



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 5SDK / pdb_00005sdk
Title : PanDDA analysis group deposition – Crystal Structure of Porphyromonas gingivalis in complex with Z416341642
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 : 1.98 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

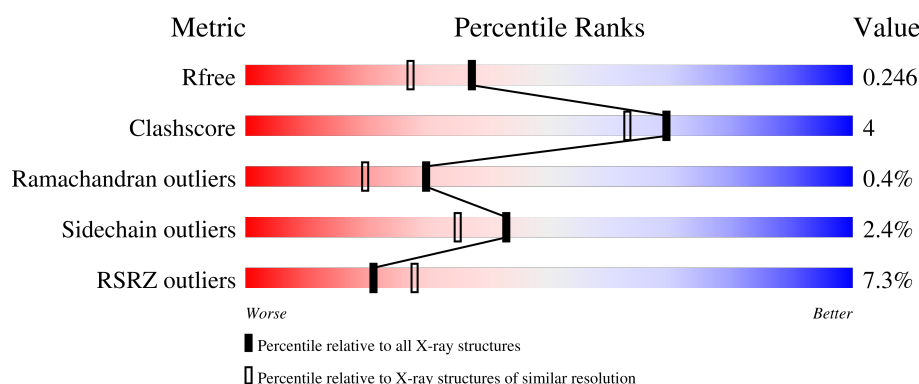
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	8% 88% 10% ..
1	B	707	6% 88% 10% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	I87	B	801[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11249 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.

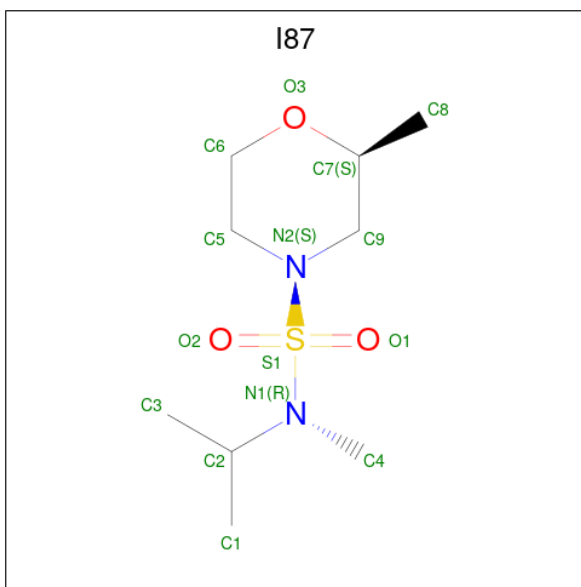
- Molecule 1 is a protein called Asp/Glu-specific dipeptidyl-peptidase.

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 (2S)-N,2-dimethyl-N-(propan-2-yl)morpholine-4-sulfonamide (CCD ID: I87) (formula: C₉H₂₀N₂O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	9	2	3	1		
2	B	1	Total	C	N	O	S	0	1
			15	9	2	3	1		

- 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		

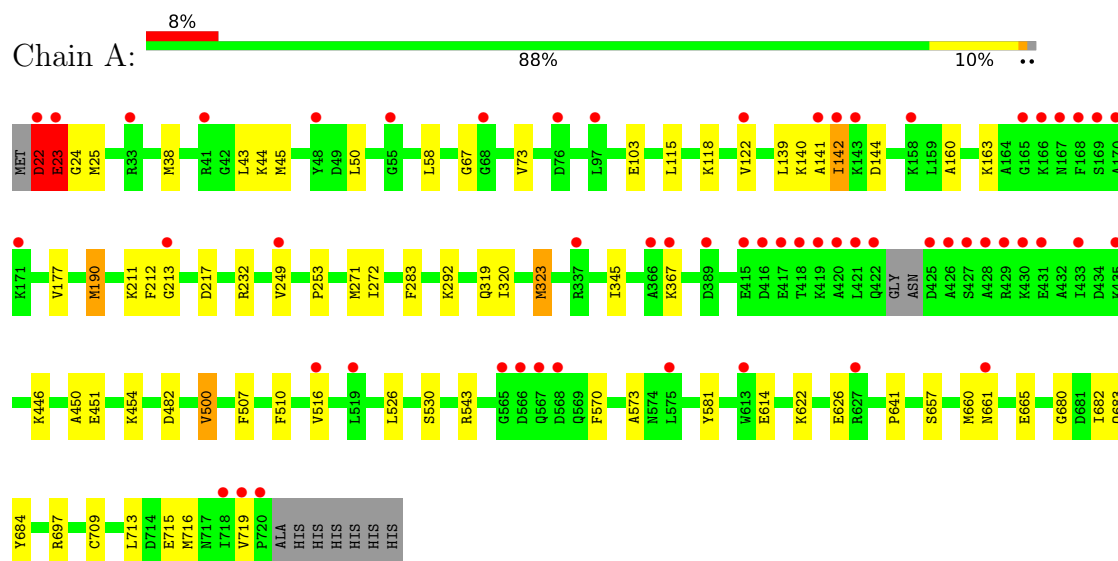
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	125	Total	O	0	0
			125	125		

