



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:53 AM UTC

PDB ID : 5SDQ / pdb_00005sdq
Title : PanDDA analysis group deposition – Crystal Structure of Porphyromonas gingivalis in complex with Z2856434887
Authors : Tham, C.T.; Coker, J.A.; Krojer, T.; Foster, W.R.; Koekemoer, L.; Douangamath, A.; Talon, R.; Fearon, D.; von Delft, F.; Yue, W.W.; Bountra, C.; Bezerra, G.A.
Deposited on : 2022-01-20
Resolution : 1.92 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](#) ①) 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

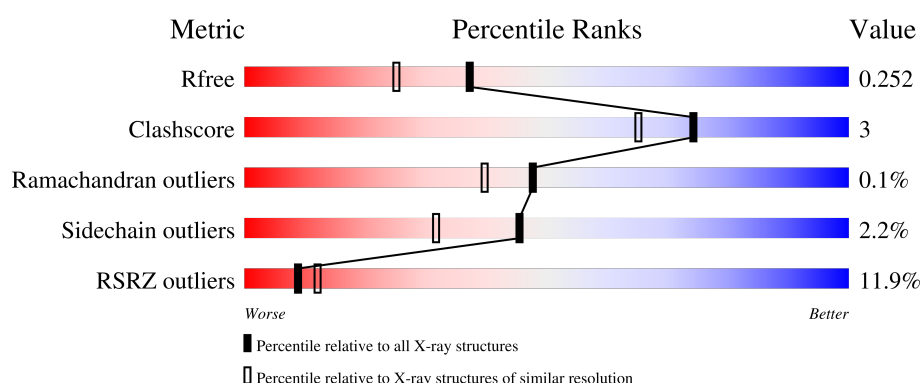
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	707	14% 88% 9% ..
1	B	707	10% 89% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11273 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.

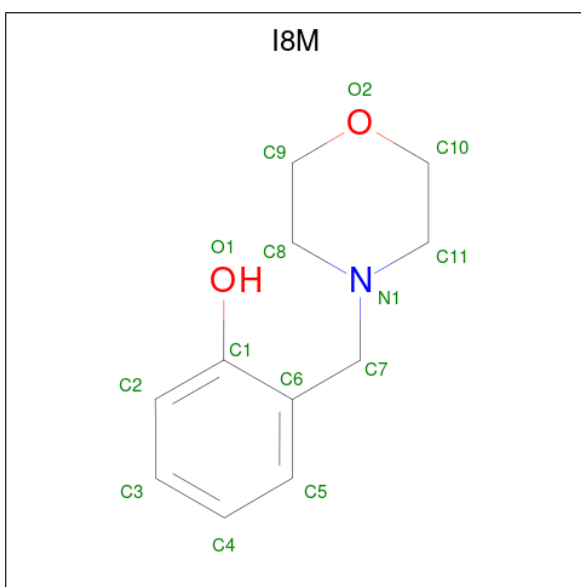
- Molecule 1 is a protein called Asp/Glu-specific dipeptidyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5493	3488	948	1030	27			
1	B	695	Total	C	N	O	S	0	1	0
			5467	3470	941	1029	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP B2RID1
A	721	ALA	-	expression tag	UNP B2RID1
A	722	HIS	-	expression tag	UNP B2RID1
A	723	HIS	-	expression tag	UNP B2RID1
A	724	HIS	-	expression tag	UNP B2RID1
A	725	HIS	-	expression tag	UNP B2RID1
A	726	HIS	-	expression tag	UNP B2RID1
A	727	HIS	-	expression tag	UNP B2RID1
B	21	MET	-	initiating methionine	UNP B2RID1
B	721	ALA	-	expression tag	UNP B2RID1
B	722	HIS	-	expression tag	UNP B2RID1
B	723	HIS	-	expression tag	UNP B2RID1
B	724	HIS	-	expression tag	UNP B2RID1
B	725	HIS	-	expression tag	UNP B2RID1
B	726	HIS	-	expression tag	UNP B2RID1
B	727	HIS	-	expression tag	UNP B2RID1

- Molecule 2 is 2-[(morpholin-4-yl)methyl]phenol (CCD ID: I8M) (formula: C₁₁H₁₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			14	11	1	2		
2	B	1	Total	C	N	O	0	1
			14	11	1	2		
2	B	1	Total	C	N	O	0	1
			14	11	1	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		

