ARG
1	C	318	GLN
1	C	368	GLU
1	C	391	GLN
1	C	454	ASN
1	C	556	THR
1	C	599	HIS
1	C	679	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	66	ASN

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	147	HIS
1	A	180	GLN
1	A	226	HIS
1	A	233	ASN
1	A	271	GLN
1	A	275	HIS
1	A	292	GLN
1	A	342	ASN
1	A	391	GLN
1	A	439	ASN
1	A	454	ASN
1	A	475	GLN
1	A	487	GLN
1	A	498	ASN
1	A	508	GLN
1	A	524	GLN
1	A	531	HIS
1	A	622	ASN
1	A	697	GLN
1	B	43	ASN
1	B	44	ASN
1	B	147	HIS
1	B	318	GLN
1	B	342	ASN
1	B	437	HIS
1	B	439	ASN
1	B	454	ASN
1	B	475	GLN
1	B	487	GLN
1	B	508	GLN
1	B	528	ASN
1	B	531	HIS
1	B	589	GLN
1	B	697	GLN
1	B	713	HIS
1	C	43	ASN
1	C	267	GLN
1	C	403	ASN
1	C	437	HIS
1	C	439	ASN
1	C	466	GLN

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Mol	Chain	Res	Type
1	C	528	ASN
1	C	589	GLN
1	C	622	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	MVL	C	802	2	14,15,15	1.35	2 (14%)	14,22,22	2.25	7 (50%)
3	MVL	A	802	2	14,15,15	1.03	1 (7%)	14,22,22	2.35	5 (35%)
3	MVL	B	802	2	14,15,15	1.28	3 (21%)	14,22,22	2.43	6 (42%)

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	MVL	C	802	2	-	0/2/22/22	0/2/2/2
3	MVL	A	802	2	-	0/2/22/22	0/2/2/2
3	MVL	B	802	2	-	0/2/22/22	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	MVL	C8-N10	-2.49	1.34	1.38
3	C	802	MVL	C8-N10	-2.44	1.34	1.38
3	B	802	MVL	C8-N10	-2.33	1.34	1.38
3	C	802	MVL	C1-N1	2.32	1.35	1.32
3	B	802	MVL	C1-N10	-2.12	1.33	1.36
3	B	802	MVL	C5-N10	2.03	1.49	1.47

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	MVL	N10-C1-N1	-4.82	108.59	111.52
3	B	802	MVL	C4-C3-C2	4.72	117.68	110.22
3	C	802	MVL	C4-C3-C2	4.56	117.43	110.22
3	A	802	MVL	C4-C3-C2	4.55	117.42	110.22
3	B	802	MVL	N10-C1-N1	-4.27	108.93	111.52
3	B	802	MVL	C7-N1-C1	3.75	108.32	104.86
3	A	802	MVL	C7-N1-C1	3.46	108.05	104.86
3	C	802	MVL	N10-C1-N1	-3.40	109.46	111.52
3	C	802	MVL	C3-C4-C5	2.98	116.41	111.37
3	C	802	MVL	C7-N1-C1	2.88	107.51	104.86
3	B	802	MVL	C8-C7-N1	-2.76	107.13	110.74
3	A	802	MVL	C3-C4-C5	2.69	115.91	111.37
3	C	802	MVL	C8-C7-N1	-2.61	107.32	110.74
3	A	802	MVL	C8-C7-N1	-2.47	107.51	110.74
3	B	802	MVL	O3-C3-C2	-2.39	104.91	109.64
3	B	802	MVL	C3-C4-C5	2.37	115.37	111.37
3	C	802	MVL	C6-C5-C4	-2.20	109.63	112.93
3	C	802	MVL	C7-C8-N10	2.09	107.71	106.18

There are no chirality outliers.

