

Full wwPDB X-ray Structure Validation Report (i)

Jan 22, 2024 – 08:20 pm GMT

PDB ID : 8PLA

Title : Thioredoxin glutathione reductase of Schistosoma mansoni fragment screen hit

11.

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Deposited on : 2023-06-27

Resolution : 1.66 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 (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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

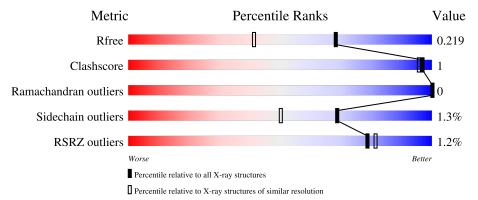
Validation Pipeline (wwPDB-VP) : 2.36

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 1.66 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	597	95%	
1	В	597	96%	

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
3	ZLI	A	602	-	-	-	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9911 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.

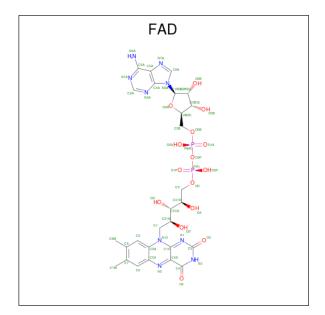
• Molecule 1 is a protein called Thioredoxin glutathione reductase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	588	Total 4503	C 2859	N 759	O 863	S 22	0	0	0
1	В	588	Total 4503	C 2859	N 759	O 863	S 22	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q962Y6
A	1	PRO	-	expression tag	UNP Q962Y6
В	0	GLY	-	expression tag	UNP Q962Y6
В	1	PRO	-	expression tag	UNP Q962Y6

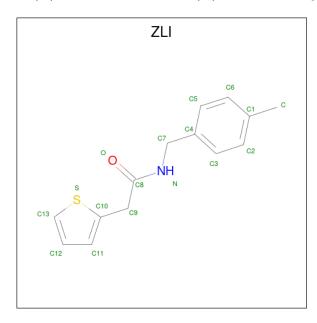
• Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





\mathbf{Mol}	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	
2	Λ	1	Total	С	N	О	Р	0	0
2	А	1	53	27	9	15	2	U	
2	D	1	Total	С	N	О	Р	0	0
2	Б	1	53	27	9	15	2	U	

• Molecule 3 is $\{N\}$ -[(4-methylphenyl)methyl]-2-thiophen-2-yl-ethanamide (three-letter code: ZLI) (formula: $C_{14}H_{15}NOS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	Λ	1	Total	С	N	О	S	0	0
3	А	1	17	14	1	1	1	0	
9	D	1	Total	С	N	О	S	0	0
3	Б	1	17	14	1	1	1	0	

• Molecule 4 is water.

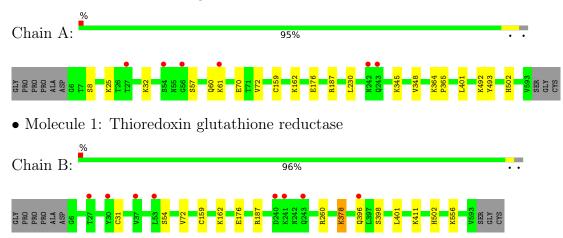
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	411	Total O 411 411	0	0
4	В	354	Total O 354 354	0	0



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: Thioredoxin glutathione reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	62.50Å 103.13Å 131.65Å	Depositor
a, b, c, α , β , γ	90.00° 92.72° 90.00°	Depositor
Resolution (Å)	57.46 - 1.66	Depositor
resolution (A)	57.46 - 1.66	EDS
% Data completeness	99.5 (57.46-1.66)	Depositor
(in resolution range)	99.6 (57.46-1.66)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.84 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0189, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.192 , 0.215	Depositor
it, it _{free}	0.198 , 0.219	DCC
R_{free} test set	9646 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 45.1	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9911	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 30.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3480e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: FAD, ZLI

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 Chair		Bond	lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.43	0/4590	0.60	0/6218	
1	В	0.41	0/4590	0.58	0/6218	
All	All	0.42	0/9180	0.59	0/12436	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4503	0	4520	9	0
1	В	4503	0	4520	7	0
2	A	53	0	31	0	0
2	В	53	0	31	0	0
3	A	17	0	0	0	0
3	В	17	0	0	0	0
4	A	411	0	0	1	0
4	В	354	0	0	2	0
All	All	9911	0	9102	16	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 1.