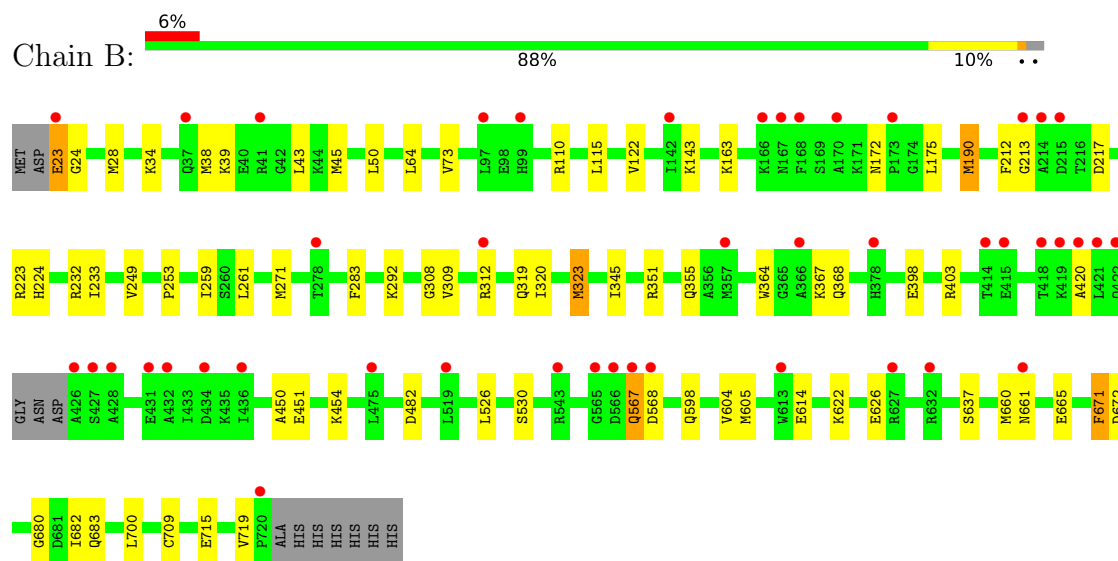
3 Residue-property plots [i](#)

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	101.59Å 117.51Å 147.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.01 – 1.98 92.01 – 1.98	Depositor EDS
% Data completeness (in resolution range)	73.4 (92.01-1.98) 73.3 (92.01-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, R_{free}	0.218 , 0.239 0.221 , 0.246	Depositor DCC
R_{free} test set	4620 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11249	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: I87, CL

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	0.74	2/5617 (0.0%)	1.07	12/7607 (0.2%)
1	B	0.76	3/5581 (0.1%)	1.07	11/7561 (0.1%)
All	All	0.75	5/11198 (0.0%)	1.07	23/15168 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	MET	SD-CE	-7.42	1.61	1.79
1	A	323	MET	SD-CE	-7.22	1.61	1.79
1	B	323	MET	SD-CE	-6.64	1.62	1.79
1	A	190	MET	SD-CE	-6.31	1.63	1.79
1	B	605	MET	SD-CE	-5.66	1.65	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLY	N-CA-C	9.18	124.46	111.42
1	A	141	ALA	CA-C-N	7.68	135.80	121.97
1	A	141	ALA	C-N-CA	7.68	135.80	121.97
1	A	660	MET	CA-C-N	6.63	132.75	120.95
1	A	660	MET	C-N-CA	6.63	132.75	120.95
1	B	23	GLU	CB-CG-CD	6.18	123.11	112.60
1	A	144	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	660	MET	CA-C-N	5.84	132.69	121.54
1	B	660	MET	C-N-CA	5.84	132.69	121.54
1	B	24	GLY	N-CA-C	5.68	122.44	112.10
1	A	67	GLY	N-CA-C	5.34	122.20	115.42
1	A	22	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	482	ASP	N-CA-C	5.25	116.81	111.14
1	B	682	ILE	N-CA-C	-5.21	107.68	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	682	ILE	N-CA-C	-5.16	107.72	111.90
1	A	115	LEU	N-CA-C	5.14	116.38	109.24
1	B	28	MET	CA-C-N	5.14	127.68	120.28
1	B	28	MET	C-N-CA	5.14	127.68	120.28
1	B	482	ASP	N-CA-C	5.13	116.68	111.14
1	A	507	PHE	CA-CB-CG	-5.09	108.70	113.80
1	B	64	LEU	N-CA-C	-5.05	100.28	108.41
1	B	115	LEU	N-CA-C	5.03	116.24	109.24

