

Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2021 – 08:03 PM GMT

PDB ID	:	6FR2
Title	:	Soluble epoxide hydrolase in complex with LK864
Authors	:	Kramer, J.S.; Pogoryelov, D.; Krasavin, M.; Proschak, E.
Deposited on		
$\operatorname{Resolution}$:	2.26 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 following versions of software and data (see references (1)) were used in the production of this report:

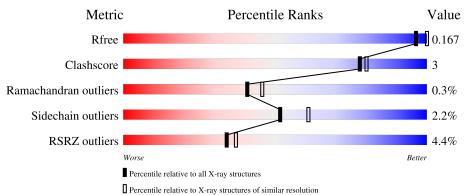
Mogul Xtriage (Phenix) EDS buster-report	······································	1.8.5 (274361), CSD as541be (2020) 1.13 2.17
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996) 2.17

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 2.26 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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		
			4%		
1	А	346	84%	7% •	8%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2735 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 Bifunctional epoxide hydrolase 2.

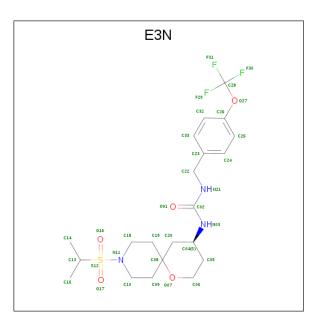
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	319	Total 2594	C 1661	N 441	O 469	S 23	0	6	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	initiating methionine	UNP P34913
A	220	ALA	-	expression tag	UNP P34913
A	221	SER	-	expression tag	UNP P34913
A	556	LEU	-	expression tag	UNP P34913
А	557	LEU	-	expression tag	UNP P34913
A	558	GLU	-	expression tag	UNP P34913
А	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913
А	562	HIS	-	expression tag	UNP P34913
А	563	HIS	-	expression tag	UNP P34913
А	564	HIS	-	expression tag	UNP P34913

• Molecule 2 is $1-[(4 {S})-9$ -propan-2-ylsulfonyl-1-oxa-9-azaspiro[5.5]undecan-4-yl]-3-[[4-(t rifluoromethyloxy)phenyl]methyl]urea (three-letter code: E3N) (formula: $C_{21}H_{30}F_3N_3O_5S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	А	1	Total 33	С 21	т	N 3	0	S 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0

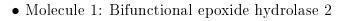
• Molecule 4 is water.

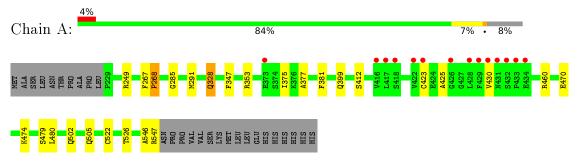
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	107	Total O 107 107	0	0



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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	80.09Å 92.18Å 107.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 - 2.26	Depositor
Resolution (A)	46.09 - 2.26	EDS
% Data completeness	98.6 (46.09-2.26)	Depositor
(in resolution range)	98.5(46.09-2.26)	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.26 (at 2.27 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R R.	0.168 , 0.210	Depositor
R, R_{free}	0.170 , 0.167	DCC
R_{free} test set	907 reflections (4.88%)	wwPDB-VP
Wilson B-factor $(Å^2)$	48.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 49.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2735	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: MG, $\rm E3N$

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	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/2675	0.57	0/3627	

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	А	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	А	291	MET	Peptide	

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	А	2594	0	2518	15	0
2	А	33	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	1	0	0	0	0
4	А	107	0	0	0	0
All	All	2735	0	2518	15	0

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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 3.

All (15) 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:347:PHE:CZ	1:A:479:SER:HB3	2.38	0.58
1:A:381:PHE:CE2	2:A:601:E3N:C15	2.87	0.58
1:A:522:CYS:SG	1:A:526:THR:HG23	2.50	0.52
1:A:470:GLU:HG2	1:A:474:LYS:HE2	1.91	0.51
1:A:328[A]:GLN:HG3	1:A:353[A]:ARG:HB2	1.93	0.50
1:A:381:PHE:CD2	2:A:601:E3N:C15	2.96	0.48
1:A:267:PHE:HA	1:A:268:PRO:HA	1.81	0.44
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.84	0.44
1:A:353[A]:ARG:HD3	1:A:546:ALA:O	2.18	0.43
1:A:502:GLN:NE2	1:A:505:GLN:OE1	2.51	0.43
1:A:470:GLU:O	1:A:474:LYS:HG3	2.19	0.42
1:A:375:ILE:C	1:A:377:ALA:N	2.73	0.42
1:A:285:GLY:O	1:A:547:ARG:NH2	2.54	0.41
1:A:425:ALA:HB1	1:A:430:VAL:HG21	2.02	0.41
1:A:375:ILE:HG12	2:A:601:E3N:C14	2.51	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	А	323/346~(93%)	314~(97%)	8 (2%)	1 (0%)	41 46	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	268	PRO

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.

M	ol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1		А	282/305~(92%)	274 (97%)	8 (3%)	43 52	

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	249	ARG
1	А	328[A]	GLN
1	А	328[B]	GLN
1	А	399	GLN
1	А	412	SER
1	А	423	CYS
1	А	460[A]	ARG
1	А	460[B]	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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).