All (16) 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	${f distance}({f A})$	overlap (Å)
1:A:364:LYS:HG3	1:A:365:PRO:HD2	1.80	0.64
1:A:176:GLU:HG3	1:A:187:ARG:HG2	1.86	0.56
1:A:60:GLN:HG2	1:A:70:GLU:O	2.11	0.51
1:A:57:SER:O	1:A:61:LYS:HD2	2.14	0.47
1:B:176:GLU:CG	1:B:187:ARG:HG2	2.47	0.44
1:A:345:LYS:HB3	4:A:880:HOH:O	2.19	0.43
1:A:230:LEU:HB3	1:A:401:LEU:HD12	2.00	0.42
1:B:260:ARG:HB2	1:B:396:GLN:HE22	1.85	0.42
1:A:364:LYS:HG3	1:A:365:PRO:CD	2.47	0.42
1:B:378:LYS:HE3	1:B:378:LYS:HB3	1.84	0.42
1:B:398:SER:N	4:B:705:HOH:O	2.48	0.41
1:B:556:LYS:HE3	4:B:716:HOH:O	2.20	0.41
1:A:25:LYS:HG3	1:A:72:VAL:HG21	2.02	0.41
1:A:492:LYS:HD3	1:A:493:TYR:CZ	2.56	0.41
1:B:31:CYS:SG	1:B:72:VAL:HG13	2.61	0.40
1:B:176:GLU:HG2	1:B:187:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

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	586/597~(98%)	572 (98%)	14 (2%)	0	100 100
1	В	586/597~(98%)	571 (97%)	15 (3%)	0	100 100
All	All	1172/1194~(98%)	1143 (98%)	29 (2%)	0	100 100

There are no Ramachandran outliers to report.



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	489/495 (99%)	483 (99%)	6 (1%)	71 53		
1	В	489/495 (99%)	482 (99%)	7 (1%)	67 46		
All	All	978/990 (99%)	965 (99%)	13 (1%)	69 50		

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	32	LYS
1	A	159	CYS
1	A	162	LYS
1	A	348	VAL
1	A	502	HIS
1	В	54	SER
1	В	159	CYS
1	В	162	LYS
1	В	378	LYS
1	В	401	LEU
1	В	411	LYS
1	В	502	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	363	ASN
1	A	396	GLN
1	В	220	GLN
1	В	396	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	Tuno	Chain	Res	es Link	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	ZLI	В	602	-	18,18,18	1.21	3 (16%)	18,23,23	1.37	2 (11%)	
3	ZLI	A	602	-	18,18,18	1.31	2 (11%)	18,23,23	0.66	0	
2	FAD	A	601	-	53,58,58	0.52	0	68,89,89	0.59	1 (1%)	
2	FAD	В	601	-	53,58,58	0.51	0	68,89,89	0.61	2 (2%)	

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
3	ZLI	В	602	-	-	1/7/9/9	0/2/2/2
3	ZLI	A	602	-	-	0/7/9/9	0/2/2/2
2	FAD	A	601	-	-	2/30/50/50	0/6/6/6
2	FAD	В	601	-	-	3/30/50/50	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	A	602	ZLI	C9-C10	-3.95	1.48	1.51

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	В	602	ZLI	C8-N	3.24	1.40	1.33
3	A	602	ZLI	C8-N	2.76	1.39	1.33
3	В	602	ZLI	C9-C10	-2.15	1.49	1.51
3	В	602	ZLI	C7-N	2.05	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	В	602	ZLI	C7-N-C8	4.43	129.23	122.34
3	В	602	ZLI	C10-C9-C8	2.70	118.76	113.39
2	В	601	FAD	O4B-C1B-C2B	-2.12	103.82	106.93
2	В	601	FAD	C5A-C6A-N6A	2.10	123.54	120.35
2	A	601	FAD	C5A-C6A-N6A	2.08	123.52	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

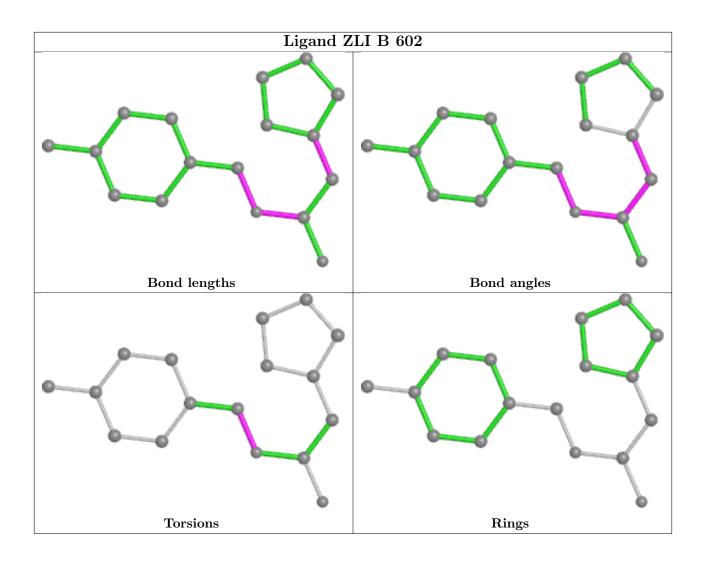
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	PA-O3P-P-O5'
2	В	601	FAD	PA-O3P-P-O5'
3	В	602	ZLI	C4-C7-N-C8
2	A	601	FAD	O4B-C4B-C5B-O5B
2	В	601	FAD	O4B-C4B-C5B-O5B
2	В	601	FAD	P-O3P-PA-O2A