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	40	0
1	B	5458	0	5231	36	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	140	0	0	0	0
4	B	125	0	0	0	0
All	All	11249	0	10513	76	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 (76) 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	1.56	0.85
1:A:319:GLN:HG3	1:A:323:MET:HE2	1.57	0.84
1:A:160:ALA:HB1	1:A:177:VAL:HG12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:HA	1:A:716:MET:HE2	1.62	0.79
1:A:213:GLY:HA3	1:A:217:ASP:HB2	1.73	0.70
1:B:261:LEU:HD21	1:B:700:LEU:HD12	1.73	0.69
1:B:172:ASN:HB3	1:B:175:LEU:HD12	1.74	0.68
1:A:25:MET:HE2	1:A:570:PHE:CE2	2.29	0.67
1:B:73:VAL:HG11	1:B:253:PRO:HG3	1.75	0.67
1:B:34:LYS:HZ1	1:B:567:GLN:HA	1.60	0.67
1:B:213:GLY:HA3	1:B:217:ASP:HB2	1.78	0.66
1:A:50:LEU:HD21	1:A:271:MET:HE1	1.77	0.66
1:B:50:LEU:HD21	1:B:271:MET:HE1	1.78	0.65
1:B:232:ARG:NH2	1:B:715:GLU:OE2	2.32	0.63
1:A:25:MET:HE1	1:A:573:ALA:HB2	1.82	0.62
1:B:223:ARG:NH2	1:B:672:ASP:OD2	2.16	0.62
1:A:232:ARG:NH2	1:A:715:GLU:OE2	2.34	0.61
1:A:500:VAL:HG22	1:A:510:PHE:HB2	1.84	0.59
1:B:232:ARG:HH22	1:B:715:GLU:CD	2.11	0.59
1:A:43:LEU:HD11	1:A:45:MET:HG2	1.85	0.59
1:B:43:LEU:HD11	1:B:45:MET:HG2	1.85	0.58
1:A:232:ARG:HH22	1:A:715:GLU:CD	2.12	0.58
1:A:526:LEU:O	1:A:530:SER:HB2	2.05	0.57
1:B:622:LYS:O	1:B:626:GLU:HG3	2.06	0.56
1:A:622:LYS:O	1:A:626:GLU:HG3	2.06	0.56
1:B:312:ARG:HG3	1:B:312:ARG:HH11	1.70	0.56
1:B:661:ASN:HD22	1:B:665:GLU:HB2	1.72	0.55
1:A:661:ASN:HD22	1:A:665:GLU:HB2	1.72	0.55
1:A:212:PHE:O	1:A:614:GLU:O	2.24	0.55
1:B:212:PHE:O	1:B:614:GLU:O	2.25	0.55
1:A:319:GLN:O	1:A:323:MET:HG3	2.07	0.55
1:B:526:LEU:O	1:B:530:SER:HB2	2.08	0.54
1:A:25:MET:HE2	1:A:570:PHE:HE2	1.70	0.54
1:A:22:ASP:O	1:A:23:GLU:O	2.26	0.54
1:B:319:GLN:O	1:B:323:MET:HG3	2.08	0.53
1:B:163:LYS:HB3	1:B:190:MET:HE1	1.90	0.53
1:A:139:LEU:O	1:A:142:ILE:HG13	2.07	0.52
1:B:309:VAL:HA	1:B:312:ARG:HD2	1.91	0.52
1:A:163:LYS:HB3	1:A:190:MET:HE1	1.92	0.51
1:B:308:GLY:O	1:B:312:ARG:HD2	2.12	0.50
1:B:320:ILE:HD13	1:B:323:MET:HE3	1.93	0.49
1:A:45:MET:HE1	1:A:58:LEU:HD22	1.94	0.49
1:A:320:ILE:HD13	1:A:323:MET:HE3	1.95	0.49
1:A:25:MET:CE	1:A:573:ALA:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLU:OE2	1:A:581:TYR:O	2.31	0.49
1:B:34:LYS:NZ	1:B:567:GLN:HA	2.25	0.48
1:B:398:GLU:O	1:B:403:ARG:HG2	2.14	0.47
1:A:680:GLY:HA2	1:A:683:GLN:O	2.15	0.47
1:B:50:LEU:CD2	1:B:271:MET:HE1	2.45	0.47
1:A:450:ALA:O	1:A:454:LYS:HG3	2.16	0.46
1:B:680:GLY:HA2	1:B:683:GLN:O	2.15	0.46
1:B:351:ARG:HH12	1:B:355:GLN:HE21	1.63	0.46
1:A:50:LEU:CD2	1:A:271:MET:HE1	2.45	0.46
1:B:292:LYS:HB2	1:B:345:ILE:HD13	1.99	0.45
1:A:292:LYS:HB2	1:A:345:ILE:HD13	1.99	0.44
1:A:160:ALA:HB1	1:A:177:VAL:CG1	2.39	0.44
1:B:450:ALA:O	1:B:454:LYS:HG3	2.18	0.44
1:A:23:GLU:HB2	1:A:684:TYR:CE2	2.53	0.44
1:A:23:GLU:HB2	1:A:684:TYR:CD2	2.53	0.43
1:B:661:ASN:ND2	1:B:665:GLU:OE1	2.52	0.43
1:B:38:MET:HE2	1:B:43:LEU:HD22	2.01	0.43
1:A:661:ASN:ND2	1:A:665:GLU:OE1	2.51	0.43
1:A:73:VAL:HG11	1:A:253:PRO:HG3	1.99	0.43
1:A:44:LYS:HE2	1:A:44:LYS:HB3	1.89	0.42
1:A:22:ASP:HB2	1:A:684:TYR:HB3	2.01	0.42
1:A:140:LYS:C	1:A:142:ILE:H	2.28	0.41
1:B:122:VAL:HG21	1:B:233:ILE:HG12	2.02	0.41
1:B:259:ILE:HG21	1:B:700:LEU:HD11	2.01	0.41
1:A:38:MET:HE2	1:A:43:LEU:HD22	2.02	0.41
1:A:641:PRO:HG3	1:A:697:ARG:CZ	2.51	0.41
1:B:364:TRP:O	1:B:368:GLN:HG2	2.21	0.41
1:B:661:ASN:ND2	1:B:665:GLU:HB2	2.36	0.41
1:B:224:HIS:HB3	1:B:604:VAL:HG22	2.03	0.40
1:A:272:ILE:HG23	1:A:657:SER:HB3	2.03	0.40
1:A:661:ASN:ND2	1:A:665:GLU:HB2	2.36	0.40
1:B:223:ARG:HG2	1:B:671:PHE:CZ	2.56	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%)	17 (2%)	2 (0%)	36	27
1	B	691/707 (98%)	667 (96%)	20 (3%)	4 (1%)	21	12
All	All	1384/1414 (98%)	1341 (97%)	37 (3%)	6 (0%)	30	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	B	143	LYS
1	B	568	ASP
1	A	142	ILE
1	B	567	GLN
1	B	420	ALA

