



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 PM UTC

PDB ID : 5SDH / pdb_00005sdh
Title : PanDDA analysis group deposition – Crystal Structure of Porphyromonas gingivalis in complex with Z2856434854
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 : 2.31 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

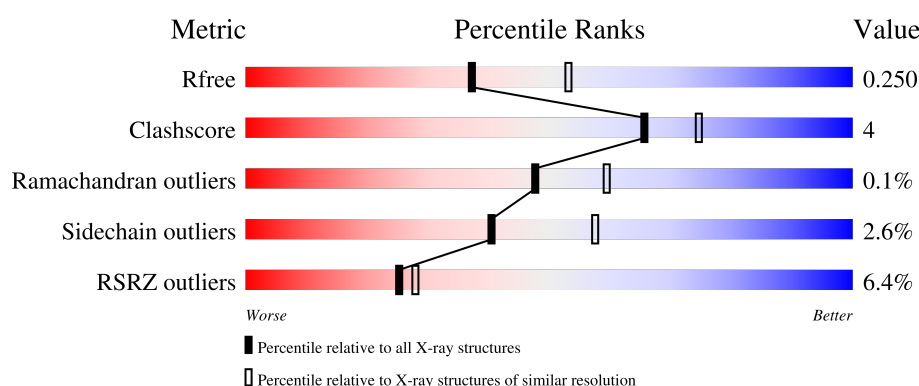
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	7% 89% 9% ..
1	B	707	5% 86% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11256 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.

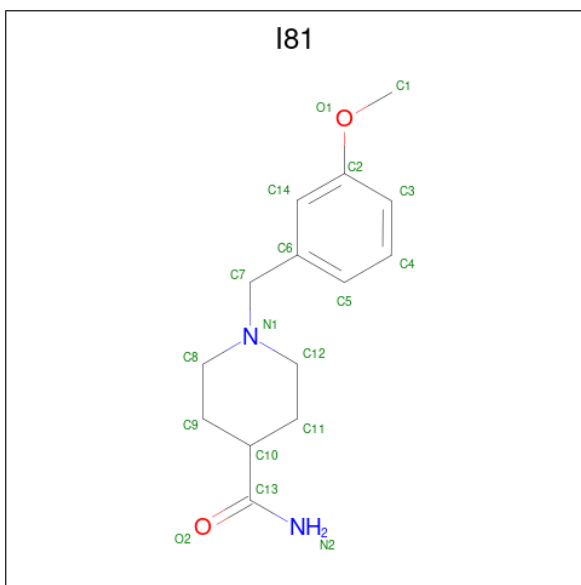
- Molecule 1 is a protein called Asp/Glu-specific dipeptidyl-peptidase.

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	0	0
			5458	3465	940	1026	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 1-[(3-methoxyphenyl)methyl]piperidine-4-carboxamide (CCD ID: I81) (formula: C₁₄H₂₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			18	14	2	2		
2	B	1	Total	C	N	O	0	1
			18	14	2	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		

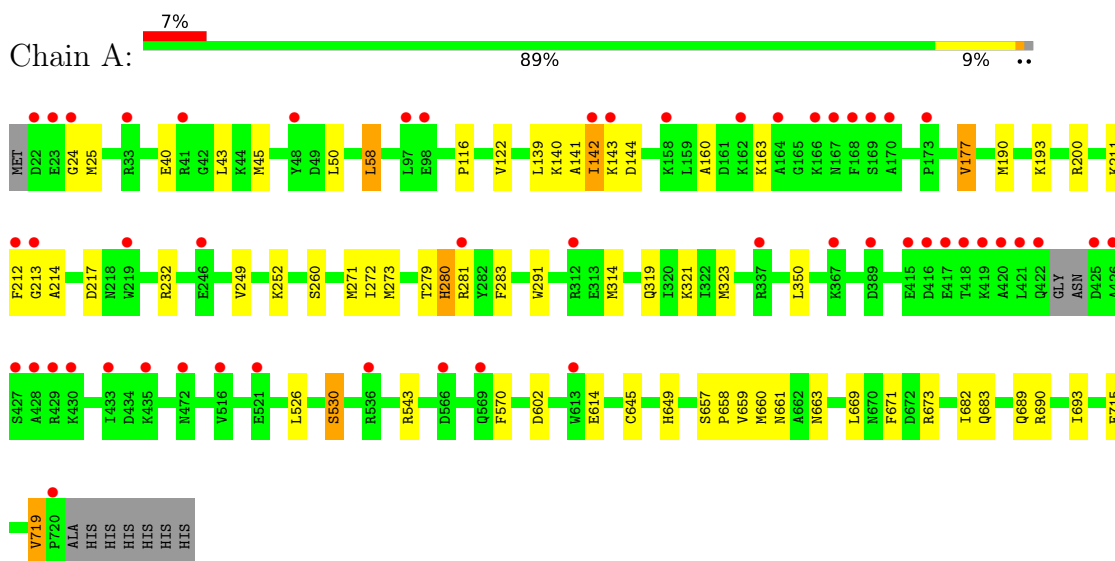
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	1
			142	142		
4	B	124	Total	O	0	0
			124	124		