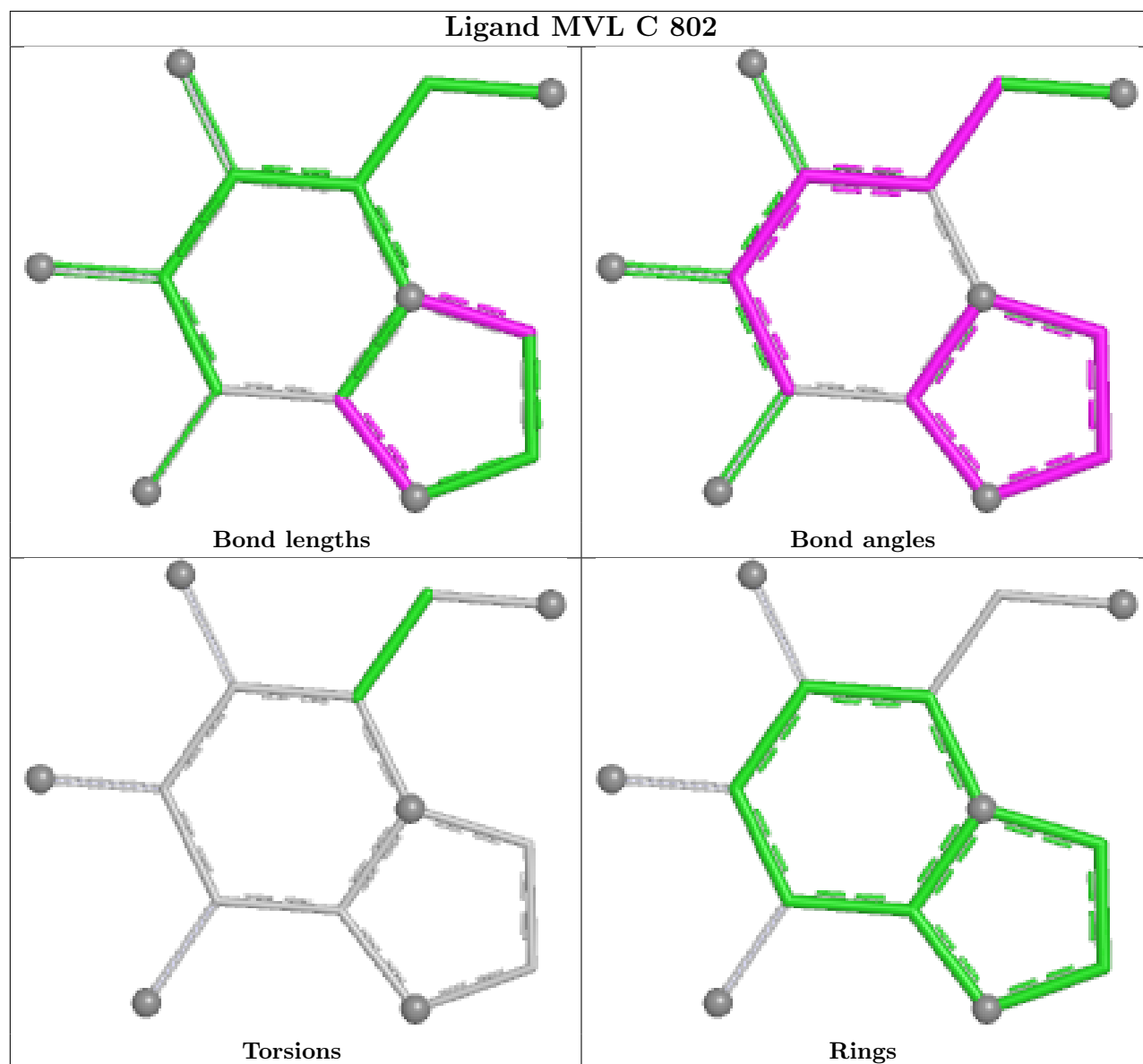
There are no torsion outliers.

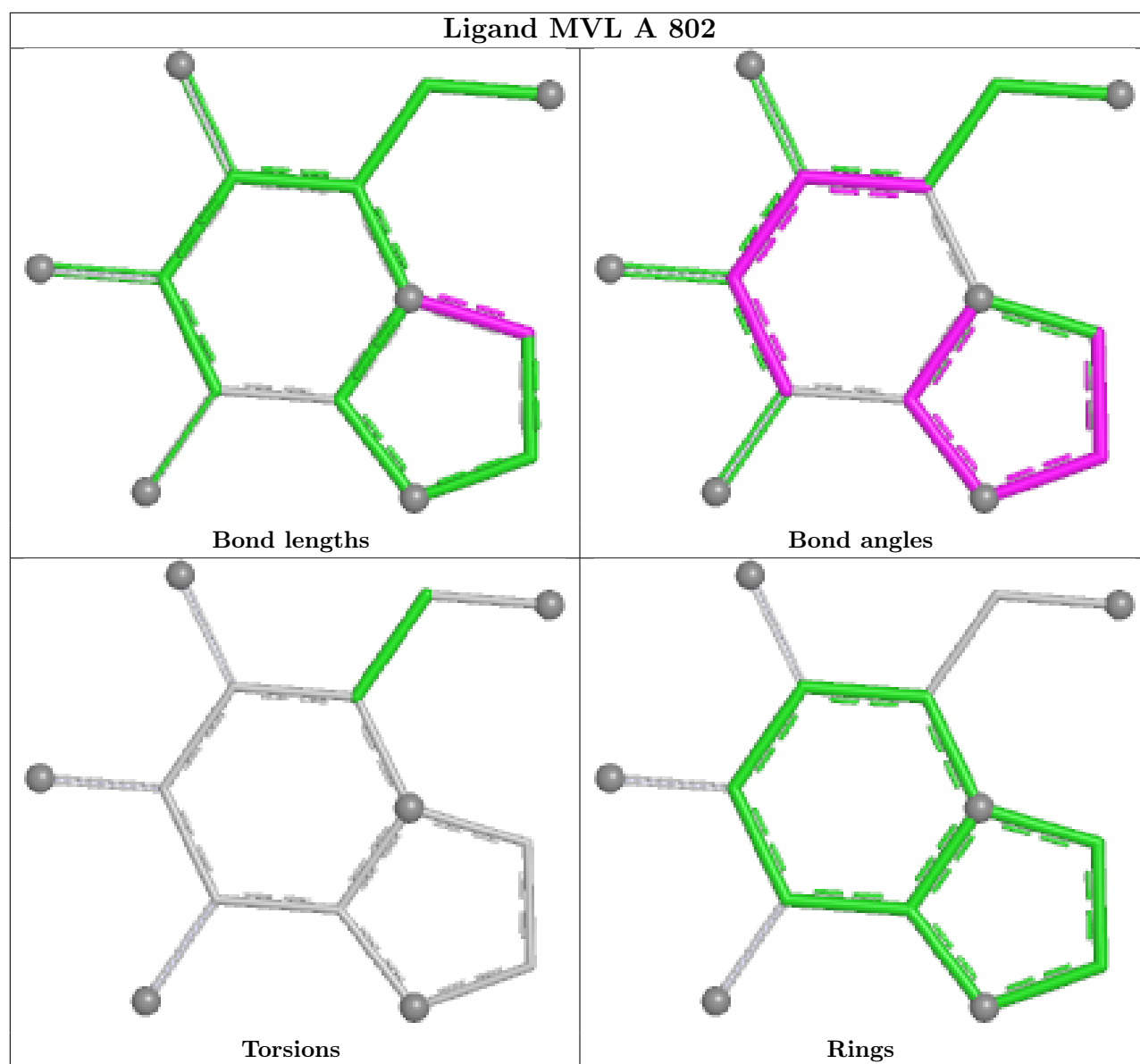
There are no ring outliers.