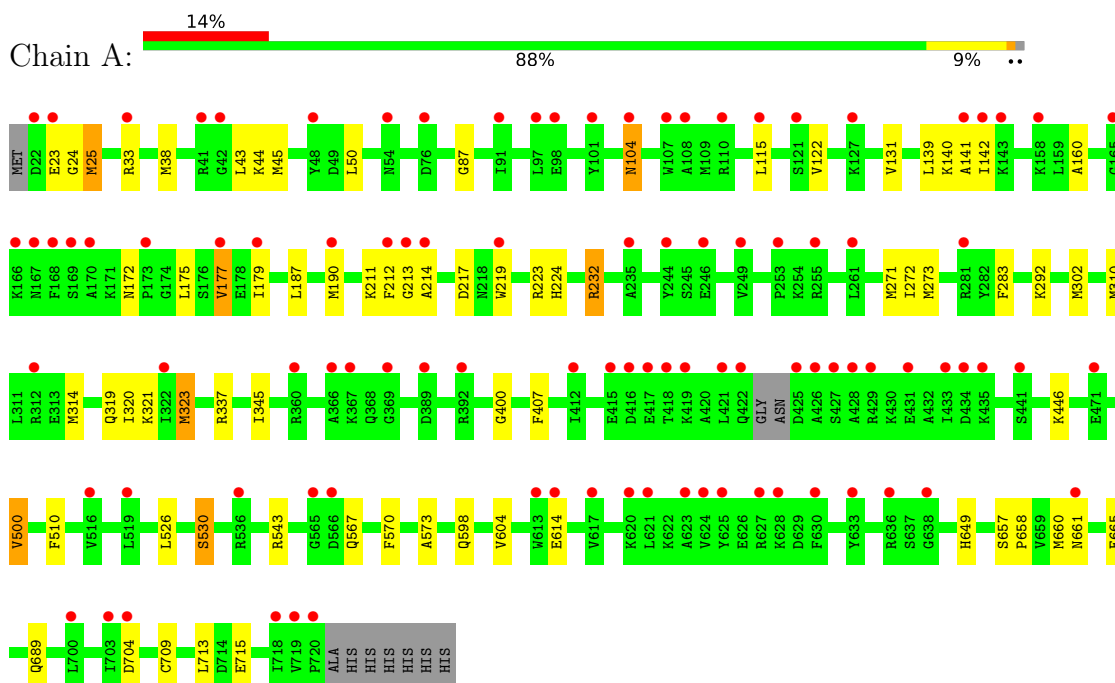
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	127	Total	O	0	1
			127	127		

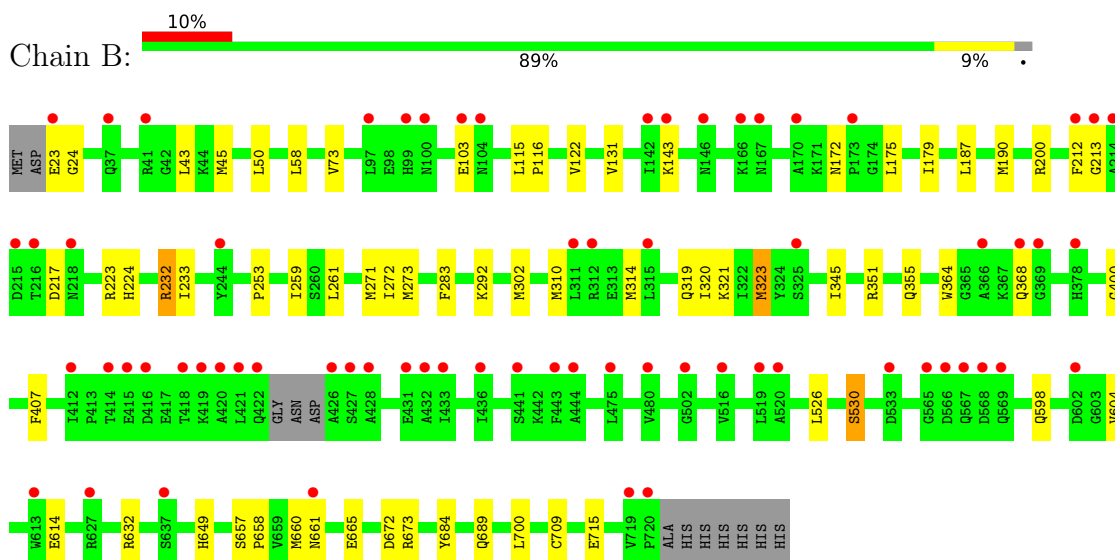
3 Residue-property plots

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: Asp/Glu-specific dipeptidyl-peptidase



• Molecule 1: Asp/Glu-specific dipeptidyl-peptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.23Å 116.88Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.52 – 1.92 76.52 – 1.92	Depositor EDS
% Data completeness (in resolution range)	80.1 (76.52-1.92) 80.1 (76.52-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, R_{free}	0.231 , 0.247 0.232 , 0.252	Depositor DCC
R_{free} test set	5504 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11273	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: CL, I8M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	3/5617 (0.1%)	1.00	10/7607 (0.1%)
1	B	0.65	1/5590 (0.0%)	0.98	5/7573 (0.1%)
All	All	0.65	4/11207 (0.0%)	0.99	15/15180 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	MET	SD-CE	-7.08	1.61	1.79
1	B	323	MET	SD-CE	-6.54	1.63	1.79
1	A	25	MET	SD-CE	-5.49	1.65	1.79
1	A	214	ALA	CA-C	5.27	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLY	N-CA-C	12.54	127.84	112.79
1	B	660	MET	CA-C-N	6.21	132.73	121.06
1	B	660	MET	C-N-CA	6.21	132.73	121.06
1	A	141	ALA	CA-C-N	6.18	133.09	121.97
1	A	141	ALA	C-N-CA	6.18	133.09	121.97
1	A	660	MET	CA-C-N	6.12	132.56	121.06
1	A	660	MET	C-N-CA	6.12	132.56	121.06
1	B	24	GLY	N-CA-C	5.80	121.66	111.57
1	A	115	LEU	N-CA-C	5.16	116.42	109.24
1	B	407	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	407	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	87	GLY	CA-C-N	5.09	127.42	120.54
1	A	87	GLY	C-N-CA	5.09	127.42	120.54
1	B	115	LEU	N-CA-C	5.09	116.31	109.24
1	A	104	ASN	CA-CB-CG	5.06	117.66	112.60