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	28
1	B	554/597 (93%)	543 (98%)	11 (2%)	48	42
All	All	1114/1194 (93%)	1087 (98%)	27 (2%)	43	35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	23	GLU
1	A	103	GLU
1	A	118	LYS
1	A	122	VAL
1	A	211	LYS

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Mol	Chain	Res	Type
1	A	249	VAL
1	A	283	PHE
1	A	367	LYS
1	A	446	LYS
1	A	451	GLU
1	A	500	VAL
1	A	516	VAL
1	A	543	ARG
1	A	709	CYS
1	A	719	VAL
1	B	23	GLU
1	B	39	LYS
1	B	110	ARG
1	B	249	VAL
1	B	283	PHE
1	B	367	LYS
1	B	451	GLU
1	B	598	GLN
1	B	637	SER
1	B	709	CYS
1	B	719	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	104	ASN
1	A	157	GLN
1	A	186	ASN
1	A	506	GLN
1	A	663	ASN
1	B	186	ASN
1	B	280	HIS
1	B	355	GLN
1	B	368	GLN
1	B	661	ASN
1	B	663	ASN

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	I87	B	801[B]	-	13,15,15	0.55	0	19,22,22	0.89	1 (5%)
2	I87	A	801	-	13,15,15	0.33	0	19,22,22	0.73	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	I87	B	801[B]	-	-	6/15/26/26	1/1/1/1
2	I87	A	801	-	-	5/15/26/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801[B]	I87	C6-C5-N2	2.06	109.74	108.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	I87	C9-N2-S1-N1
2	A	801	I87	C9-N2-S1-O2
2	B	801[B]	I87	C5-N2-S1-N1
2	B	801[B]	I87	C9-N2-S1-N1
2	B	801[B]	I87	C9-N2-S1-O1
2	A	801	I87	C4-N1-S1-O1
2	B	801[B]	I87	C1-C2-N1-S1
2	B	801[B]	I87	C5-N2-S1-O2
2	B	801[B]	I87	C2-N1-S1-O2
2	A	801	I87	C4-N1-S1-O2
2	A	801	I87	C4-N1-S1-N2