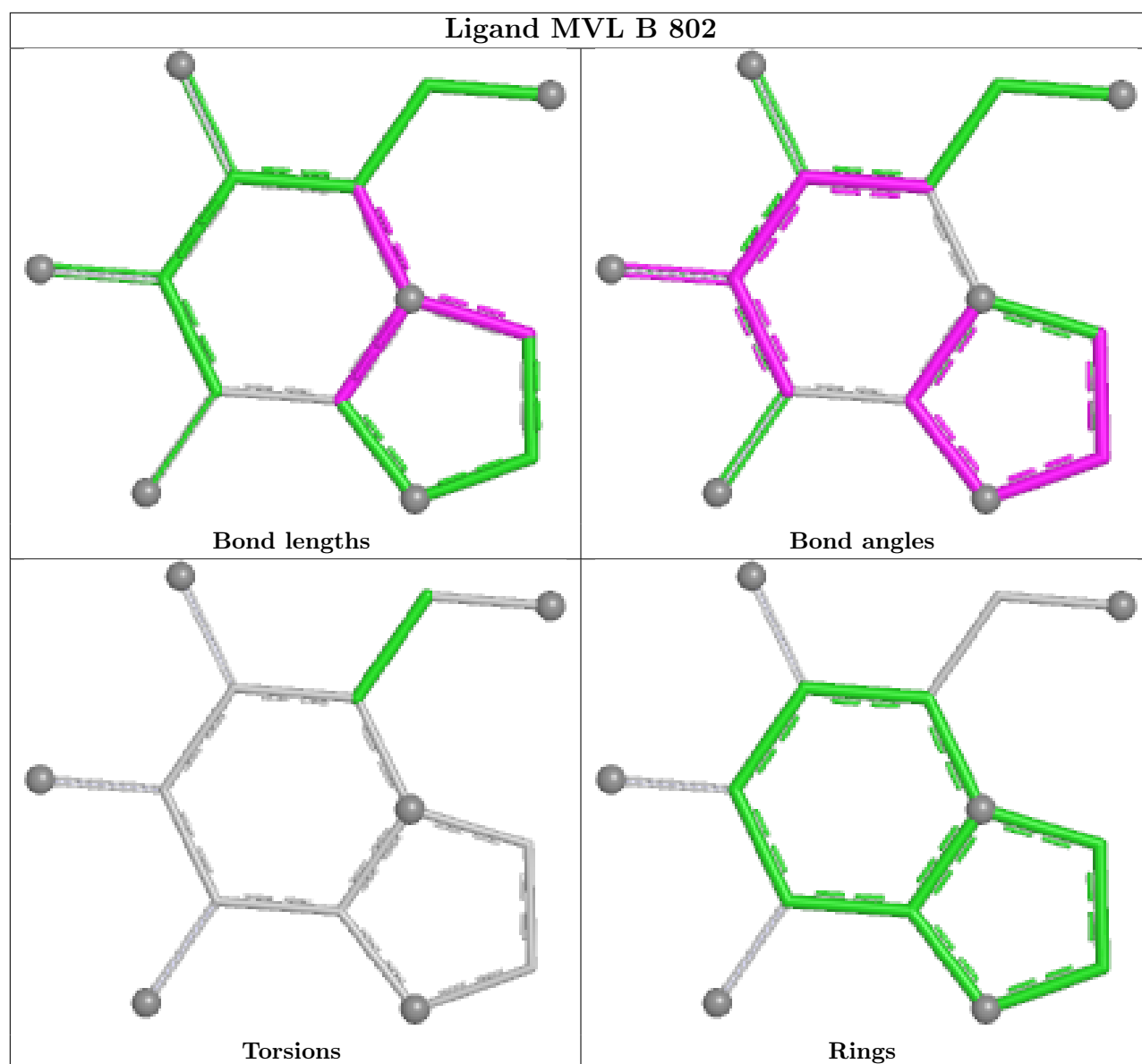
No monomer is involved in short contacts.