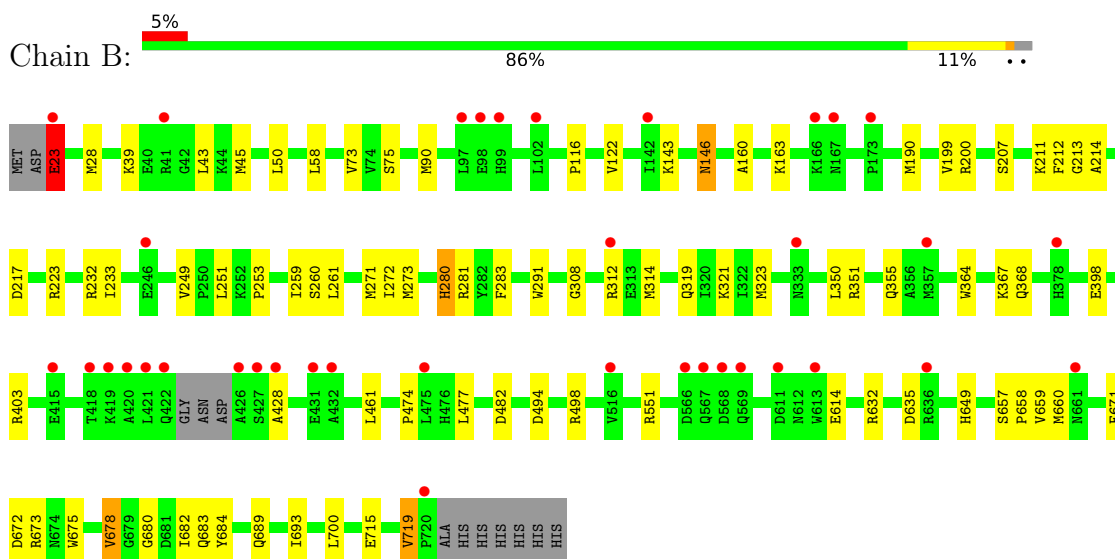
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	102.49Å 116.71Å 147.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.70 – 2.31 73.70 – 2.31	Depositor EDS
% Data completeness (in resolution range)	78.2 (73.70-2.31) 78.2 (73.70-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, R_{free}	0.213 , 0.246 0.219 , 0.250	Depositor DCC
R_{free} test set	3082 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11256	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, I81