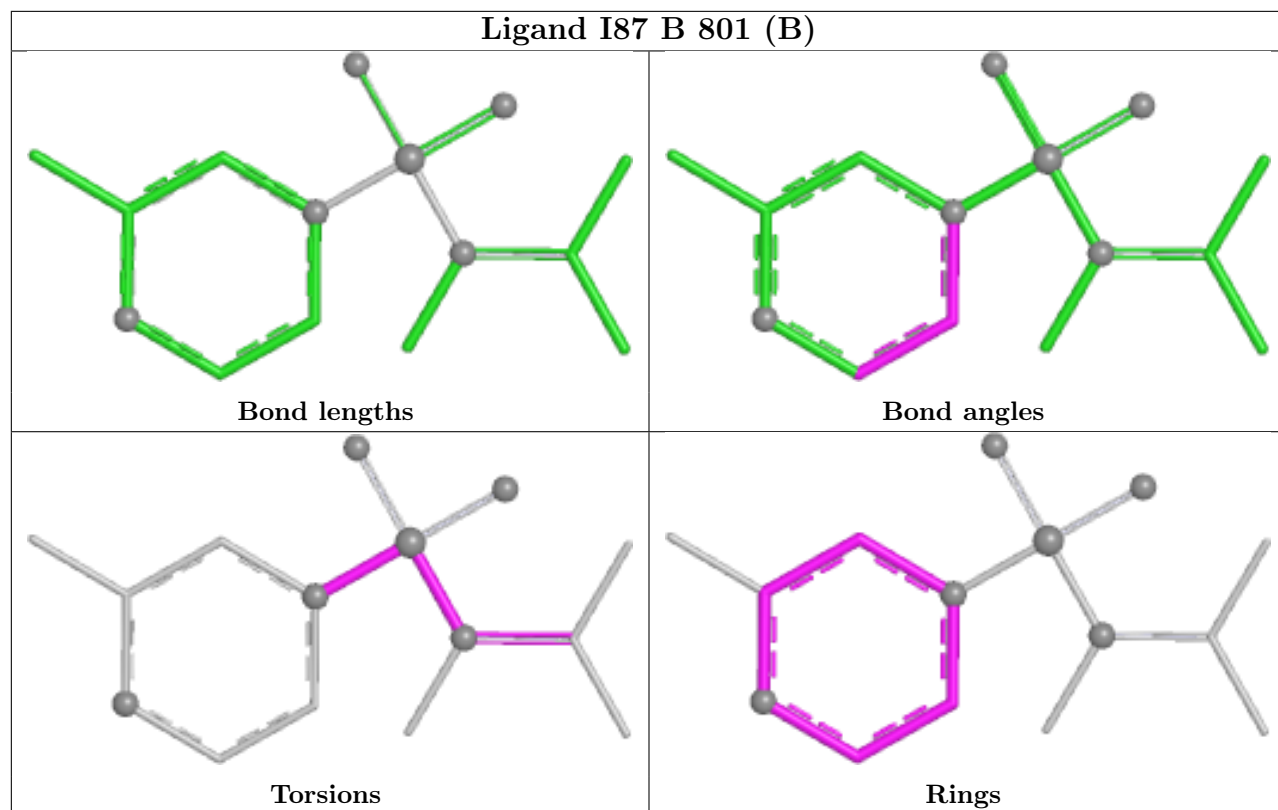
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801[B]	I87	C5-C6-C7-C9-N2-O3

