



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:18 AM UTC

PDB ID : 8R1B / pdb_00008r1b
Title : Crystal structure of recombinant LasB from *Pseudomonas aeruginosa* PAO1
in complex with 6466
Authors : Kolling, D.; Koehnke, J.
Deposited on : 2023-11-01
Resolution : 1.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

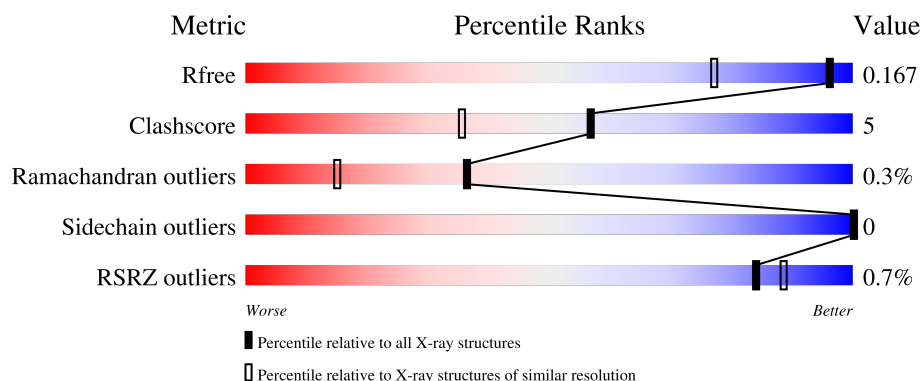
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.31 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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

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	514	

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
6	XI5	A	407	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4897 atoms, of which 2192 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 Pro-elastase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	298	4503	1467	2165	402	454	15	0	3	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-197	MET	-	initiating methionine	UNP P14756
A	-196	LYS	-	expression tag	UNP P14756
A	-195	TYR	-	expression tag	UNP P14756
A	-194	LEU	-	expression tag	UNP P14756
A	-193	LEU	-	expression tag	UNP P14756
A	-192	PRO	-	expression tag	UNP P14756
A	-191	THR	-	expression tag	UNP P14756
A	-190	ALA	-	expression tag	UNP P14756
A	-189	ALA	-	expression tag	UNP P14756
A	-188	ALA	-	expression tag	UNP P14756
A	-187	GLY	-	expression tag	UNP P14756
A	-186	LEU	-	expression tag	UNP P14756
A	-185	LEU	-	expression tag	UNP P14756
A	-184	LEU	-	expression tag	UNP P14756
A	-183	LEU	-	expression tag	UNP P14756
A	-182	ALA	-	expression tag	UNP P14756
A	-181	ALA	-	expression tag	UNP P14756
A	-180	GLN	-	expression tag	UNP P14756
A	-179	PRO	-	expression tag	UNP P14756
A	-178	ALA	-	expression tag	UNP P14756
A	-177	MET	-	expression tag	UNP P14756
A	-176	ALA	-	expression tag	UNP P14756
A	-175	MET	-	expression tag	UNP P14756
A	-174	GLY	-	expression tag	UNP P14756
A	302	GLU	-	expression tag	UNP P14756
A	303	ASN	-	expression tag	UNP P14756
A	304	LEU	-	expression tag	UNP P14756

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Chain	Residue	Modelled	Actual	Comment	Reference
A	305	TYR	-	expression tag	UNP P14756
A	306	PHE	-	expression tag	UNP P14756
A	307	GLN	-	expression tag	UNP P14756
A	308	GLY	-	expression tag	UNP P14756
A	309	LEU	-	expression tag	UNP P14756
A	310	GLU	-	expression tag	UNP P14756
A	311	HIS	-	expression tag	UNP P14756
A	312	HIS	-	expression tag	UNP P14756
A	313	HIS	-	expression tag	UNP P14756
A	314	HIS	-	expression tag	UNP P14756
A	315	HIS	-	expression tag	UNP P14756
A	316	HIS	-	expression tag	UNP P14756