Γ	Mol	Tuno	Chain	\mathbf{Res}	Res	Link	Bo	ond leng	ths	B	ond ang	gles
1V.	101	Type Chain Res Li		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2			
	2	E3N	А	601	-	32,35,35	1.68	4 (12%)	42,52,52	2.96	19 (45%)	

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	E3N	А	601	-	-	12/26/50/50	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	601	E3N	O07-C06	-5.16	1.36	1.44
2	А	601	E3N	O16-S12	-4.64	1.39	1.43
2	А	601	E3N	O17-S12	-3.75	1.40	1.43
2	А	601	E3N	C09-C08	-2.26	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	А	601	E3N	C19-C18-N11	7.90	118.89	109.14
2	А	601	E3N	O17-S12-O16	-6.90	114.78	119.22
2	А	601	E3N	C06-O07-C08	6.42	124.39	114.70
2	А	601	E3N	C09-C10-N11	5.88	116.39	109.14
2	А	601	E3N	C10-N11-S12	4.42	126.12	116.93

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	601	E3N	O07-C08-C19	-4.40	94.04	108.69
2	А	601	E3N	N21-C02-N03	4.02	125.18	115.92
2	А	601	E3N	C14-C13-C15	-3.85	105.78	112.85
2	А	601	E3N	C19-C08-C09	-3.79	104.66	109.56
2	А	601	E3N	O01-C02-N03	-3.31	116.58	122.62
2	А	601	E3N	C20-C04-C05	-3.10	105.80	108.80
2	А	601	E3N	C20-C04-N03	3.02	114.02	110.29
2	А	601	E3N	C18-N11-S12	2.77	122.70	116.93
2	А	601	E3N	C33-C23-C24	-2.76	113.83	118.17
2	А	601	E3N	C04-N03-C02	2.75	128.84	123.02
2	А	601	E3N	C22-N21-C02	2.61	126.84	121.53
2	А	601	E3N	C32-C33-C23	2.52	124.49	121.03
2	А	601	E3N	O01-C02-N21	-2.45	118.23	122.50
2	А	601	E3N	C14-C13-S12	2.00	114.62	109.92

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There are no chirality outliers.

All (12)	All (12) torsion outliers are listed below:								
Mol	Chain	Res	Type	Atoms					
2	А	601	E3N	C15-C13-S12-N11					
2	А	601	E3N	C15-C13-S12-O16					
2	А	601	E3N	C14-C13-S12-N11					
2	А	601	E3N	C14-C13-S12-O16					
2	А	601	E3N	C14-C13-S12-O17					
2	А	601	E3N	C18-N11-S12-C13					
2	А	601	E3N	C18-N11-S12-O16					
2	А	601	E3N	C18-N11-S12-O17					
2	А	601	E3N	C15-C13-S12-O17					
2	А	601	E3N	C25-C26-O27-C28					
2	А	601	E3N	C32-C26-O27-C28					
2	А	601	E3N	C23-C22-N21-C02					

There are no ring outliers.

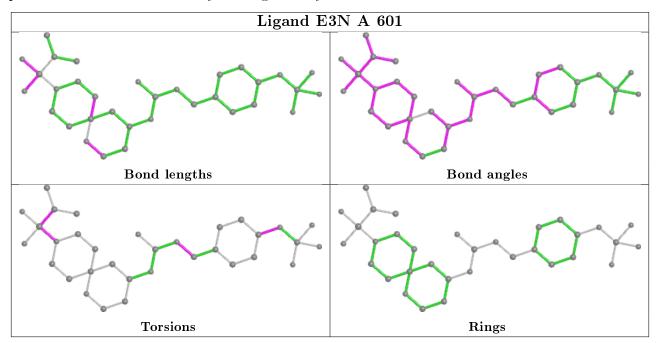
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	601	E3N	3	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, 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	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	319/346~(92%)	0.15	14 (4%) 34 37	33, 49, 91, 108	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	430	VAL	4.6
1	А	416	VAL	4.2
1	А	423	CYS	4.0
1	А	417	LEU	3.8
1	А	428	LEU	3.4
1	А	431	ASN	3.2
1	А	434	GLU	3.2
1	А	432	SER	3.0
1	А	433	PRO	2.7
1	А	422	VAL	2.5
1	А	373	GLU	2.4
1	А	429	PHE	2.2
1	А	426	GLY	2.2
1	А	418	SER	2.1

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.

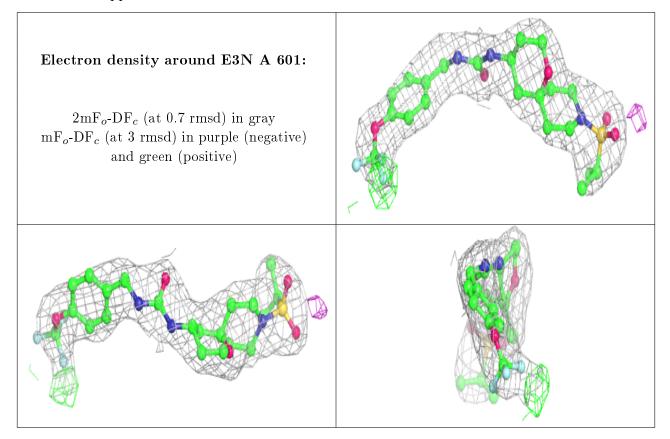


6.4 Ligands (i)

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	${f B} ext{-factors}({f A}^2)$	$Q{<}0.9$
3	MG	А	602	1/1	0.78	0.16	$62,\!62,\!62,\!62$	0
2	E3N	А	601	33/33	0.95	0.14	$44,\!63,\!85,\!103$	3

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.