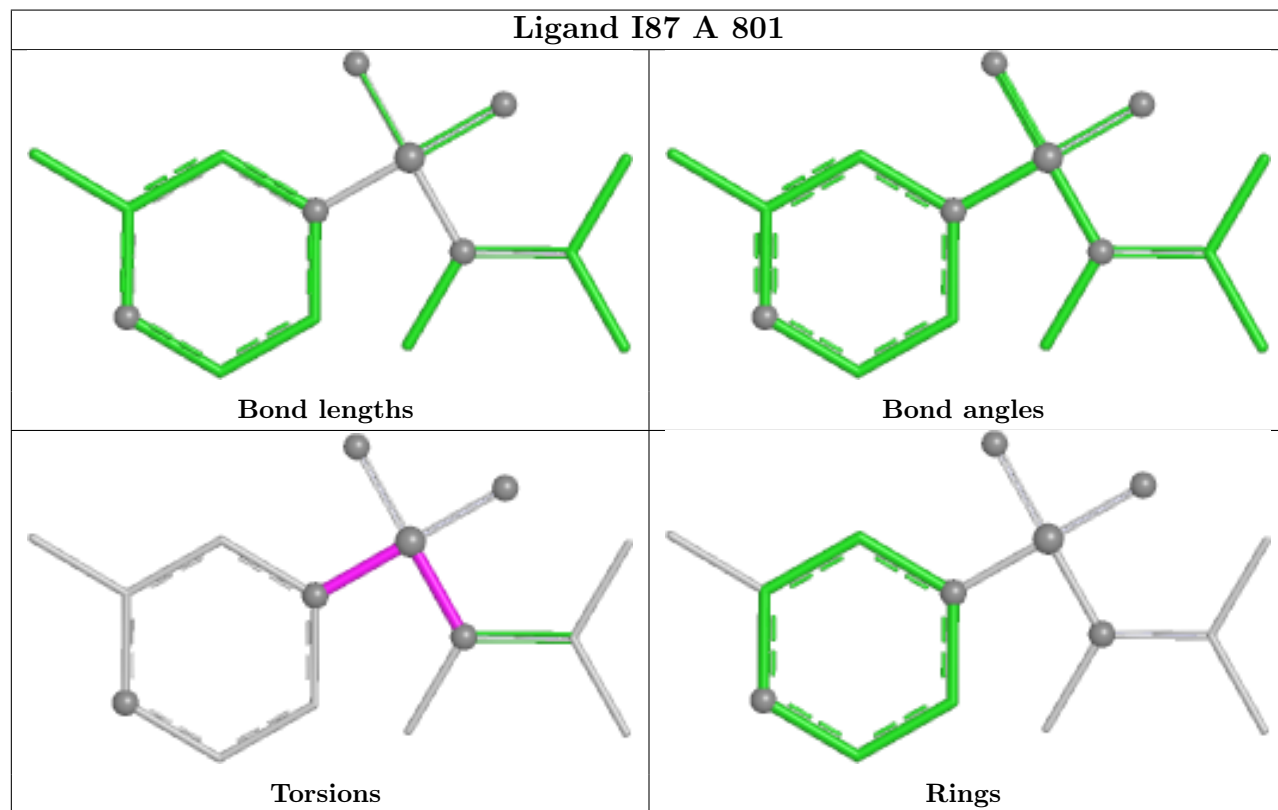
No monomer is involved in short contacts.

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.

Ligand I87 B 801 (B)



Ligand I87 A 801



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%)	0.69	57 (8%) 17 24	30, 43, 64, 79	0
1	B	695/707 (98%)	0.60	45 (6%) 25 33	29, 42, 62, 83	0
All	All	1392/1414 (98%)	0.65	102 (7%) 21 28	29, 43, 63, 83	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	ASP	8.1
1	A	142	ILE	6.7
1	A	23	GLU	6.4
1	B	420	ALA	5.8
1	B	426	ALA	5.8
1	B	422	GLN	5.6
1	B	566	ASP	5.5
1	A	426	ALA	5.4
1	A	22	ASP	5.3
1	A	418	THR	5.2
1	B	428	ALA	5.2
1	B	418	THR	5.0
1	A	613	TRP	5.0
1	B	568	ASP	4.8
1	A	425	ASP	4.8
1	A	422	GLN	4.6
1	B	167	ASN	4.5
1	B	720	PRO	4.3
1	A	167	ASN	4.2
1	A	427	SER	4.0
1	A	428	ALA	3.9
1	B	421	LEU	3.8
1	A	48	TYR	3.8
1	B	142	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	720	PRO	3.7
1	A	33	ARG	3.7
1	B	613	TRP	3.7
1	B	427	SER	3.6
1	A	169	SER	3.6
1	A	168	PHE	3.5
1	B	170	ALA	3.5
1	B	173	PRO	3.5
1	A	170	ALA	3.5
1	A	213	GLY	3.4
1	A	97	LEU	3.4
1	A	417	GLU	3.4
1	B	415	GLU	3.3
1	A	141	ALA	3.3
1	B	166	LYS	3.3
1	B	419	LYS	3.3
1	A	568	ASP	3.3
1	B	567	GLN	3.2
1	A	165	GLY	3.2
1	B	661	ASN	3.1
1	B	431	GLU	3.1
1	B	97	LEU	3.0
1	A	171	LYS	3.0
1	B	213	GLY	3.0
1	A	567	GLN	2.9
1	B	432	ALA	2.9
1	A	416	ASP	2.9
1	B	475	LEU	2.8
1	A	420	ALA	2.8
1	B	99	HIS	2.8
1	A	389	ASP	2.7
1	A	415	GLU	2.7
1	B	378	HIS	2.7
1	B	627	ARG	2.7
1	A	143	LYS	2.7
1	B	519	LEU	2.6
1	A	433	ILE	2.6
1	A	429	ARG	2.6
1	B	312	ARG	2.6
1	B	357	MET	2.6
1	B	414	THR	2.6
1	A	435	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	661	ASN	2.6
1	A	367	LYS	2.5
1	A	55	GLY	2.5
1	A	575	LEU	2.5
1	B	23	GLU	2.4
1	A	719	VAL	2.4
1	A	158	LYS	2.4
1	A	249	VAL	2.4
1	B	168	PHE	2.4
1	A	419	LYS	2.4
1	B	214	ALA	2.3
1	A	565	GLY	2.3
1	B	41	ARG	2.3
1	B	565	GLY	2.3
1	A	516	VAL	2.3
1	A	431	GLU	2.2
1	A	430	LYS	2.2
1	B	278	THR	2.2
1	A	76	ASP	2.2
1	A	421	LEU	2.2
1	A	337	ARG	2.2
1	B	632	ARG	2.2
1	A	366	ALA	2.1
1	A	68	GLY	2.1
1	A	519	LEU	2.1
1	B	366	ALA	2.1
1	B	215	ASP	2.1
1	A	41	ARG	2.1
1	B	543	ARG	2.1
1	A	718	ILE	2.0
1	B	436	ILE	2.0
1	B	37	GLN	2.0
1	A	122	VAL	2.0
1	B	434	ASP	2.0
1	A	166	LYS	2.0
1	A	627	ARG	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 [i](#)