There are no ring outliers.

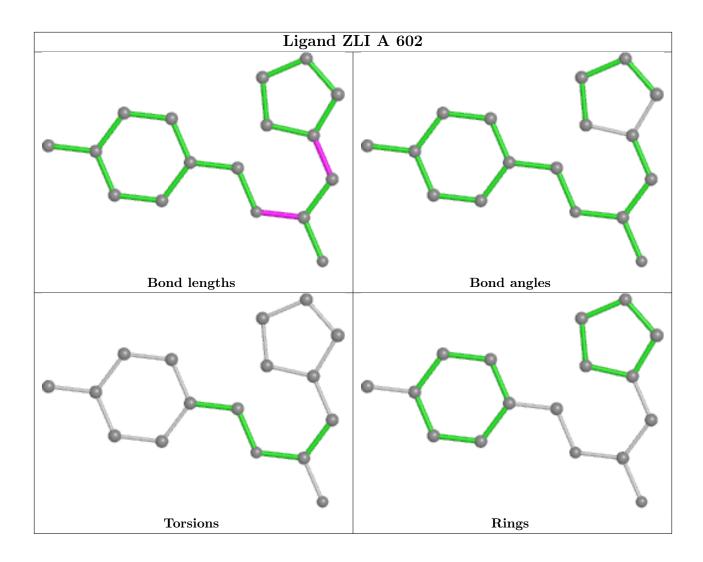
No monomer is involved in short contacts.

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 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.