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	5493	0	5282	35	0
1	B	5467	0	5236	31	0
2	A	14	0	0	0	0
2	B	28	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	141	0	0	0	0
4	B	127	0	0	1	0
All	All	11273	0	10518	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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:B:319:GLN:HG3	1:B:323:MET:HE2	1.62	0.80
1:A:319:GLN:HG3	1:A:323:MET:HE2	1.63	0.78
1:B:50:LEU:HD21	1:B:271:MET:HE1	1.64	0.77
1:B:223:ARG:NH2	1:B:672:ASP:OD2	2.18	0.77
1:A:160:ALA:HB1	1:A:177:VAL:HG12	1.67	0.76
1:A:139:LEU:O	1:A:142:ILE:HG13	1.86	0.76
1:A:50:LEU:HD21	1:A:271:MET:HE1	1.68	0.75
1:B:213:GLY:HA3	1:B:217:ASP:HB2	1.69	0.75
1:A:213:GLY:HA3	1:A:217:ASP:HB2	1.71	0.73
1:B:131:VAL:HG11	1:B:190:MET:HE3	1.80	0.62
1:A:25:MET:HE1	1:A:573:ALA:HB2	1.82	0.61
1:A:649:HIS:CD2	1:A:689:GLN:HE22	2.19	0.60
1:A:131:VAL:HG11	1:A:190:MET:HE3	1.83	0.60
1:A:25:MET:HE2	1:A:570:PHE:CE2	2.38	0.59
1:B:649:HIS:CD2	1:B:689:GLN:HE22	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ILE:HD11	1:B:190:MET:HE2	1.87	0.57
1:B:212:PHE:O	1:B:614:GLU:O	2.23	0.57
1:A:25:MET:HE2	1:A:570:PHE:HE2	1.71	0.56
1:B:73:VAL:HG11	1:B:253:PRO:HG3	1.87	0.56
1:A:179:ILE:HD11	1:A:190:MET:HE2	1.88	0.56
1:B:261:LEU:HD21	1:B:700:LEU:HD12	1.88	0.54
1:A:314:MET:HG2	1:A:321:LYS:HA	1.90	0.54
1:B:351:ARG:HH12	1:B:355:GLN:HE21	1.54	0.54
1:B:314:MET:HG2	1:B:321:LYS:HA	1.90	0.53
1:B:320:ILE:HD13	1:B:323:MET:HE3	1.90	0.53
1:B:172:ASN:HB3	1:B:175:LEU:HD12	1.90	0.53
1:A:160:ALA:HB1	1:A:177:VAL:CG1	2.37	0.52
1:A:320:ILE:HD13	1:A:323:MET:HE3	1.91	0.52
1:A:661:ASN:HD22	1:A:665:GLU:HB2	1.76	0.51
1:B:661:ASN:HD22	1:B:665:GLU:HB2	1.76	0.51
1:A:25:MET:CE	1:A:573:ALA:HB2	2.39	0.51
1:A:212:PHE:O	1:A:614:GLU:O	2.28	0.50
1:B:364:TRP:O	1:B:368:GLN:HG2	2.12	0.49
1:B:259:ILE:HG21	1:B:700:LEU:HD11	1.94	0.48
1:B:673:ARG:HD2	4:B:905:HOH:O	2.13	0.48
1:B:23:GLU:HG2	1:B:684:TYR:CD2	2.50	0.47
1:A:292:LYS:HB2	1:A:345:ILE:HD13	1.98	0.46
1:B:43:LEU:HD11	1:B:45:MET:HG2	1.97	0.46
1:A:232:ARG:NH2	1:A:715:GLU:OE2	2.49	0.45
1:B:292:LYS:HB2	1:B:345:ILE:HD13	1.97	0.45
1:B:526:LEU:O	1:B:530:SER:HB2	2.17	0.45
1:A:526:LEU:O	1:A:530:SER:HB2	2.17	0.45
1:B:232:ARG:NH2	1:B:715:GLU:OE2	2.50	0.44
1:B:224:HIS:HB3	1:B:604:VAL:HG22	1.99	0.44
1:A:500:VAL:HG22	1:A:510:PHE:HB2	2.00	0.43
1:A:224:HIS:HB3	1:A:604:VAL:HG22	1.99	0.43
1:A:140:LYS:C	1:A:142:ILE:H	2.26	0.43
1:A:219:TRP:HZ2	1:A:337:ARG:HE	1.67	0.43
1:A:272:ILE:HG23	1:A:657:SER:HB3	2.01	0.43
1:A:172:ASN:HB3	1:A:175:LEU:HD12	2.01	0.42
1:A:302:MET:HE2	1:A:400:GLY:HA2	2.01	0.42
1:A:43:LEU:HD11	1:A:45:MET:HG2	2.01	0.42
1:A:33:ARG:HB2	1:A:567:GLN:OE1	2.19	0.42
1:B:272:ILE:HG23	1:B:657:SER:HB3	2.01	0.41
1:A:44:LYS:HE2	1:A:44:LYS:HB3	1.70	0.41
1:B:122:VAL:HG21	1:B:233:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASP:HB2	1:A:713:LEU:HD11	2.02	0.41
1:A:38:MET:HE2	1:A:43:LEU:HD22	2.03	0.41
1:A:232:ARG:HH22	1:A:715:GLU:CD	2.29	0.41
1:B:261:LEU:HD13	1:B:632:ARG:HG3	2.03	0.41
1:A:273:MET:O	1:A:658:PRO:HD2	2.22	0.40
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.96	0.40
1:B:302:MET:HE2	1:B:400:GLY:HA2	2.02	0.40
1:A:649:HIS:HD2	1:A:689:GLN:HE22	1.68	0.40
1:B:116:PRO:HA	1:B:200:ARG:HG2	2.02	0.40
1:B:273:MET:O	1:B:658:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	693/707 (98%)	674 (97%)	19 (3%)	0	100	100
1	B	692/707 (98%)	667 (96%)	24 (4%)	1 (0%)	48	40
All	All	1385/1414 (98%)	1341 (97%)	43 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	LYS