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	0.66	1/5617 (0.0%)	1.07	11/7607 (0.1%)
1	B	0.67	2/5581 (0.0%)	1.07	13/7561 (0.2%)
All	All	0.66	3/11198 (0.0%)	1.07	24/15168 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ALA	CA-C	6.84	1.59	1.52
1	B	214	ALA	CA-C	6.01	1.58	1.52
1	B	90	MET	SD-CE	-5.50	1.65	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLY	N-CA-C	9.12	127.31	112.89
1	A	141	ALA	CA-C-N	7.61	135.67	121.97
1	A	141	ALA	C-N-CA	7.61	135.67	121.97
1	B	23	GLU	CB-CG-CD	6.00	122.81	112.60
1	B	660	MET	CA-C-N	5.86	132.07	121.06
1	B	660	MET	C-N-CA	5.86	132.07	121.06
1	A	660	MET	CA-C-N	5.83	132.02	121.06
1	A	660	MET	C-N-CA	5.83	132.02	121.06
1	A	280	HIS	CA-C-N	5.75	128.56	120.28
1	A	280	HIS	C-N-CA	5.75	128.56	120.28
1	B	280	HIS	CA-C-N	5.66	128.43	120.28
1	B	280	HIS	C-N-CA	5.66	128.43	120.28
1	B	671	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	143	LYS	CA-C-N	5.56	130.01	122.56
1	A	143	LYS	C-N-CA	5.56	130.01	122.56
1	B	428	ALA	CA-C-N	5.56	128.19	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ALA	C-N-CA	5.56	128.19	120.29
1	B	482	ASP	N-CA-C	5.28	116.72	111.07
1	A	144	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	146	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	671	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	635	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	28	MET	CA-C-N	5.01	127.49	120.28
1	B	28	MET	C-N-CA	5.01	127.49	120.28

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	38	0
1	B	5458	0	5231	44	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	142	0	0	0	0
4	B	124	0	0	0	0
All	All	11256	0	10513	82	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 4.