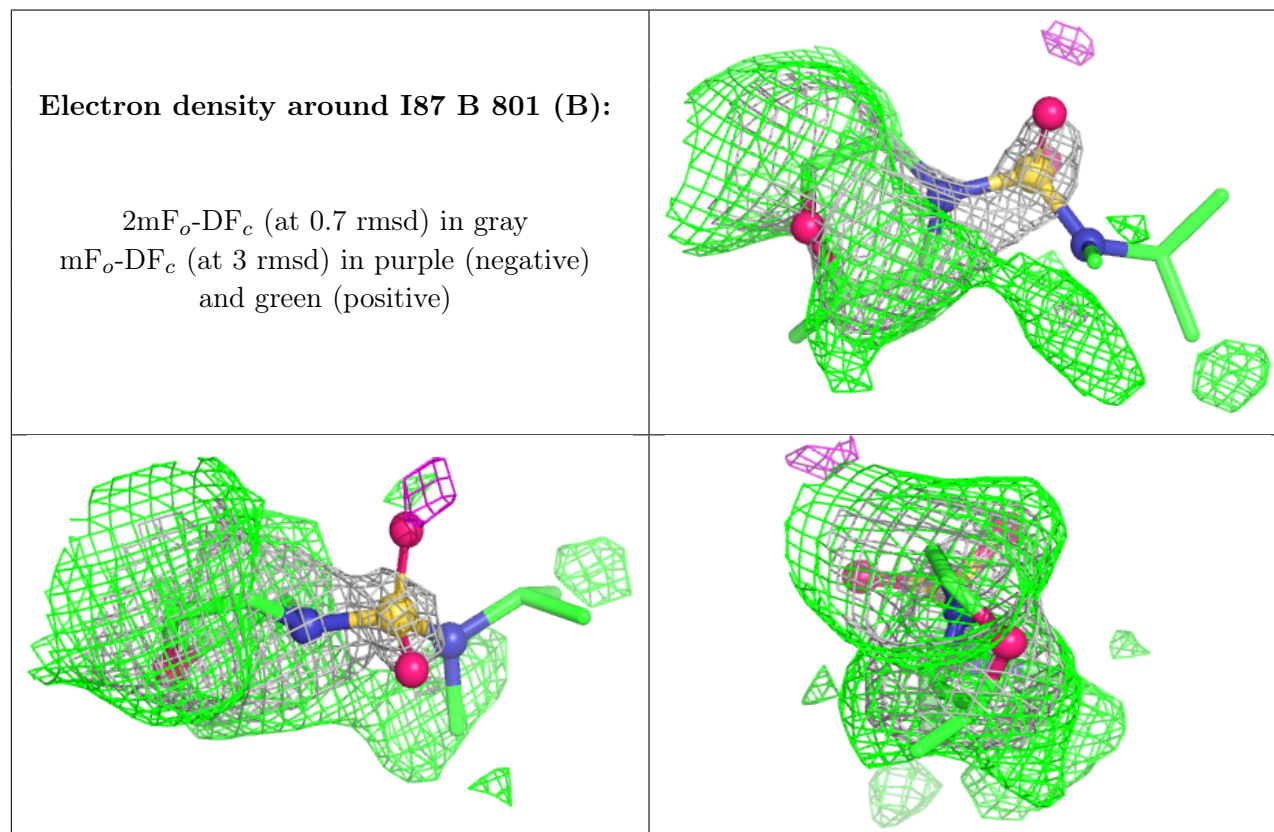
There are no oligosaccharides in this entry.

