

Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2024 – 05:47 pm BST

PDB ID : 8R1B

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.orgA user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.003 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

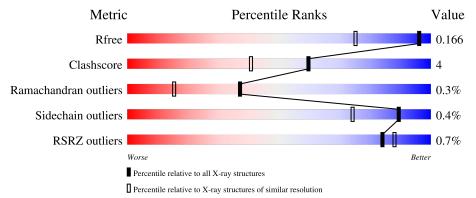
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance (i)

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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (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 <=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	54%	•	42%					

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 (i)

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.

\mathbf{Mol}	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace	
1	A	298	Total 4503	C 1467	H 2165	N 402	O 454	S 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
Α	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

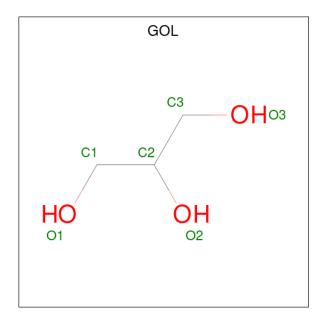
• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

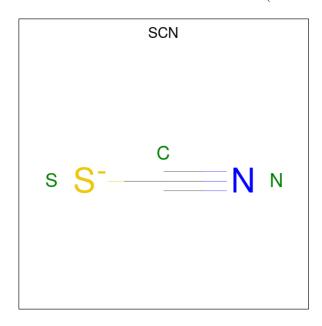
• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





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

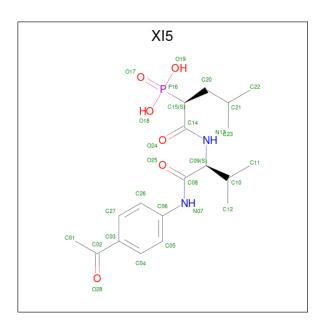
• Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

• Molecule 6 is $[(2 \{S\})-1-[[1-[(4-ethanoylphenyl)amino]-3-methyl-1-oxidanylidene-butan-2-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]phosphonic acid (three-letter code: XI5) (formula: <math>C_{19}H_{29}N_2O_6P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	Λ	1	Total	С	Н	N	О	Р	0	0
О	A	1	55	19	27	2	6	1	U	0

• Molecule 7 is water.

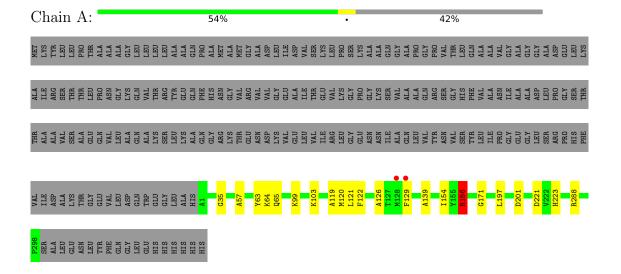
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	316	Total O 316 316	0	0



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: Pro-elastase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	39.37Å 89.98Å 40.83Å	Depositor
a, b, c, α , β , γ	90.00° 114.08° 90.00°	Depositor
Resolution (Å)	44.99 - 1.31	Depositor
resolution (A)	44.99 - 1.31	EDS
% Data completeness	99.0 (44.99-1.31)	Depositor
(in resolution range)	98.6 (44.99-1.31)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 \; (at \; 1.31\text{Å})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.145 , 0.167	Depositor
it, it _{free}	0.144 , 0.166	DCC
R_{free} test set	3212 reflections (5.16%)	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, 35.7	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	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.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: GOL, CA, ZN, XI5, SCN

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).

Mal	Mol Chain Bond lengths		Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.66	0/2403	0.84	$1/3255 \ (0.0\%)$

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 maintain 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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	201	ASP	CB-CG-OD1	5.51	123.26	118.30

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	19	0
2	A	1	0	0	0	0
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	19	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 4.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	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
1:A:35:GLY:O	1:A:99:LYS:NZ	2.20	0.74
1:A:223:HIS:ND1	7:A:501:HOH:O	1.82	0.73
1:A:288:ARG:NH1	7:A:506:HOH:O	2.34	0.61
1:A:65:GLN:HG3	7:A:503:HOH:O	2.01	0.52
1:A:57:ALA:O	7:A:504:HOH:O	2.18	0.50
1:A:63:TYR:HA	1:A:64:LYS:HA	1.85	0.45
1:A:139:ALA:HB3	1:A:171:GLY:HA2	1.99	0.44
1:A:119:ALA:HB2	4:A:405:GOL:C1	2.43	0.43
1:A:288:ARG:NH2	7:A:512:HOH:O	2.51	0.43
1:A:129:PHE:HE1	1:A:197:LEU:HD21	1.84	0.42
1:A:154:ILE:HD12	1:A:156:ARG:HG2	2.01	0.42
1:A:103:LYS:HB2	1:A:121:LEU:HD23	2.02	0.42
1:A:120[A]:MET:HE2	1:A:122:PHE:CZ	2.54	0.42
1:A:65:GLN:CD	7:A:503:HOH:O	2.46	0.42

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	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.