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	560/597 (94%)	544 (97%)	16 (3%)	37	21
1	B	555/597 (93%)	546 (98%)	9 (2%)	55	44
All	All	1115/1194 (93%)	1090 (98%)	25 (2%)	45	32

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	104	ASN
1	A	122	VAL
1	A	177	VAL
1	A	187	LEU
1	A	211	LYS
1	A	223	ARG
1	A	232	ARG
1	A	283	PHE
1	A	310	MET
1	A	446	LYS
1	A	500	VAL
1	A	530	SER
1	A	543	ARG
1	A	598	GLN
1	A	709	CYS
1	B	103[A]	GLU
1	B	103[B]	GLU
1	B	187	LEU
1	B	232	ARG
1	B	283	PHE
1	B	310	MET
1	B	530	SER
1	B	598	GLN
1	B	709	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	649	HIS

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Mol	Chain	Res	Type
1	A	661	ASN
1	B	146	ASN
1	B	280	HIS
1	B	355	GLN
1	B	583	GLN
1	B	598	GLN
1	B	661	ASN
1	B	689	GLN

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	$\# Z > 2$
2	I8M	B	801[B]	-	15,15,15	0.25	0	19,19,19	0.47	0
2	I8M	A	801[B]	-	15,15,15	0.25	0	19,19,19	0.40	0
2	I8M	B	802[B]	-	15,15,15	0.26	0	19,19,19	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I8M	B	801[B]	-	-	2/4/12/12	0/2/2/2
2	I8M	A	801[B]	-	-	2/4/12/12	0/2/2/2
2	I8M	B	802[B]	-	-	2/4/12/12	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