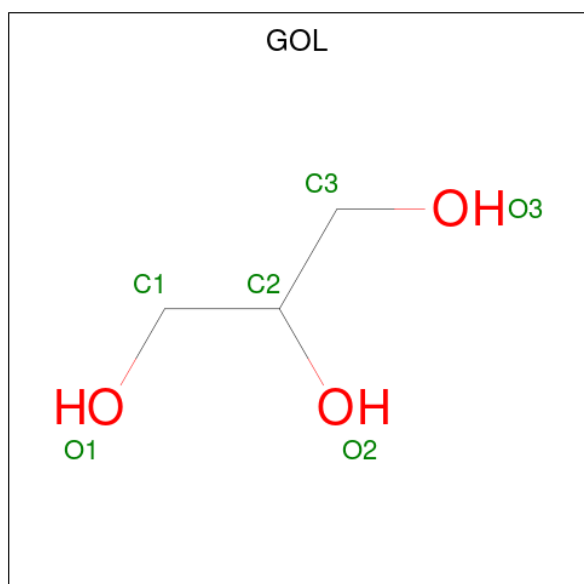
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

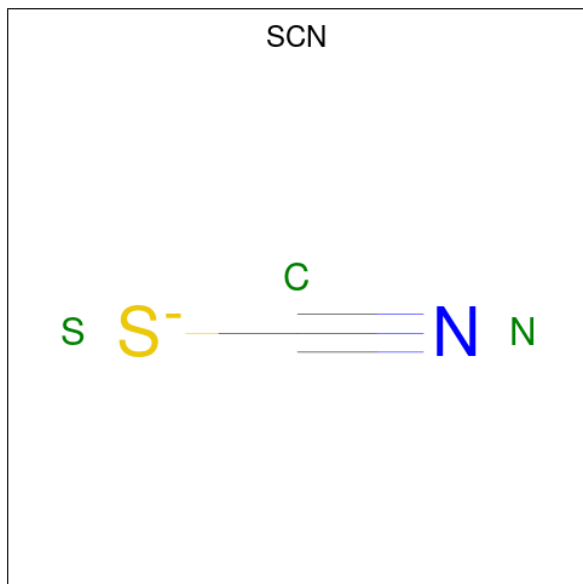
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



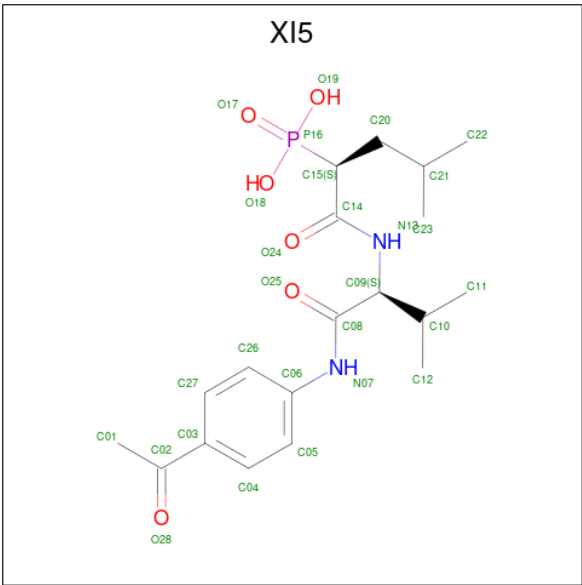
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 6 is [(2 {S})-1-[[1-[(4-ethanoylphenyl)amino]-3-methyl-1-oxidanylidene-butan-2-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]phosphonic acid (CCD ID: XI5) (formula: C₁₉H₂₉N₂O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	P	0	0
			55	19	27	2	6	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	316	Total	O	0	0
			316	316		

- Molecule 1: Pro-elastase

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.37Å 89.98Å 40.83Å 90.00° 114.08° 90.00°	Depositor
Resolution (Å)	44.99 – 1.31 44.99 – 1.31	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.99-1.31) 98.6 (44.99-1.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.145 , 0.167 0.146 , 0.167	Depositor DCC
R_{free} test set	3200 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4897	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.06% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XI5, SCN, GOL, ZN, CA

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	0/2403	0.75	0/3255

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	2338	2165	2166	21	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	18	0	24	2	0
5	A	3	0	0	0	0
6	A	28	27	0	0	0
7	A	316	0	0	10	1
All	All	2705	2192	2190	21	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 5.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH2	7:A:502:HOH:O	1.99	0.95
1:A:221:ASP:OD2	7:A:501:HOH:O	1.83	0.94
1:A:65:GLN:NE2	7:A:503:HOH:O	2.12	0.82
1:A:119:ALA:HB2	4:A:405:GOL:H12	1.62	0.80
1:A:65:GLN:CG	7:A:503:HOH:O	2.32	0.77

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)
7:A:718:HOH:O	7:A:759:HOH:O[1_455]	2.13	0.07

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	299/514 (58%)	290 (97%)	8 (3%)	1 (0%)	36 15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ALA