All (82) 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:223:ARG:NH2	1:B:672:ASP:OD2	1.94	1.01
1:B:50:LEU:HD21	1:B:271:MET:HE1	1.64	0.78
1:A:50:LEU:HD21	1:A:271:MET:HE1	1.66	0.77
1:B:314:MET:HG2	1:B:321:LYS:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:MET:HG2	1:A:321:LYS:HA	1.67	0.77
1:A:160:ALA:HB1	1:A:177:VAL:HG12	1.67	0.76
1:B:213:GLY:HA3	1:B:217:ASP:HB2	1.69	0.75
1:B:308:GLY:O	1:B:312:ARG:HD2	1.88	0.74
1:A:213:GLY:HA3	1:A:217:ASP:HB2	1.70	0.73
1:A:649:HIS:HD2	1:A:689:GLN:HE22	1.40	0.69
1:B:649:HIS:HD2	1:B:689:GLN:HE22	1.43	0.67
1:A:116:PRO:HA	1:A:200:ARG:HG2	1.78	0.66
1:B:116:PRO:HA	1:B:200:ARG:HG2	1.78	0.66
1:A:45:MET:HE1	1:A:58:LEU:HD22	1.79	0.65
1:A:25:MET:HE1	1:A:279:THR:CG2	2.27	0.65
1:A:25:MET:HE1	1:A:279:THR:HG21	1.77	0.65
1:A:163:LYS:HB3	1:A:190:MET:HE1	1.79	0.65
1:A:649:HIS:CD2	1:A:689:GLN:HE22	2.14	0.64
1:B:163:LYS:HB3	1:B:190:MET:HE1	1.80	0.64
1:B:649:HIS:CD2	1:B:689:GLN:HE22	2.16	0.63
1:B:319:GLN:HG3	1:B:323:MET:HE2	1.80	0.63
1:A:319:GLN:HG3	1:A:323:MET:HE2	1.82	0.60
1:B:494:ASP:OD1	1:B:498:ARG:NH1	2.36	0.58
1:A:649:HIS:HD2	1:A:689:GLN:NE2	2.01	0.57
1:B:319:GLN:HG3	1:B:323:MET:CE	2.34	0.57
1:B:261:LEU:HD21	1:B:700:LEU:HD12	1.86	0.57
1:A:319:GLN:HG3	1:A:323:MET:CE	2.36	0.56
1:B:649:HIS:HD2	1:B:689:GLN:NE2	2.03	0.56
1:B:232:ARG:NH2	1:B:715:GLU:OE2	2.40	0.55
1:B:351:ARG:HH12	1:B:355:GLN:HE21	1.56	0.54
1:A:139:LEU:O	1:A:142:ILE:HG13	2.08	0.54
1:A:25:MET:CE	1:A:279:THR:HG21	2.38	0.53
1:A:232:ARG:NH2	1:A:715:GLU:OE2	2.42	0.53
1:A:319:GLN:O	1:A:323:MET:HG3	2.09	0.52
1:B:23:GLU:HG2	1:B:684:TYR:CD2	2.44	0.52
1:B:319:GLN:O	1:B:323:MET:HG3	2.09	0.52
1:A:291:TRP:CZ3	1:A:682:ILE:HG13	2.45	0.52
1:B:50:LEU:CD2	1:B:271:MET:HE1	2.39	0.51
1:B:259:ILE:HG21	1:B:700:LEU:HD11	1.92	0.51
1:A:50:LEU:CD2	1:A:271:MET:HE1	2.40	0.50
1:A:140:LYS:C	1:A:142:ILE:H	2.19	0.50
1:B:398:GLU:O	1:B:403:ARG:HG2	2.12	0.49
1:A:526:LEU:O	1:A:530:SER:HB2	2.12	0.49
1:B:291:TRP:CZ3	1:B:682:ILE:HG13	2.48	0.49
1:A:43:LEU:HD11	1:A:45:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:VAL:HG11	1:B:253:PRO:HG3	1.96	0.47
1:B:260:SER:HA	1:B:719:VAL:HG22	1.97	0.47
1:A:272:ILE:HG23	1:A:657:SER:HB3	1.97	0.46
1:B:251:LEU:O	1:B:253:PRO:HD3	2.15	0.46
1:A:25:MET:HE2	1:A:570:PHE:CE2	2.51	0.46
1:B:232:ARG:HH22	1:B:715:GLU:CD	2.24	0.46
1:B:122:VAL:HG21	1:B:233:ILE:HG12	1.97	0.46
1:A:280:HIS:HB2	1:A:682:ILE:CD1	2.46	0.45
1:B:272:ILE:HG23	1:B:657:SER:HB3	1.97	0.45
1:B:43:LEU:HD11	1:B:45:MET:HG2	1.98	0.45
1:A:25:MET:HE2	1:A:570:PHE:HE2	1.81	0.45
1:B:146:ASN:HB2	1:B:551:ARG:CZ	2.47	0.45
1:A:232:ARG:HH22	1:A:715:GLU:CD	2.25	0.45
1:B:280:HIS:HB2	1:B:682:ILE:CD1	2.48	0.44
1:B:675:TRP:O	1:B:678:VAL:HG13	2.17	0.44
1:A:260:SER:HA	1:A:719:VAL:HG22	1.99	0.44
1:B:659:VAL:HG21	1:B:693:ILE:HG12	2.00	0.44
1:A:350:LEU:HD22	1:A:683:GLN:HB3	1.99	0.44
1:B:350:LEU:HD22	1:B:683:GLN:HB3	2.00	0.43
1:B:212:PHE:O	1:B:614:GLU:O	2.37	0.43
1:B:160:ALA:HA	1:B:190:MET:HE2	2.01	0.43
1:A:280:HIS:HB2	1:A:682:ILE:HD13	2.02	0.42
1:B:122:VAL:HG13	1:B:199:VAL:HG21	2.02	0.42
1:A:160:ALA:HA	1:A:190:MET:HE2	2.02	0.42
1:B:364:TRP:O	1:B:368:GLN:HG2	2.20	0.42
1:B:474:PRO:HD2	1:B:477:LEU:HD12	2.01	0.42
1:B:673:ARG:HE	1:B:673:ARG:HB3	1.67	0.42
1:B:271:MET:HE3	1:B:271:MET:HB2	1.90	0.41
1:A:212:PHE:O	1:A:614:GLU:O	2.38	0.41
1:A:673:ARG:HE	1:A:673:ARG:HB3	1.70	0.41
1:A:659:VAL:HG21	1:A:693:ILE:HG12	2.02	0.41
1:A:661:ASN:HB3	1:A:663:ASN:H	1.86	0.41
1:A:645:CYS:HB2	1:A:690:ARG:HB3	2.03	0.41
1:B:680:GLY:HA2	1:B:683:GLN:O	2.21	0.40
1:B:280:HIS:HB2	1:B:682:ILE:HD13	2.04	0.40
1:A:273:MET:O	1:A:658:PRO:HD2	2.22	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%)	672 (97%)	20 (3%)	1 (0%)	48	59
1	B	691/707 (98%)	668 (97%)	22 (3%)	1 (0%)	48	59
All	All	1384/1414 (98%)	1340 (97%)	42 (3%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	143	LYS
1	A	142	ILE