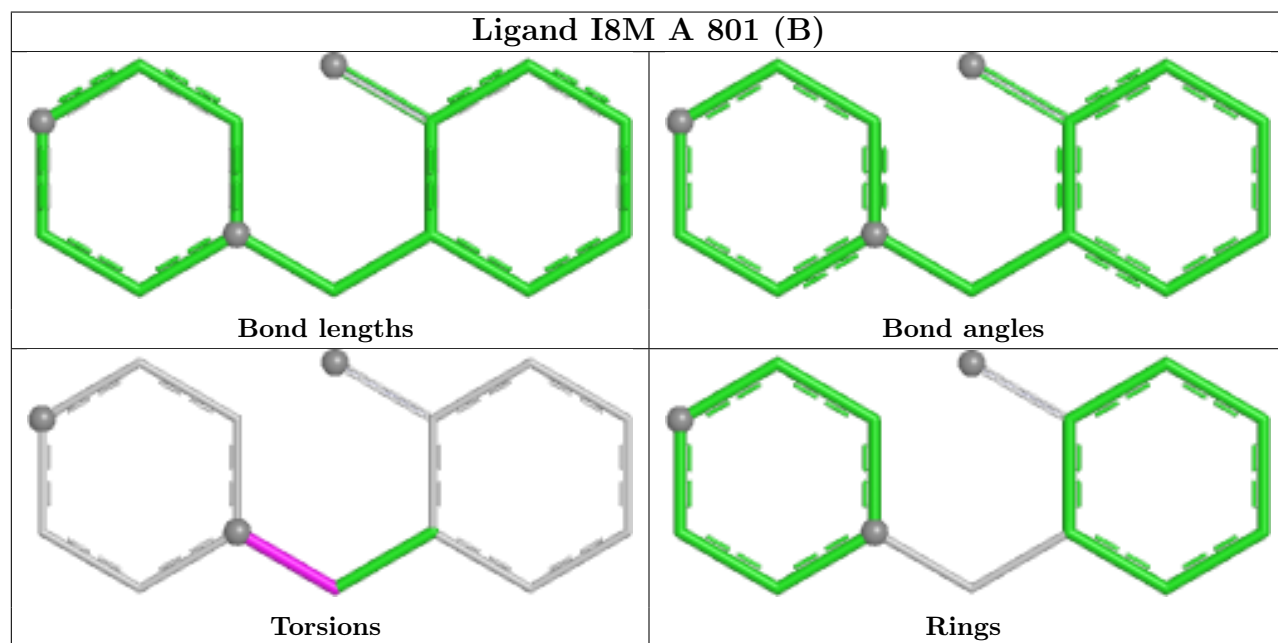
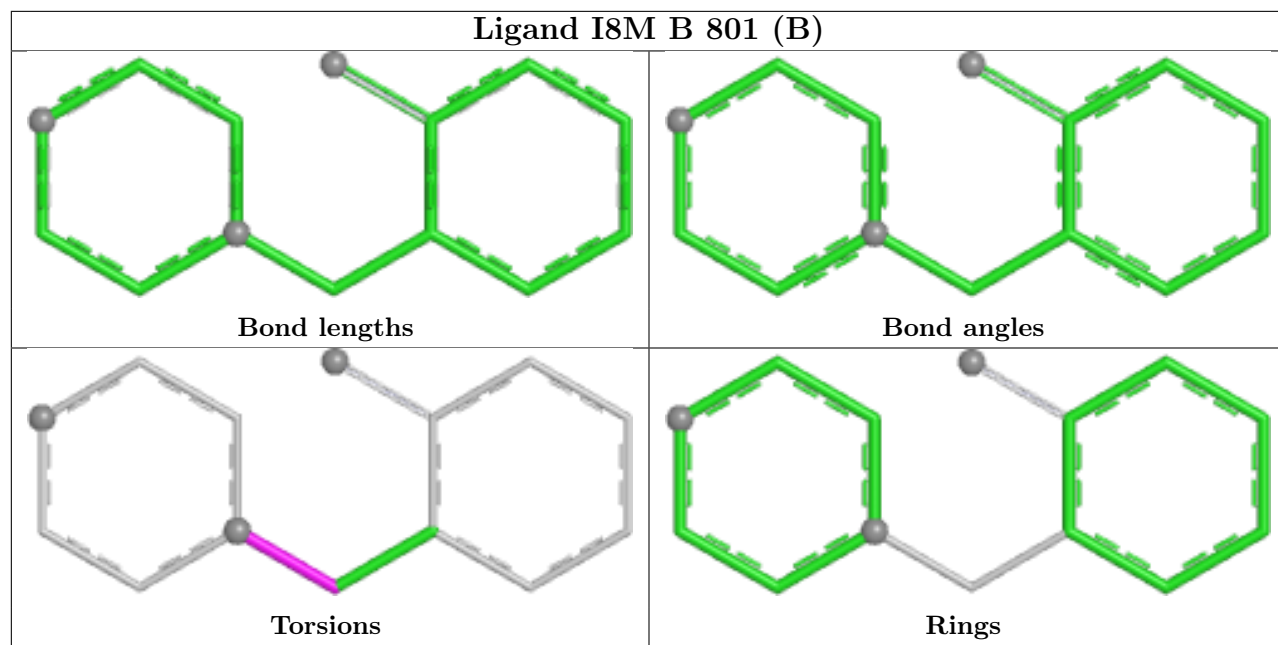
All (6) torsion outliers are listed below:

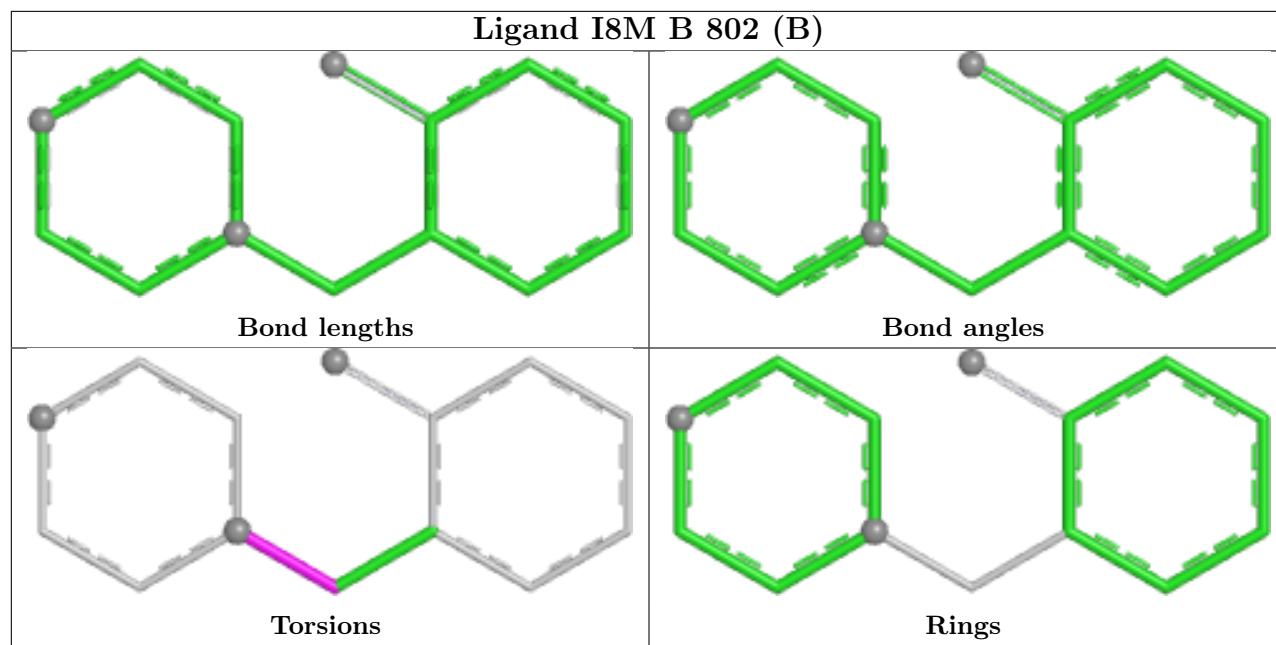
Mol	Chain	Res	Type	Atoms
2	B	801[B]	I8M	C6-C7-N1-C11
2	B	801[B]	I8M	C6-C7-N1-C8
2	A	801[B]	I8M	C6-C7-N1-C8
2	A	801[B]	I8M	C6-C7-N1-C11
2	B	802[B]	I8M	C6-C7-N1-C8
2	B	802[B]	I8M	C6-C7-N1-C11