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	714/727 (98%)	-0.33	14 (1%) 65 60	24, 37, 58, 116	1 (0%)
1	B	708/727 (97%)	0.68	59 (8%) 17 14	31, 60, 93, 131	0
1	C	692/727 (95%)	2.40	423 (61%) 0 0	43, 97, 126, 159	3 (0%)
All	All	2114/2181 (96%)	0.90	496 (23%) 2 1	24, 61, 115, 159	4 (0%)

All (496) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	624	LEU	6.8
1	C	544	TYR	6.7
1	C	732	GLY	6.6
1	C	643	ALA	6.5
1	C	669	LEU	6.0
1	C	464	LEU	5.8
1	C	29	PRO	5.8
1	C	535[A]	GLU	5.8
1	C	586	PHE	5.8
1	C	355	PHE	5.7
1	C	674	LEU	5.6
1	C	34	GLY	5.6
1	B	20	ALA	5.4
1	C	599	HIS	5.1
1	C	543	TRP	5.1
1	C	600	VAL	5.1
1	C	691	PRO	5.0
1	C	585	GLY	5.0
1	C	48	ALA	5.0
1	C	75	TYR	5.0
1	C	172[A]	TRP	4.9
1	A	579	MET	4.9
1	C	677	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	52	PHE	4.9
1	C	711	ILE	4.9
1	C	122	PRO	4.9
1	C	541	TYR	4.8
1	C	409	ILE	4.8
1	A	38	GLY	4.8
1	C	113	PHE	4.8
1	C	572	SER	4.7
1	C	114	THR	4.7
1	C	341	ASN	4.7
1	C	644	TRP	4.6
1	C	623	THR	4.6
1	A	576	SER	4.6
1	C	297	GLU	4.6
1	C	658	ALA	4.6
1	C	277	ASP	4.6
1	C	639	GLY	4.5
1	C	149	TYR	4.5
1	C	596	PRO	4.5
1	C	123	GLY	4.4
1	A	39	GLY	4.4
1	C	304	GLN	4.4
1	C	617	VAL	4.3
1	C	88	LEU	4.3
1	C	603	LEU	4.3
1	C	89	SER	4.3
1	A	37	ASP	4.3
1	C	349	PHE	4.2
1	C	506	PHE	4.2
1	C	431	ASN	4.2
1	C	47	GLY	4.2
1	C	625	TYR	4.2
1	C	417	ILE	4.2
1	C	363	THR	4.2
1	C	591	ALA	4.2
1	C	346	TYR	4.1
1	C	649	ALA	4.1
1	B	734	GLY	4.1
1	C	684	ILE	4.1
1	C	414	LEU	4.1
1	C	303	VAL	4.0
1	C	250	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	734	GLY	4.0
1	C	483	ASP	4.0
1	C	410	THR	4.0
1	C	215	LEU	3.9
1	C	45	TYR	3.9
1	C	487	GLN	3.9
1	C	26	TYR	3.9
1	C	319	PRO	3.9
1	C	112	ALA	3.9
1	A	36	ILE	3.9
1	C	22	GLU	3.8
1	C	524	GLN	3.8
1	C	592	HIS	3.8
1	C	315	THR	3.8
1	B	579	MET	3.8
1	C	542	PHE	3.8
1	C	593	GLY	3.8
1	C	638	CYS	3.8
1	C	507	PHE	3.8
1	C	621	LEU	3.8
1	C	120	ALA	3.7
1	C	80	ILE	3.7
1	C	105	SER	3.7
1	C	157	ALA	3.7
1	B	246	LEU	3.7
1	C	296	ILE	3.7
1	C	549	ILE	3.7
1	C	54	MET	3.7
1	C	301	THR	3.7
1	B	677	ALA	3.7
1	B	186	ASP	3.7
1	C	91	THR	3.7
1	C	602	TYR	3.7
1	C	723	VAL	3.6
1	C	133	ASN	3.6
1	C	175[A]	ARG	3.6
1	C	408	VAL	3.6
1	B	40	LEU	3.6
1	C	312	LEU	3.6
1	C	552	LEU	3.6
1	C	23	ILE	3.6
1	C	281	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	309	TYR	3.6
1	B	181	ILE	3.6
1	B	581	HIS	3.6
1	C	73	TYR	3.6
1	C	545	VAL	3.6
1	C	316	MET	3.6
1	C	55	ILE	3.6
1	C	81	PHE	3.6
1	C	716	ILE	3.6
1	B	341	ASN	3.6
1	C	330	MET	3.5
1	C	145	GLY	3.5
1	C	709	PHE	3.5
1	C	664	ILE	3.5
1	C	78	ASN	3.5
1	C	109	THR	3.5
1	A	731	SER	3.5
1	C	527	GLY	3.5
1	C	657	PRO	3.5
1	B	230	ALA	3.5
1	C	406	ILE	3.4
1	C	496	TYR	3.4
1	B	116	ASP	3.4
1	C	659	ASP	3.4
1	C	49	THR	3.4
1	C	365	LEU	3.4
1	C	676	LEU	3.4
1	C	42	GLY	3.4
1	C	300	GLY	3.4
1	C	413	ILE	3.4
1	C	694	ILE	3.4
1	C	278	PHE	3.4
1	C	606	PHE	3.4
1	C	692	GLU	3.4
1	C	528	ASN	3.4
1	C	159	ILE	3.4
1	C	83	PHE	3.4
1	C	724	PHE	3.4
1	C	129	LEU	3.4
1	C	595	GLU	3.4
1	C	151	TYR	3.3
1	C	539	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	529	GLY	3.3
1	C	311	ALA	3.3
1	C	632	TYR	3.3
1	C	471	TRP	3.3
1	C	27	VAL	3.3
1	C	24	THR	3.3
1	C	633	ALA	3.3
1	C	717	MET	3.3
1	C	362	TYR	3.3
1	C	590	TYR	3.3
1	C	364	LEU	3.3
1	C	160	ILE	3.3
1	C	468	PHE	3.2
1	C	525	TYR	3.2
1	C	371	THR	3.2
1	C	526	GLY	3.2
1	C	31	ILE	3.2
1	C	378	ILE	3.2
1	C	668	LEU	3.2
1	C	295	LYS	3.2
1	C	655	VAL	3.2
1	B	35	ALA	3.2
1	C	138	LEU	3.2
1	C	360	PRO	3.2
1	C	486	TYR	3.2
1	B	189	VAL	3.2
1	C	339	VAL	3.2
1	C	79	THR	3.2
1	C	504	THR	3.2
1	C	663	ILE	3.2
1	B	153	ALA	3.2
1	C	136	ALA	3.2
1	C	648	SER	3.2
1	C	305	LYS	3.2
1	C	730	PRO	3.2
1	C	385	GLY	3.2
1	C	699	VAL	3.2
1	C	620	ILE	3.2
1	C	687	ILE	3.2
1	B	527	GLY	3.1
1	C	460	VAL	3.1
1	C	389	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	661	ARG	3.1
1	C	438	PRO	3.1
1	C	153	ALA	3.1
1	C	701	LEU	3.1
1	C	650	MET	3.0
1	C	731	SER	3.0
1	C	294	GLY	3.0
1	C	422	MET	3.0
1	C	653	TYR	3.0
1	C	547	HIS	3.0
1	B	215	LEU	3.0
1	C	636	ASP	3.0
1	C	629	SER	3.0
1	C	247	ASN	3.0
1	C	320	ASN	3.0
1	C	317	ILE	3.0
1	C	462	ILE	3.0
1	C	473	VAL	3.0
1	C	517	ILE	3.0
1	C	152	PRO	3.0
1	C	476	LEU	3.0
1	C	71	SER	3.0
1	C	587	VAL	3.0
1	C	59	PRO	3.0
1	C	351	LEU	3.0
1	C	479	LYS	3.0
1	C	28	ASN	3.0
1	C	342	ASN	3.0
1	C	176	ILE	2.9
1	C	534	THR	2.9
1	C	125	TYR	2.9
1	C	30	PHE	2.9
1	C	597	SER	2.9
1	C	641	MET	2.9
1	C	252	THR	2.9
1	C	77	ARG	2.9
1	C	121	ARG	2.9
1	C	546	PRO	2.9
1	C	728	LYS	2.9
1	C	619	HIS	2.9
1	C	675	LYS	2.9
1	C	308	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	247	ASN	2.9
1	B	247	ASN	2.9
1	C	255	VAL	2.9
1	C	46	PRO	2.9
1	C	532	PRO	2.9
1	C	673	THR	2.9