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%)	545 (97%)	15 (3%)	39	56
1	B	554/597 (93%)	540 (98%)	14 (2%)	42	59
All	All	1114/1194 (93%)	1085 (97%)	29 (3%)	40	57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	58	LEU
1	A	122	VAL
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	193	LYS
1	A	211	LYS
1	A	249	VAL
1	A	252	LYS
1	A	281	ARG
1	A	283	PHE
1	A	530	SER
1	A	543	ARG
1	A	602	ASP
1	A	669	LEU
1	A	719	VAL
1	B	23	GLU
1	B	39	LYS
1	B	58	LEU
1	B	75	SER
1	B	207	SER
1	B	211	LYS
1	B	249	VAL
1	B	281	ARG
1	B	283	PHE
1	B	367	LYS
1	B	461	LEU
1	B	632	ARG
1	B	678	VAL
1	B	719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	100	ASN
1	A	104	ASN
1	A	157	GLN
1	A	218	ASN
1	A	280	HIS
1	A	506	GLN
1	A	649	HIS
1	A	654	ASN
1	A	663	ASN
1	B	146	ASN
1	B	218	ASN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	583	GLN
1	B	612	ASN
1	B	649	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	I81	A	801[B]	-	19,19,19	0.17	0	25,25,25	0.55	0
2	I81	B	801[B]	-	19,19,19	0.17	0	25,25,25	0.56	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	I81	A	801[B]	-	-	5/10/20/20	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	I81	B	801[B]	-	-	2/10/20/20	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

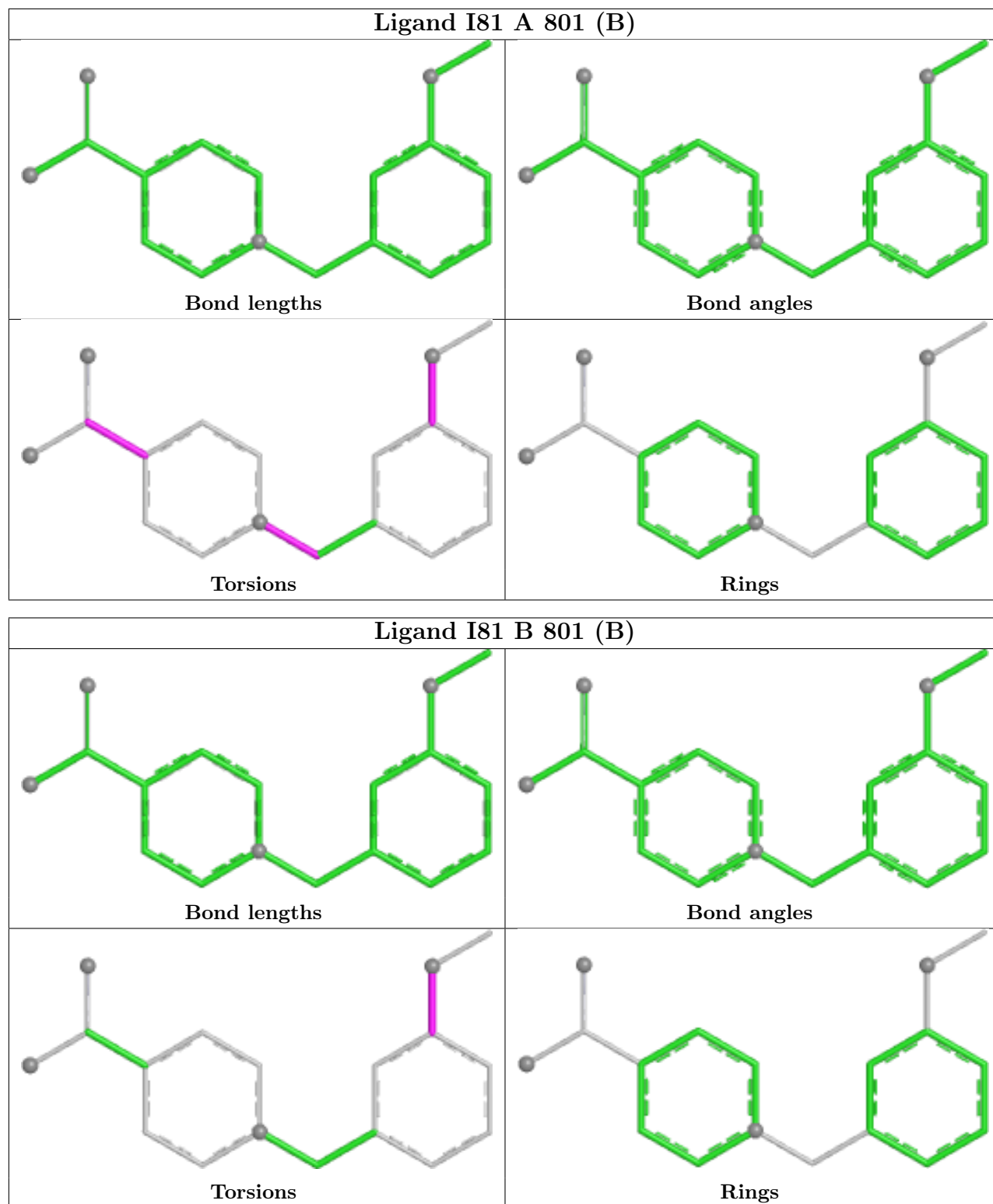
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801[B]	I81	C14-C2-O1-C1
2	A	801[B]	I81	C3-C2-O1-C1
2	B	801[B]	I81	C14-C2-O1-C1
2	A	801[B]	I81	C6-C7-N1-C8
2	B	801[B]	I81	C3-C2-O1-C1
2	A	801[B]	I81	C9-C10-C13-O2
2	A	801[B]	I81	C9-C10-C13-N2