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	242/402 (60%)	242 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	XI5	A	407	2	27,28,28	1.73	4 (14%)	34,40,40	1.24	4 (11%)
4	GOL	A	405	-	5,5,5	0.59	0	5,5,5	0.71	0
5	SCN	A	406	-	1,2,2	0.57	0	0,1,1	-	-
4	GOL	A	403	-	5,5,5	0.38	0	5,5,5	0.51	0
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.62	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
6	XI5	A	407	2	1/1/10/10	11/33/34/34	0/1/1/1
4	GOL	A	405	-	-	3/4/4/4	-
4	GOL	A	403	-	-	0/4/4/4	-
4	GOL	A	404	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	XI5	C14-N13	4.57	1.43	1.34
6	A	407	XI5	C08-N07	4.47	1.45	1.35
6	A	407	XI5	P16-C15	4.13	1.87	1.81
6	A	407	XI5	O25-C08	-2.47	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	XI5	O19-P16-O17	-2.99	105.94	113.45
6	A	407	XI5	C15-C20-C21	-2.64	112.11	116.52
6	A	407	XI5	C08-C09-N13	-2.43	103.73	110.32
6	A	407	XI5	O24-C14-C15	2.06	122.01	119.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	407	XI5	C15

5 of 14 torsion outliers are listed below:

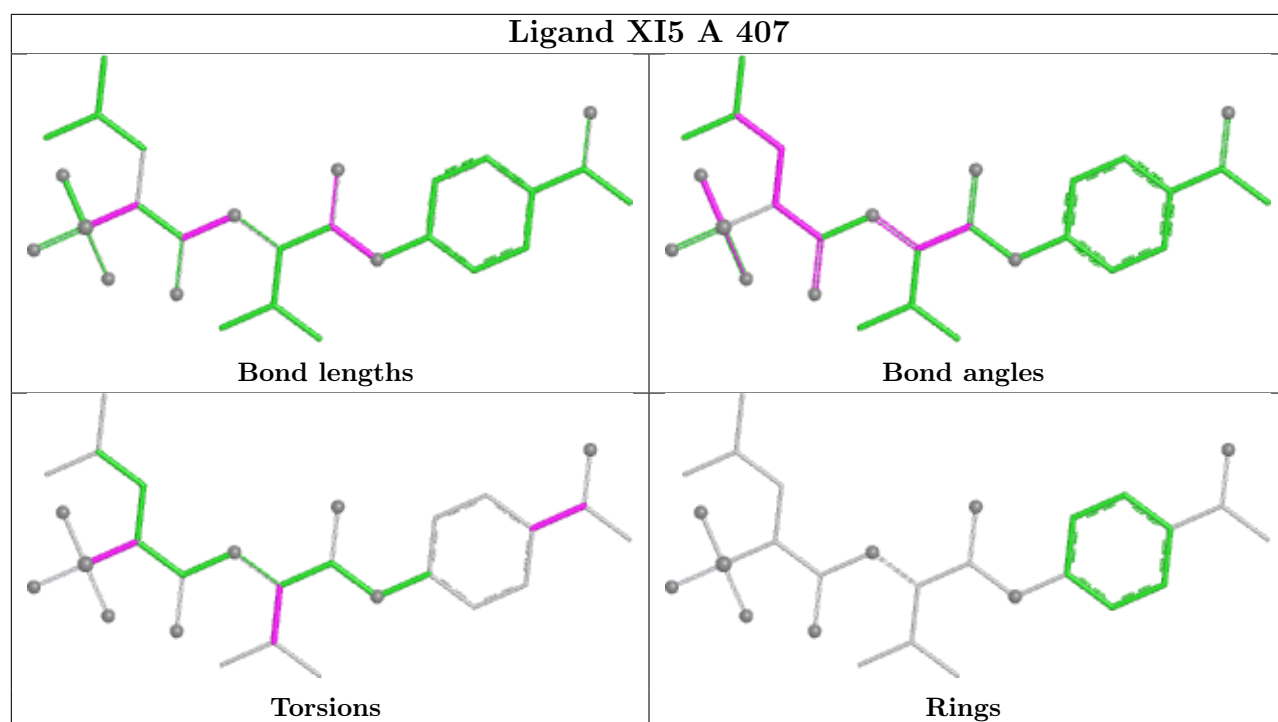
Mol	Chain	Res	Type	Atoms
4	A	405	GOL	C1-C2-C3-O3
6	A	407	XI5	C14-C15-P16-O18
6	A	407	XI5	C14-C15-P16-O19
6	A	407	XI5	N13-C09-C10-C11
6	A	407	XI5	N13-C09-C10-C12

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	GOL	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	298/514 (57%)	-0.24	2 (0%) 84 88	10, 16, 28, 40	3 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128[A]	MET	2.5
1	A	129	PHE	2.2

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.