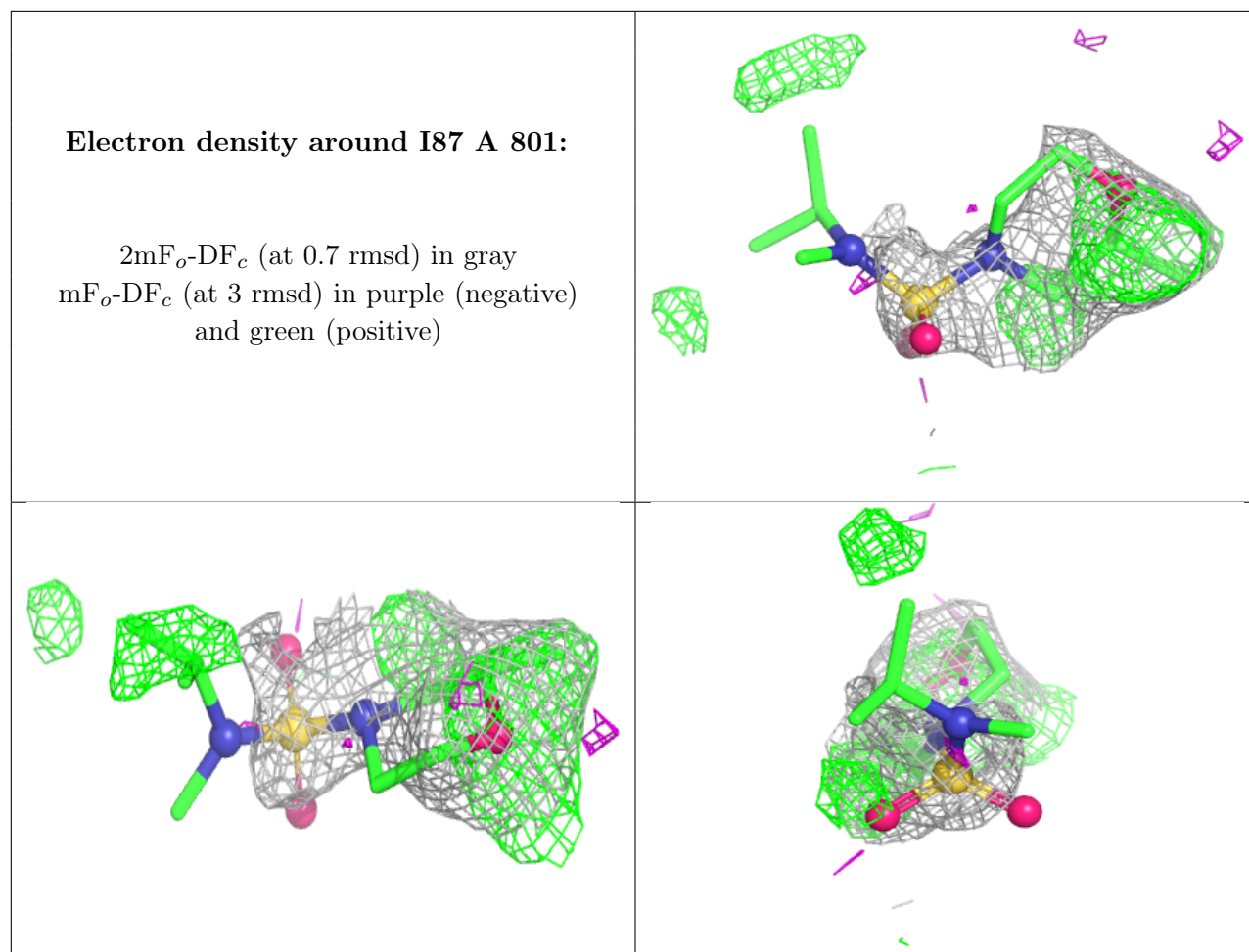
6.4 Ligands [i](#)

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
2	I87	B	801[B]	15/15	0.61	0.67	68,68,68,68	15
2	I87	A	801	15/15	0.67	0.40	140,141,142,142	0
3	CL	A	802	1/1	0.82	0.19	75,75,75,75	0
3	CL	B	802	1/1	0.92	0.23	70,70,70,70	0
3	CL	A	803	1/1	0.94	0.10	50,50,50,50	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 ⓘ

There are no such residues in this entry.