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.50	52 (7%)	20 23	32, 51, 72, 85	0
1	B	695/707 (98%)	0.44	37 (5%)	32 34	31, 49, 69, 85	0
All	All	1392/1414 (98%)	0.47	89 (6%)	25 28	31, 50, 71, 85	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	422	GLN	6.3
1	A	23	GLU	5.9
1	A	22	ASP	5.6
1	B	566	ASP	5.4
1	A	425	ASP	5.2
1	B	426	ALA	4.8
1	A	566	ASP	4.8
1	B	420	ALA	4.5
1	A	422	GLN	4.4
1	A	142	ILE	4.3
1	B	613	TRP	4.2
1	A	219	TRP	4.2
1	A	426	ALA	3.9
1	B	427	SER	3.9
1	A	418	THR	3.7
1	A	427	SER	3.7
1	B	428	ALA	3.6
1	A	417	GLU	3.5
1	B	567	GLN	3.4
1	B	720	PRO	3.4
1	A	169	SER	3.3
1	B	568	ASP	3.3
1	B	475	LEU	3.1
1	A	415	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	415	GLU	3.1
1	B	418	THR	3.0
1	B	167	ASN	3.0
1	A	613	TRP	3.0
1	B	99	HIS	3.0
1	B	378	HIS	3.0
1	B	97	LEU	2.8
1	B	661	ASN	2.8
1	A	168	PHE	2.8
1	B	142	ILE	2.7
1	B	23	GLU	2.7
1	A	33	ARG	2.7
1	A	569	GLN	2.7
1	B	569	GLN	2.7
1	A	167	ASN	2.7
1	A	389	ASP	2.7
1	A	720	PRO	2.7
1	A	48	TYR	2.6
1	A	162	LYS	2.6
1	A	312	ARG	2.6
1	A	433	ILE	2.6
1	A	416	ASP	2.6
1	A	41	ARG	2.6
1	B	41	ARG	2.6
1	A	472	ASN	2.6
1	A	420	ALA	2.5
1	B	98	GLU	2.5
1	A	166	LYS	2.5
1	A	435	LYS	2.5
1	A	164	ALA	2.4
1	A	97	LEU	2.4
1	A	521	GLU	2.4
1	A	212	PHE	2.4
1	A	419	LYS	2.4
1	B	312	ARG	2.4
1	B	431	GLU	2.4
1	A	516	VAL	2.4
1	A	246	GLU	2.4
1	A	430	LYS	2.3
1	A	98	GLU	2.3
1	A	143	LYS	2.3
1	A	213	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	428	ALA	2.3
1	A	421	LEU	2.3
1	A	173	PRO	2.3
1	A	170	ALA	2.3
1	B	421	LEU	2.3
1	A	281	ARG	2.2
1	B	246	GLU	2.2
1	B	102	LEU	2.2
1	A	536	ARG	2.2
1	A	367	LYS	2.2
1	B	419	LYS	2.2
1	B	333	ASN	2.2
1	B	173	PRO	2.2
1	B	636	ARG	2.1
1	B	166	LYS	2.1
1	B	357	MET	2.1
1	A	24	GLY	2.1
1	A	429	ARG	2.1
1	A	337	ARG	2.0
1	B	516	VAL	2.0
1	A	158	LYS	2.0
1	B	432	ALA	2.0
1	B	611	ASP	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](#)