1	C	710	PHE	2.9
1	C	490	HIS	2.8
1	C	216	THR	2.8
1	C	372	ASP	2.8
1	C	647	PHE	2.8
1	C	652	PHE	2.8
1	C	313	TYR	2.8
1	C	103	PRO	2.8
1	C	721	THR	2.8
1	C	101	LEU	2.8
1	C	243	PHE	2.8
1	C	352	TRP	2.8
1	C	222	GLY	2.8
1	C	44	ASN	2.8
1	C	455	ILE	2.8
1	C	367	PRO	2.8
1	C	253	CYS	2.8
1	C	722	MET	2.8
1	C	119	LYS	2.8
1	C	390	TRP	2.8
1	A	679	ASN	2.8
1	C	135	ASN	2.8
1	C	150	GLN	2.8
1	C	391	GLN	2.8
1	C	396	ASP	2.8
1	C	165	HIS	2.8
1	C	195	ILE	2.7
1	B	172	TRP	2.7
1	B	276	TRP	2.7
1	B	575	LYS	2.7
1	B	193	ARG	2.7
1	C	370	VAL	2.7
1	C	523	TYR	2.7
1	C	70	ALA	2.7
1	C	357	ALA	2.7
1	B	67	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	192	TYR	2.7
1	C	293	LEU	2.7
1	A	732	GLY	2.7
1	C	373	PHE	2.7
1	C	325	VAL	2.7
1	C	392	LEU	2.7
1	C	630	SER	2.7
1	B	574	TYR	2.7
1	C	484	ALA	2.7
1	C	700	THR	2.7
1	B	108	ARG	2.6
1	C	106	SER	2.6
1	B	530	GLY	2.6
1	C	707	LYS	2.6
1	C	51	PRO	2.6
1	C	210	PHE	2.6
1	C	682	PHE	2.6
1	C	672	CYS	2.6
1	C	96	LEU	2.6
1	C	282	VAL	2.6
1	B	180	GLN	2.6
1	C	466	GLN	2.6
1	C	384	TYR	2.6
1	C	448	TYR	2.6
1	C	645	TYR	2.6
1	C	65	PRO	2.6
1	B	177	ILE	2.6
1	C	146	ILE	2.6
1	B	81	PHE	2.6
1	C	562	PHE	2.6
1	C	569	PHE	2.6
1	C	66	ASN	2.6
1	C	627	ASN	2.6
1	C	618	SER	2.6
1	C	283	ALA	2.6
1	C	474	ALA	2.6
1	C	289	TRP	2.6
1	B	244	GLY	2.6
1	C	519	PRO	2.6
1	C	241	PHE	2.6
1	B	212	SER	2.6
1	C	683	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	67	TRP	2.5
1	C	134	ILE	2.5
1	C	442	PHE	2.5
1	C	439	ASN	2.5
1	C	226	HIS	2.5
1	C	332	ALA	2.5
1	C	244	GLY	2.5
1	C	198	TRP	2.5
1	C	553	MET	2.5
1	C	608	GLY	2.5
1	C	288	ASP	2.5
1	C	533	PHE	2.5
1	C	566	LEU	2.5
1	C	609	GLN	2.5
1	C	212	SER	2.5
1	C	686	THR	2.5
1	C	60	ASP	2.5
1	C	161	LEU	2.5
1	B	78	ASN	2.5
1	B	231	VAL	2.5
1	C	211	SER	2.5
1	C	376	SER	2.5
1	C	368	GLU	2.4
1	B	156	ASP	2.4
1	C	192	TYR	2.4
1	C	670	ASP	2.4
1	C	695	TYR	2.4
1	B	679	ASN	2.4
1	C	403	ASN	2.4
1	B	171	SER	2.4
1	C	94	SER	2.4
1	B	82	GLY	2.4
1	C	130	LYS	2.4
1	C	387	LEU	2.4
1	C	398	TYR	2.4
1	C	640	GLN	2.4
1	B	187	HIS	2.4
1	C	646	VAL	2.4
1	C	377	MET	2.4
1	C	558	GLY	2.4
1	B	214	ILE	2.4
1	C	279	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	420	ILE	2.4
1	C	475	GLN	2.4
1	C	314	HIS	2.4
1	C	531	HIS	2.4
1	C	662	TYR	2.4
1	C	500	PHE	2.4
1	C	428	ALA	2.4
1	C	601	ALA	2.4
1	B	526	GLY	2.4
1	B	150	GLN	2.4
1	C	174	ARG	2.4
1	C	246	LEU	2.4
1	C	331	ALA	2.4
1	C	607	ALA	2.4
1	C	354	THR	2.3
1	C	610	PRO	2.3
1	B	440	SER	2.3
1	B	232	ILE	2.3
1	C	156	ASP	2.3
1	C	404	HIS	2.3
1	C	127	VAL	2.3
1	B	582	ASN	2.3
1	C	626	ASN	2.3
1	C	93	ALA	2.3
1	C	33	THR	2.3
1	C	463	THR	2.3
1	C	556	THR	2.3
1	C	642	SER	2.3
1	C	183	ILE	2.3
1	C	399	CYS	2.3
1	C	298	VAL	2.3
1	C	502	PRO	2.3
1	C	148	ARG	2.3
1	C	154	GLY	2.3
1	C	203	LYS	2.3
1	C	302	GLU	2.3
1	C	616	TYR	2.3
1	C	706	HIS	2.3
1	C	719	GLY	2.3
1	C	201	LEU	2.3
1	C	611	TRP	2.3
1	C	689	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	374	VAL	2.3
1	C	321	THR	2.2
1	C	457	THR	2.2
1	C	665	GLY	2.2
1	C	169	LYS	2.2
1	C	322	MET	2.2
1	C	499	LEU	2.2
1	B	445	TRP	2.2
1	C	467	ALA	2.2
1	C	56	GLN	2.2
1	C	437	HIS	2.2
1	C	99	ILE	2.2
1	C	405	SER	2.2
1	A	733	TRP	2.2
1	B	733	TRP	2.2
1	C	118	GLU	2.2
1	C	489	PHE	2.2
1	C	64	ALA	2.2
1	C	275	HIS	2.2
1	C	383	TYR	2.2
1	C	386	TYR	2.2
1	C	510	LYS	2.2
1	B	163	MET	2.2
1	B	240	CYS	2.2
1	C	451	MET	2.2
1	C	571	THR	2.2
1	C	223	GLY	2.2
1	C	480	LEU	2.2
1	C	588	GLY	2.2
1	C	84	SER	2.2
1	B	206	PHE	2.2
1	C	520	PHE	2.2
1	C	654	PRO	2.2
1	C	444	VAL	2.2
1	C	482	LYS	2.2
1	B	245	GLN	2.2
1	C	102	MET	2.2
1	A	678	GLY	2.2
1	C	68	GLY	2.2
1	C	124	TYR	2.2
1	C	402	GLY	2.2
1	C	666	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	488	ARG	2.2
1	C	688	ARG	2.2
1	C	213	PRO	2.2
1	C	225	VAL	2.1
1	A	341	ASN	2.1
1	B	233	ASN	2.1
1	B	191	GLY	2.1
1	C	237	LEU	2.1
1	C	361	LEU	2.1
1	C	411	ASP	2.1
1	C	509	SER	2.1
1	B	155	LYS	2.1
1	C	345	HIS	2.1
1	C	598	HIS	2.1
1	C	538	ALA	2.1
1	B	580	ASN	2.1
1	C	72	GLY	2.1
1	C	170	GLY	2.1
1	C	251	LEU	2.1
1	C	678	GLY	2.1
1	C	110	SER	2.1
1	C	186	ASP	2.1
1	C	340	ALA	2.1
1	C	477	ALA	2.1
1	C	605	ASN	2.1
1	C	32	GLY	2.1
1	C	57	LEU	2.1
1	C	651	GLY	2.1
1	C	155	LYS	2.1
1	C	501	HIS	2.1
1	C	318	GLN	2.1
1	C	53	GLY	2.1
1	C	685	ARG	2.1
1	C	205	TYR	2.1
1	C	407	PRO	2.1
1	C	128	MET	2.1
1	B	550	GLN	2.0
1	C	589	GLN	2.0
1	B	266	ARG	2.0
1	C	144	ASN	2.0
1	C	703	GLY	2.0
1	C	435	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	448	TYR	2.0
1	C	358	SER	2.0
1	C	388	PRO	2.0
1	C	472	CYS	2.0
1	C	63	GLU	2.0
1	B	133	ASN	2.0
1	C	505	LYS	2.0
1	C	536	GLY	2.0
1	C	612	LYS	2.0
1	C	350	SER	2.0
1	C	381	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