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	697/707 (98%)	1.03	98 (14%) 6 8	30, 48, 67, 83	0
1	B	695/707 (98%)	0.83	68 (9%) 13 16	26, 44, 62, 86	1 (0%)
All	All	1392/1414 (98%)	0.93	166 (11%) 9 12	26, 46, 65, 86	1 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	7.2
1	A	418	THR	6.1
1	A	22	ASP	5.7
1	B	428	ALA	5.5
1	A	566	ASP	5.5
1	A	425	ASP	5.5
1	A	426	ALA	5.2
1	A	23	GLU	5.2
1	B	426	ALA	5.1
1	B	420	ALA	5.0
1	B	422	GLN	4.9
1	B	103[A]	GLU	4.8
1	B	213	GLY	4.7
1	A	427	SER	4.7
1	B	720	PRO	4.6
1	B	142	ILE	4.3
1	A	48	TYR	4.3
1	A	422	GLN	4.2
1	B	418	THR	4.2
1	A	213	GLY	3.9
1	B	568	ASP	3.9
1	A	613	TRP	3.8
1	A	167	ASN	3.8
1	A	661	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	97	LEU	3.7
1	B	427	SER	3.7
1	B	661	ASN	3.7
1	A	97	LEU	3.7
1	B	475	LEU	3.7
1	B	519	LEU	3.7
1	B	378	HIS	3.6
1	A	419	LYS	3.6
1	B	143	LYS	3.6
1	B	166	LYS	3.5
1	A	428	ALA	3.5
1	B	415	GLU	3.5
1	B	613	TRP	3.5
1	B	566	ASP	3.4
1	A	415	GLU	3.4
1	A	718	ILE	3.3
1	A	219	TRP	3.3
1	B	431	GLU	3.2
1	A	143	LYS	3.2
1	B	567	GLN	3.2
1	B	421	LEU	3.2
1	B	167	ASN	3.2
1	A	417	GLU	3.2
1	B	419	LYS	3.2
1	A	170	ALA	3.1
1	A	720	PRO	3.1
1	A	433	ILE	3.1
1	A	107	TRP	3.1
1	A	621	LEU	3.1
1	A	416	ASP	3.0
1	B	502	GLY	3.0
1	A	214	ALA	3.0
1	A	168	PHE	2.9
1	A	516	VAL	2.9
1	B	41	ARG	2.8
1	B	215	ASP	2.8
1	A	33	ARG	2.8
1	B	520	ALA	2.8
1	A	169	SER	2.8
1	A	623	ALA	2.8
1	B	146	ASN	2.8
1	B	23	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	141	ALA	2.7
1	A	246	GLU	2.7
1	A	431	GLU	2.7
1	A	719	VAL	2.7
1	B	214	ALA	2.6
1	A	244	TYR	2.6
1	B	533	ASP	2.6
1	A	190	MET	2.6
1	B	170	ALA	2.6
1	A	435	LYS	2.6
1	A	636	ARG	2.6
1	B	173	PRO	2.5
1	A	158	LYS	2.5
1	B	432	ALA	2.5
1	A	367	LYS	2.5
1	B	436	ILE	2.5
1	B	312	ARG	2.5
1	B	368	GLN	2.5
1	B	480	VAL	2.5
1	B	516	VAL	2.5
1	B	719	VAL	2.5
1	A	127	LYS	2.5
1	A	212	PHE	2.4
1	A	703	ILE	2.4
1	B	433	ILE	2.4
1	A	617	VAL	2.4
1	A	41	ARG	2.4
1	A	165	GLY	2.4
1	B	37	GLN	2.4
1	A	76	ASP	2.4
1	B	416	ASP	2.4
1	A	312	ARG	2.4
1	A	322	ILE	2.4
1	B	412	ILE	2.4
1	B	627	ARG	2.4
1	B	325	SER	2.4
1	A	628	LYS	2.4
1	B	311	LEU	2.3
1	A	253	PRO	2.3
1	B	369	GLY	2.3
1	A	177	VAL	2.3
1	A	441	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	392	ARG	2.3
1	A	429	ARG	2.3
1	A	261	LEU	2.3
1	B	443	PHE	2.3
1	A	366	ALA	2.3
1	A	627	ARG	2.3
1	A	624	VAL	2.3
1	A	471	GLU	2.3
1	A	369	GLY	2.3
1	A	412	ILE	2.3
1	B	441	SER	2.3
1	B	569	GLN	2.3
1	A	249	VAL	2.3
1	A	166	LYS	2.3
1	A	519	LEU	2.3
1	A	281	ARG	2.2
1	A	638	GLY	2.2
1	B	99	HIS	2.2
1	A	255	ARG	2.2
1	A	360	ARG	2.2
1	A	98	GLU	2.2
1	A	421	LEU	2.2
1	A	565	GLY	2.2
1	B	444	ALA	2.2
1	A	104	ASN	2.2
1	B	602	ASP	2.2
1	A	101	TYR	2.2
1	A	434	ASP	2.2
1	A	115	LEU	2.2
1	A	700	LEU	2.2
1	B	366	ALA	2.2
1	A	54	ASN	2.1
1	A	630	PHE	2.1
1	A	633	TYR	2.1
1	A	91	ILE	2.1
1	B	216	THR	2.1
1	A	42	GLY	2.1
1	B	244	TYR	2.1
1	A	389	ASP	2.1
1	B	414	THR	2.1
1	B	104	ASN	2.1
1	A	108	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	2.1
1	A	121	SER	2.1
1	A	614	GLU	2.1
1	B	565	GLY	2.1
1	A	173	PRO	2.1
1	B	315	LEU	2.1
1	A	704	ASP	2.1
1	A	536	ARG	2.1
1	A	620	LYS	2.0
1	B	637	SER	2.0
1	B	100	ASN	2.0
1	B	218	ASN	2.0
1	A	235	ALA	2.0
1	B	212	PHE	2.0
1	A	625	TYR	2.0
1	A	110	ARG	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](#)

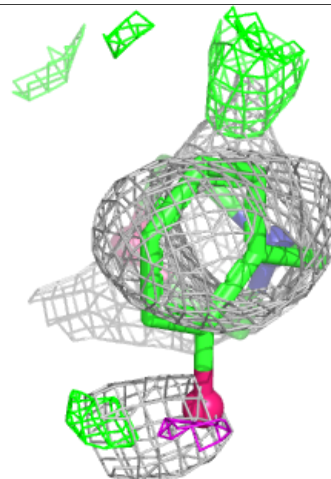
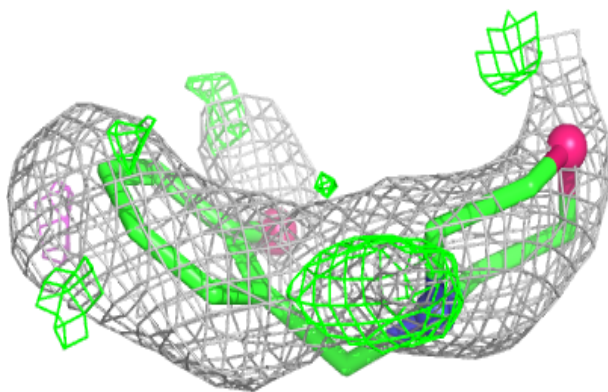
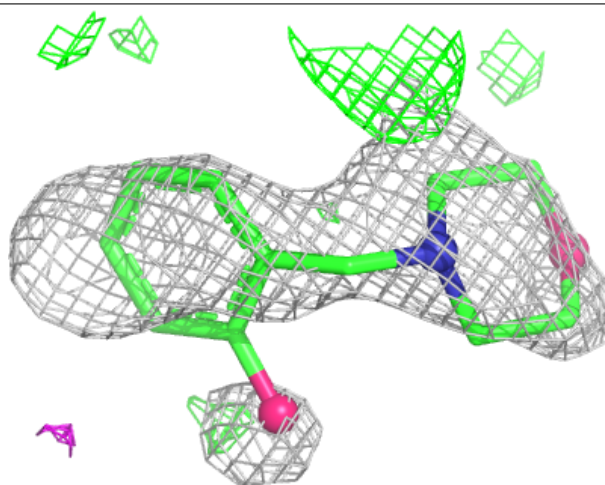
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	802	1/1	0.82	0.20	76,76,76,76	0
2	I8M	B	802[B]	14/14	0.83	0.28	60,61,61,61	14
2	I8M	A	801[B]	14/14	0.84	0.34	49,50,50,50	14
2	I8M	B	801[B]	14/14	0.88	0.19	45,46,48,48	14
3	CL	B	803	1/1	0.90	0.26	67,67,67,67	0
3	CL	A	803	1/1	0.96	0.10	45,45,45,45	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.