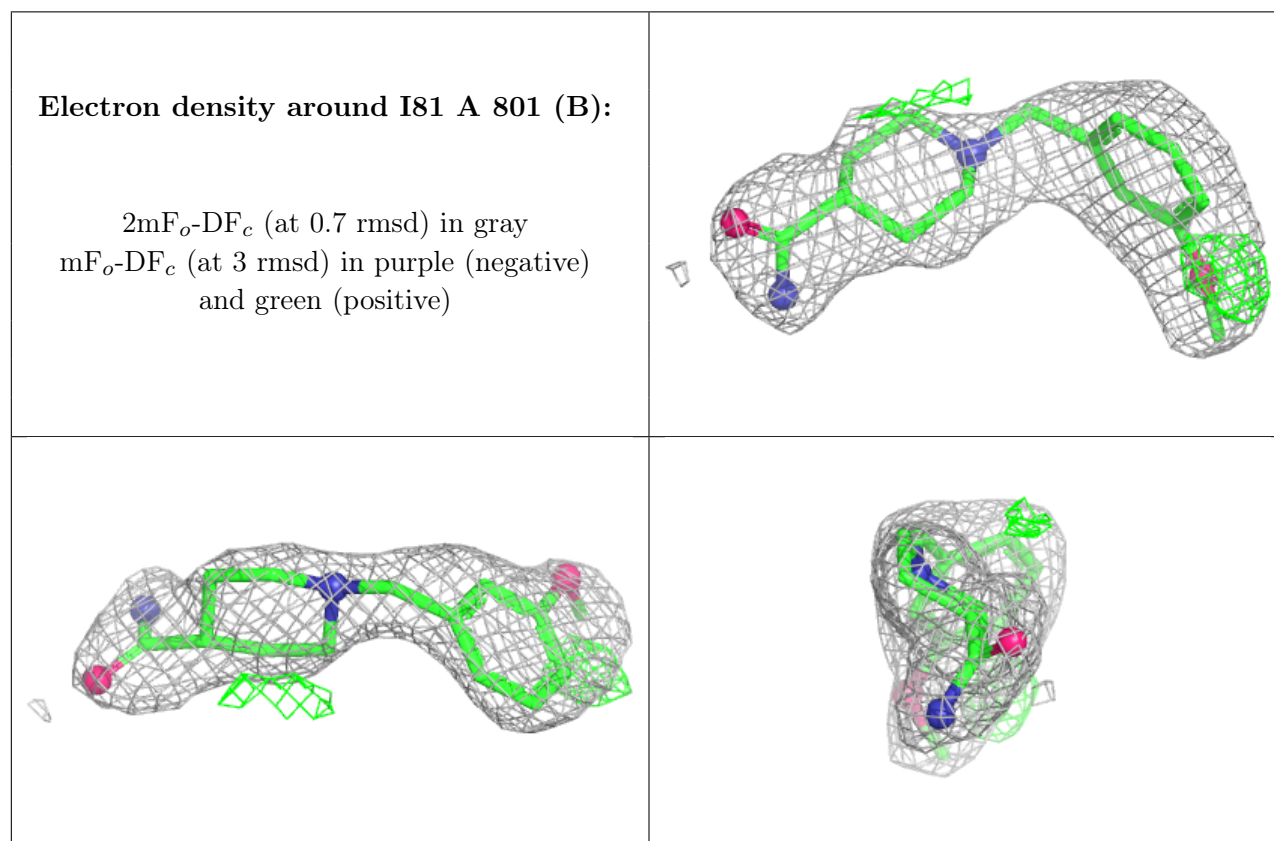
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