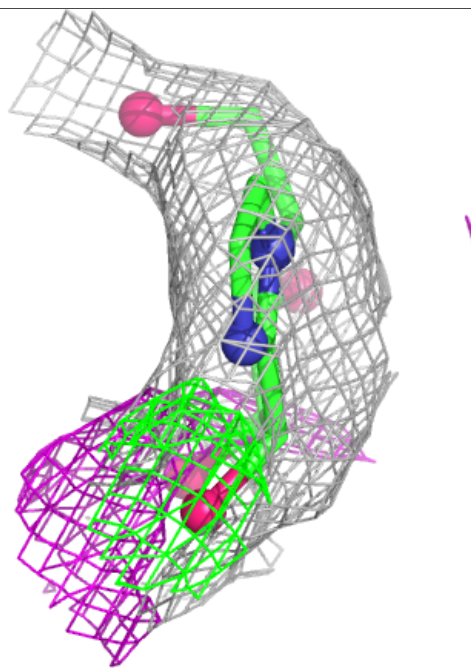
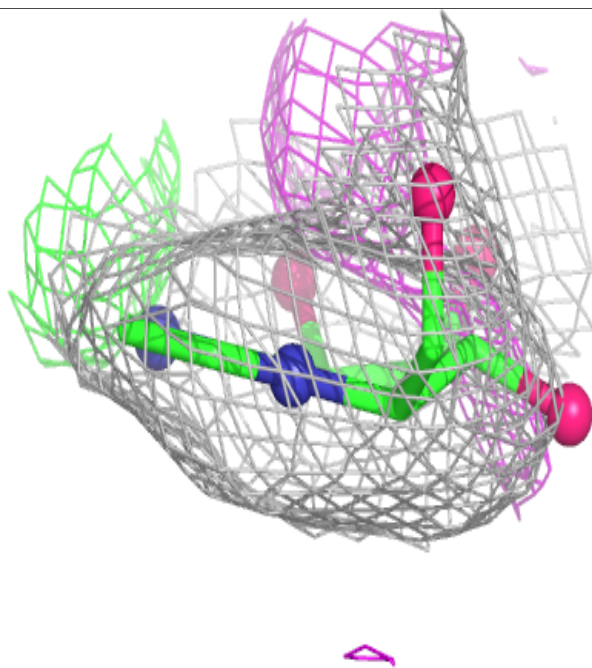
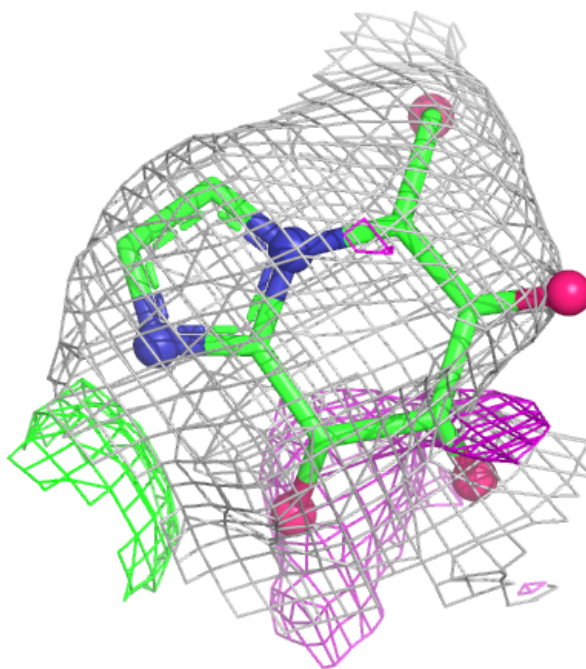
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	MVL	C	802	14/14	0.77	0.19	90,97,101,103	0
3	MVL	B	802	14/14	0.89	0.14	54,68,70,70	0
2	CA	C	801	1/1	0.95	0.18	100,100,100,100	0
3	MVL	A	802	14/14	0.97	0.06	30,33,34,35	0
2	CA	B	801	1/1	0.99	0.05	55,55,55,55	0
2	CA	A	801	1/1	1.00	0.04	33,33,33,33	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.