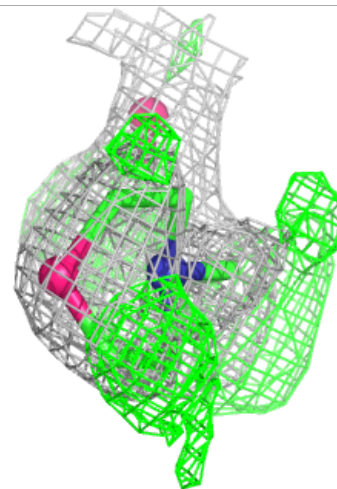
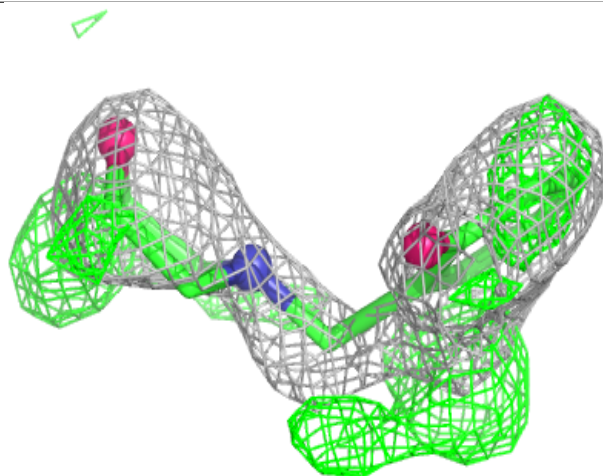
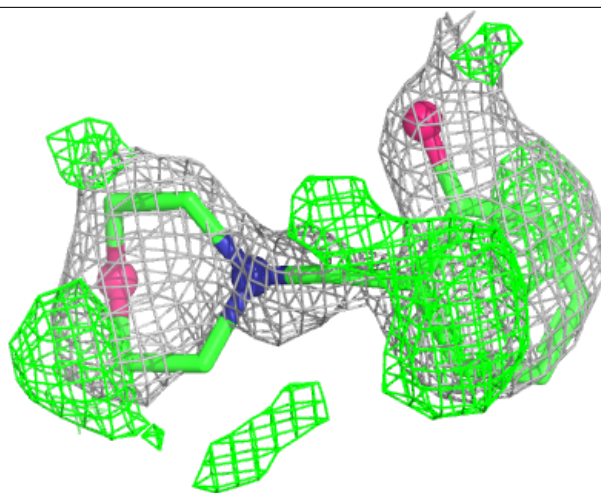
Electron density around I8M B 802 (B):

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



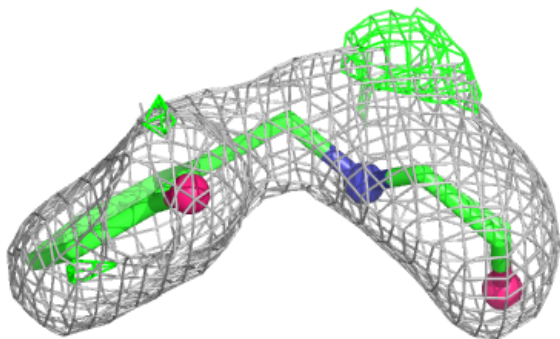
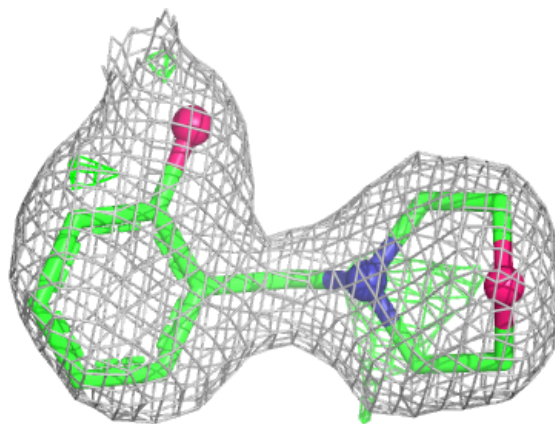
Electron density around I8M A 801 (B):

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



Electron density around I8M B 801 (B):

$2mF_o-DF_c$ (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.