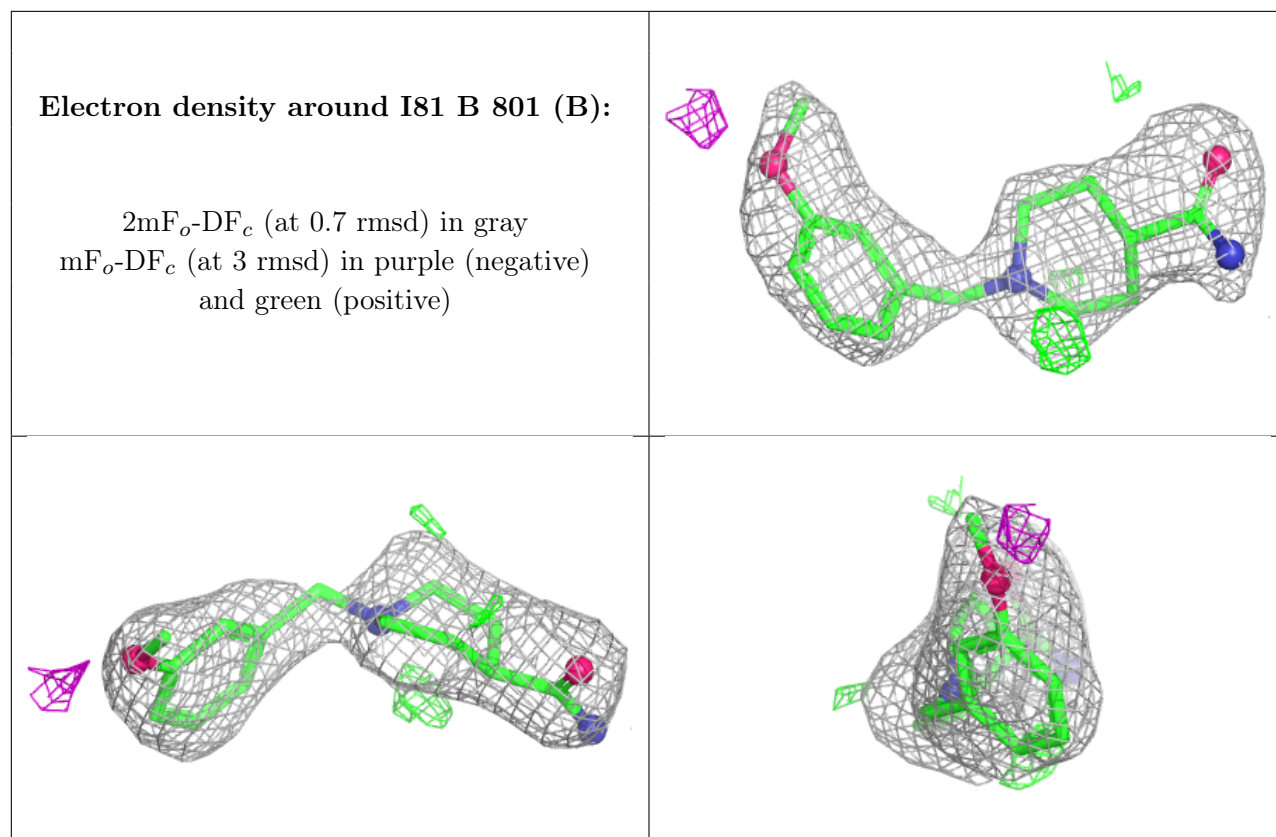
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	I81	A	801[B]	18/18	0.84	0.19	50,51,52,52	18
2	I81	B	801[B]	18/18	0.87	0.15	57,60,62,62	18
3	CL	A	802	1/1	0.89	0.17	85,85,85,85	0
3	CL	A	803	1/1	0.89	0.13	65,65,65,65	0
3	CL	B	802	1/1	0.91	0.26	64,64,64,64	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.