Mo	l Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	299/514 (58%)	290 (97%)	8 (3%)	1 (0%)	37 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%)	241 (100%)	1 (0%)	89 74

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	Вс	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	GOL	A	404	-	5,5,5	0.33	0	5,5,5	0.56	0	
4	GOL	A	405	-	5,5,5	0.57	0	5,5,5	0.69	0	
5	SCN	A	406	-	1,2,2	0.60	0	0,1,1	-	-	
6	XI5	A	407	2	27,28,28	1.71	4 (14%)	35,40,40	1.10	2 (5%)	
4	GOL	A	403	-	5,5,5	0.37	0	5,5,5	0.47	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
4	GOL	A	404	-	-	0/4/4/4	-
4	GOL	A	403	_	-	0/4/4/4	-
6	XI5	A	407	2	1/1/10/10	10/33/34/34	0/1/1/1
4	GOL	A	405	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
6	A	407	XI5	C08-N07	4.49	1.45	1.35

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(A)
6	A	407	XI5	C14-N13	4.46	1.43	1.34
6	A	407	XI5	P16-C15	4.13	1.87	1.81
6	A	407	XI5	O25-C08	-2.38	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
6	A	407	XI5	O19-P16-O17	-2.99	105.94	113.45
6	A	407	XI5	C08-C09-N13	-2.44	103.73	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	407	XI5	C15

All (13) 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
6	A	407	XI5	C08-C09-C10-C11
4	A	405	GOL	O2-C2-C3-O3
6	A	407	XI5	C08-C09-C10-C12
4	A	405	GOL	O1-C1-C2-C3
6	A	407	XI5	O28-C02-C03-C04
6	A	407	XI5	O28-C02-C03-C27
6	A	407	XI5	C01-C02-C03-C04
6	A	407	XI5	C01-C02-C03-C27

There are no ring outliers.

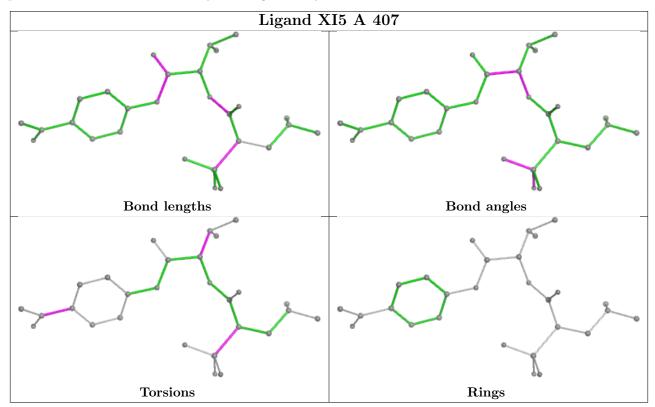
1 monomer is involved in 2 short contacts:

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 then 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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9
1	A	298/514 (57%)	-0.26	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	2.6	
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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	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

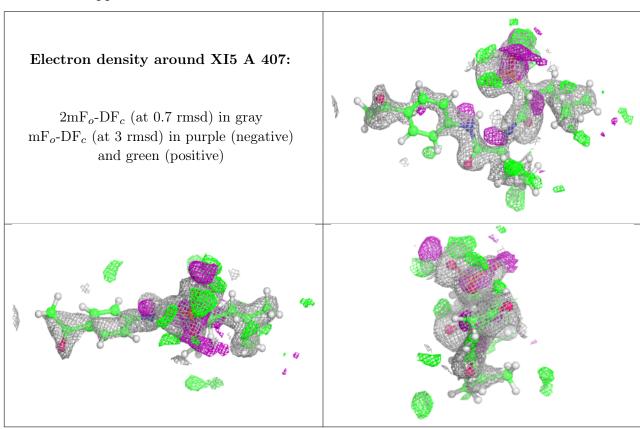
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	ZN	A	401	1/1	0.98	0.04	11,11,11,11	0
3	CA	A	402	1/1	0.99	0.03	12,12,12,12	0

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 (i)

There are no such residues in this entry.