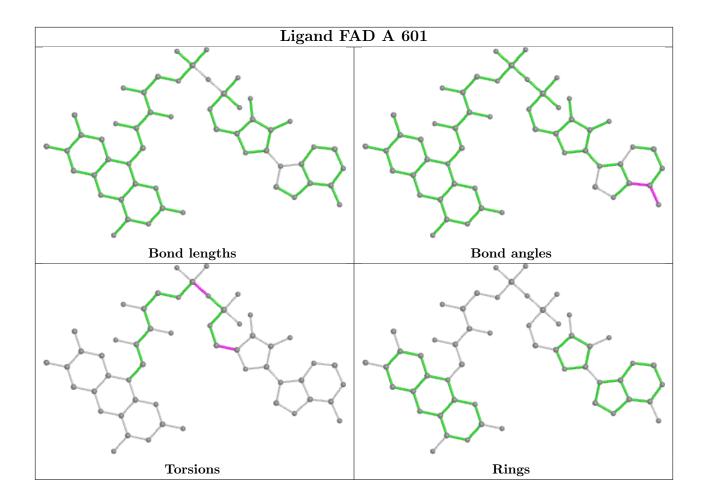




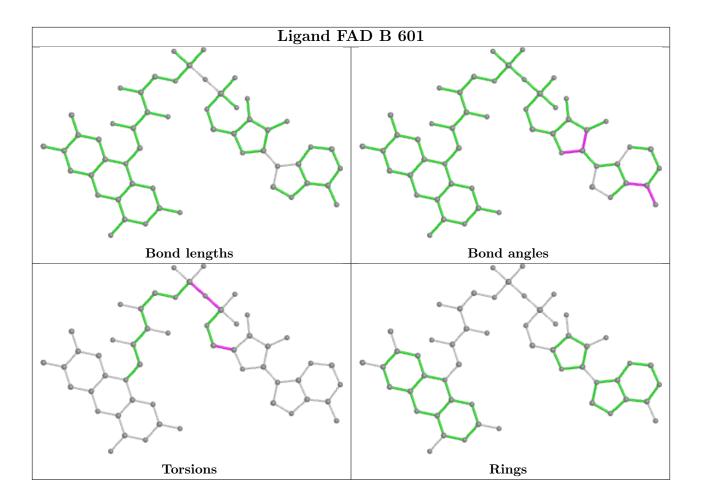












5.7 Other polymers (i)

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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	588/597 (98%)	-0.30	6 (1%) 82 85	13, 20, 38, 52	0
1	В	588/597 (98%)	-0.22	8 (1%) 75 79	13, 23, 40, 58	0
All	All	1176/1194 (98%)	-0.26	14 (1%) 79 81	13, 21, 39, 58	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	THR	3.0
1	В	241	LYS	2.9
1	A	54	SER	2.7
1	В	30	TYR	2.7
1	В	243	GLN	2.7
1	A	61	LYS	2.6
1	В	53	LEU	2.6
1	В	396	GLN	2.6
1	В	240	ASP	2.3
1	В	27	THR	2.3
1	A	243	GLN	2.1
1	A	242	ASN	2.1
1	В	37	VAL	2.1
1	A	56	GLY	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 monosaccharides in this entry.

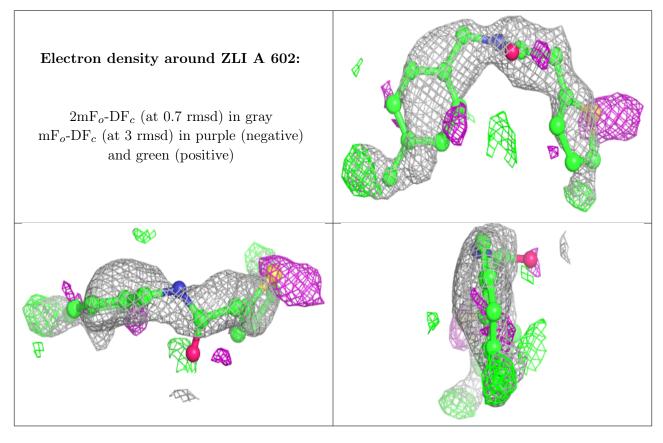


6.4 Ligands (i)

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
3	ZLI	A	602	17/17	0.57	0.41	54,66,78,86	0
3	ZLI	В	602	17/17	0.69	0.30	54,62,72,75	0
2	FAD	В	601	53/53	0.96	0.07	16,20,23,24	0
2	FAD	A	601	53/53	0.97	0.07	15,17,21,21	0

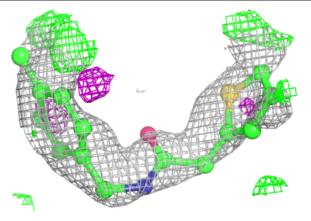
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

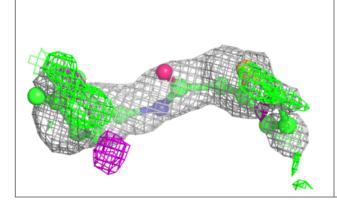


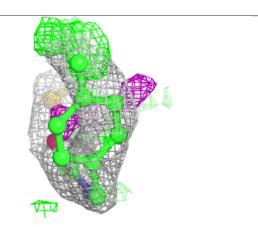


Electron density around ZLI B 602:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

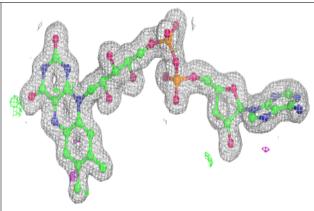


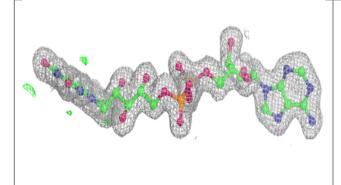


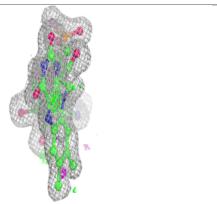


Electron density around FAD B 601:

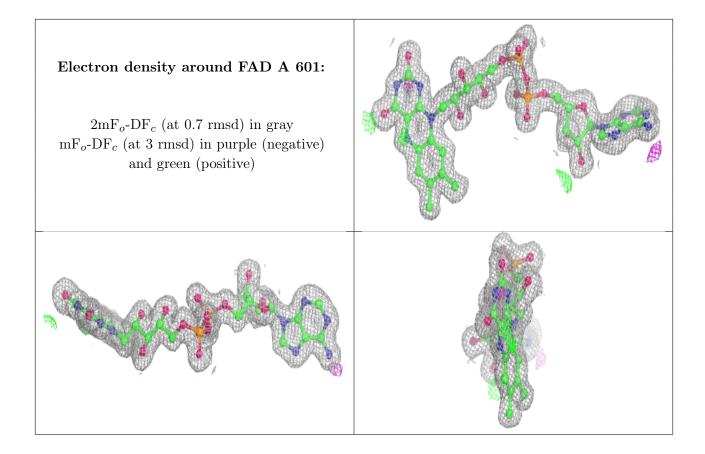
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