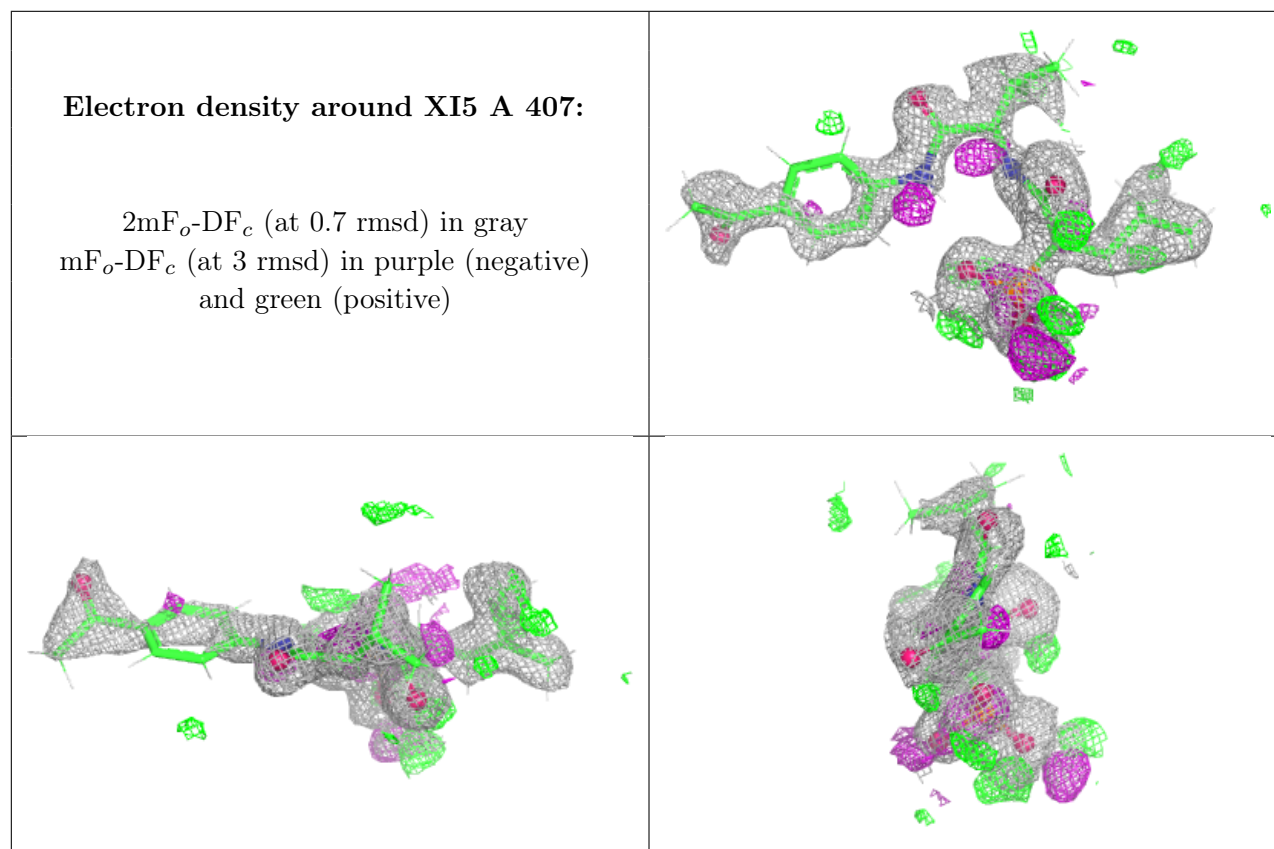
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	405	6/6	0.82	0.14	29,35,42,51	0
6	XI5	A	407	28/28	0.86	0.15	21,39,58,67	0
4	GOL	A	403	6/6	0.90	0.10	21,26,30,35	0
4	GOL	A	404	6/6	0.96	0.08	17,20,24,28	0
5	SCN	A	406	3/3	0.98	0.09	14,14,21,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	401	1/1	0.98	0.04	11,11,11,11	0
3	CA	A	402	1/1	0.99	0.02	12,12,12,12	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.