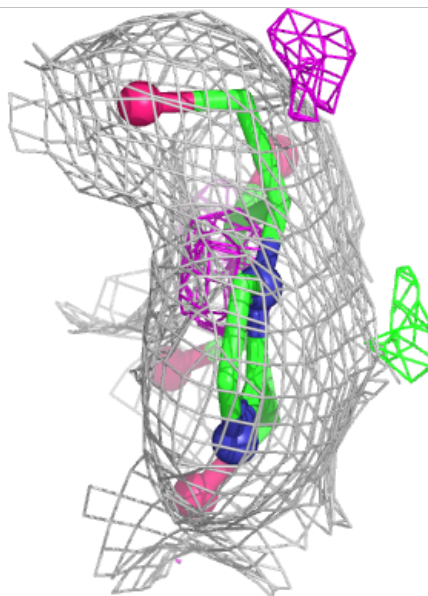
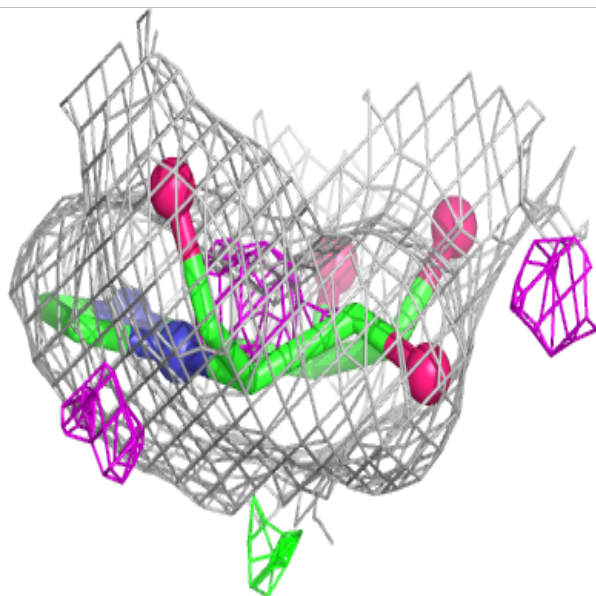
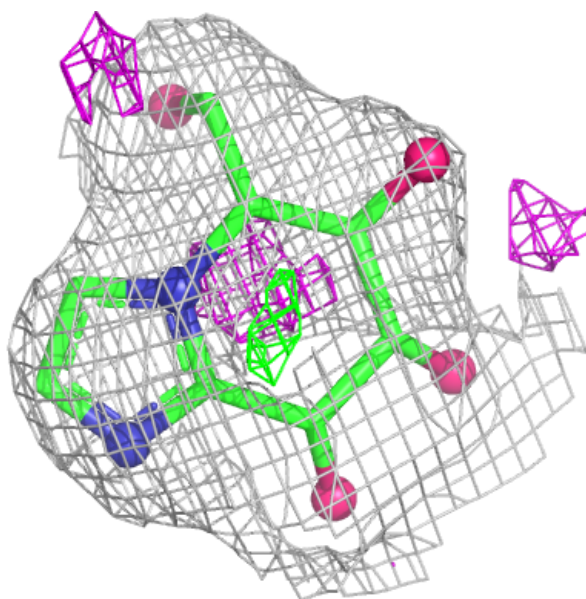
Electron density around MVL C 802:

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



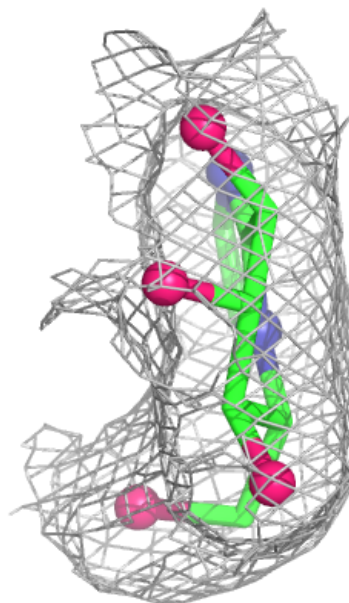
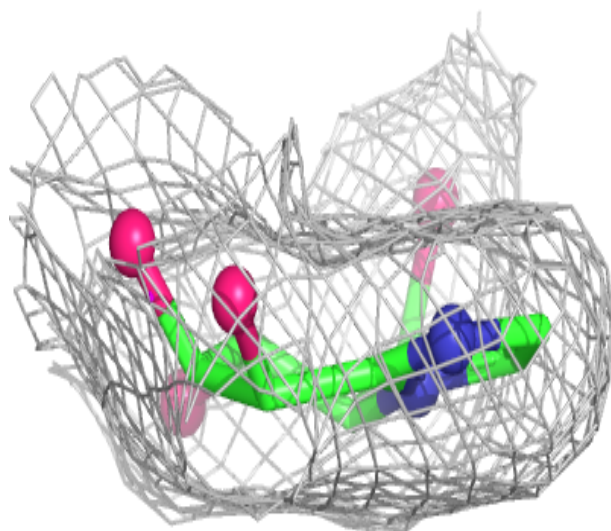
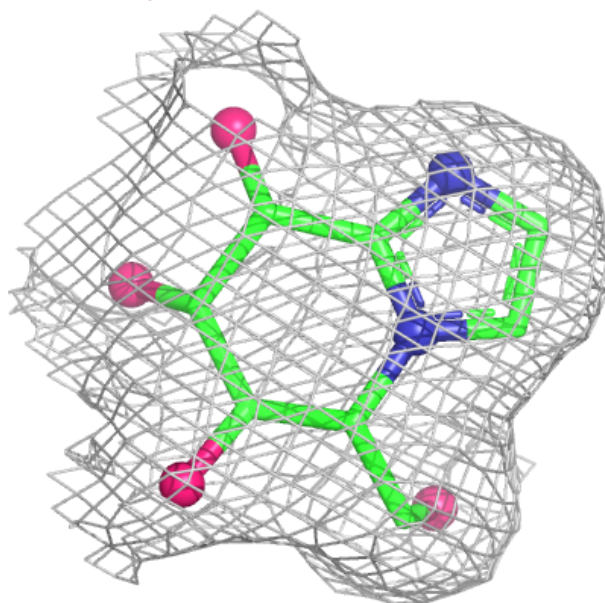
Electron density around MVL B 802:

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



Electron density around MVL A 802:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.