

wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 07:02 AM EDT

PDB ID : 3PGS

Title : Phe3Gly mutant of EcFadL Authors : van den Berg, B.; Lepore, B.W.

Deposited on : 2010-11-02

Resolution : 1.90 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 (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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35

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)

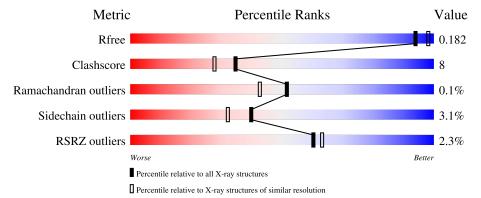
Validation Pipeline (wwPDB-VP) : 2.35

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	427	87%	12%	•		
1	В	427	82%	17%			



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8014 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 Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	427	Total 3459	C 2194	N 592	O 666	S 7	3	23	0
1	В	426	Total 3411	C 2167	N 583	O 654	S 7	5	19	0

There are 14 discrepancies between the modelled and reference sequences:

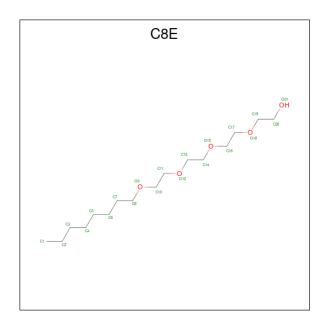
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	PHE	engineered mutation	UNP P10384
A	422	HIS	-	expression tag	UNP P10384
A	423	HIS	-	expression tag	UNP P10384
A	424	HIS	-	expression tag	UNP P10384
A	425	HIS	-	expression tag	UNP P10384
A	426	HIS	-	expression tag	UNP P10384
A	427	HIS	-	expression tag	UNP P10384
В	3	GLY	PHE	engineered mutation	UNP P10384
В	422	HIS	-	expression tag	UNP P10384
В	423	HIS	-	expression tag	UNP P10384
В	424	HIS	-	expression tag	UNP P10384
В	425	HIS	-	expression tag	UNP P10384
В	426	HIS	-	expression tag	UNP P10384
В	427	HIS	-	expression tag	UNP P10384

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mo	ıl	Chain	Residues	Aton	ns	ZeroOcc	AltConf
2		A	1	Total 1	Ca 1	0	0

• Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



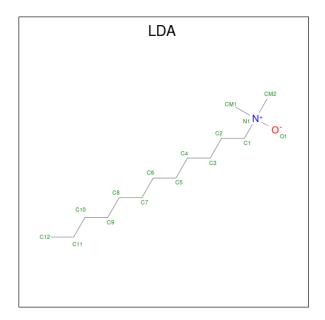


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 20 15 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 21 16 5	0	0
3	A	1	Total C O 13 11 2	0	0
3	В	1	Total C O 21 16 5	0	0
3	В	1	Total C O 21 16 5	0	0
3	В	1	Total C O 21 16 5	0	0
3	В	1	Total C O 15 10 5	0	0
3	В	1	Total C O 21 16 5	0	0

 \bullet Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:



 $\mathrm{C}_{14}\mathrm{H}_{31}\mathrm{NO}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 11 11	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 10 10	0	0
4	В	1	Total C 10 10	0	0
4	В	1	Total C 10 10	0	0

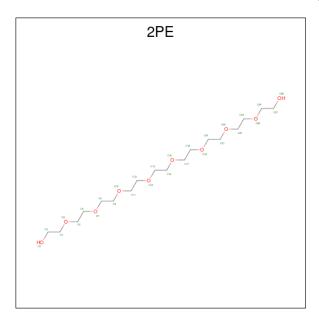
 \bullet Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	В	1	Total C O 4 2 2	0	0

 \bullet Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $\mathrm{C}_{18}\mathrm{H}_{38}\mathrm{O}_{10}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	В	1	Total C 28 18	O 10	0	0

• Molecule 7 is water.



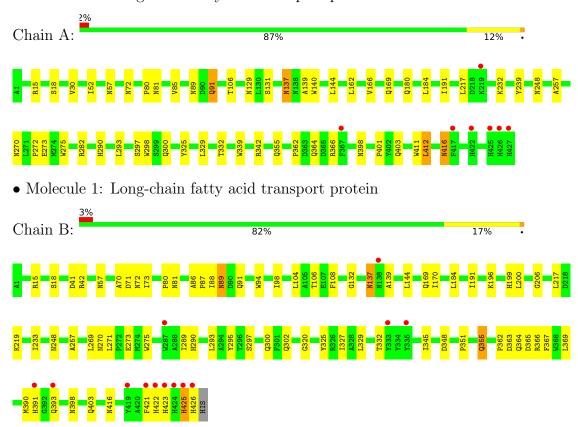
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	394	Total O 394 394	0	0
7	В	383	Total O 383 383	0	0



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: Long-chain fatty acid transport protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	63.07Å 147.51Å 151.09Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 - 1.90	Depositor
rtesolution (A)	38.78 - 1.85	EDS
% Data completeness	99.0 (38.78-1.90)	Depositor
(in resolution range)	93.9 (38.78-1.85)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	2.14 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_572)	Depositor
R, R_{free}	0.167 , 0.192	Depositor
it, it free	0.161 , 0.182	DCC
R_{free} test set	1987 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35\;,60.5$	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8014	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.17% 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: 2PE, ACT, LDA, C8E, 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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.39	0/3607	0.55	0/4903	
1	В	0.37	0/3553	0.54	0/4834	
All	All	0.38	0/7160	0.54	0/9737	

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	3459	0	3266	44	0
1	В	3411	0	3220	59	0
2	A	1	0	0	0	0
3	A	144	0	226	22	0
3	В	99	0	155	17	0
4	A	67	0	124	5	0
4	В	20	0	38	3	0
5	A	4	0	3	1	0
5	В	4	0	3	0	0
6	В	28	0	38	2	0
7	A	394	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	В	383	0	0	5	0
All	All	8014	0	7073	118	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 8.

The worst 5 of 118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:191:ILE:HG21	3:B:434:C8E:H202	1.40	1.02
3:A:443:C8E:H32	1:B:169:GLN:HE22	1.26	0.98
1:B:248:ASN:HD21	1:B:257:ALA:H	1.10	0.97
1:A:248:ASN:HD21	1:A:257:ALA:H	1.15	0.94
1:B:355:GLN:H	1:B:355:GLN:HE21	1.07	0.93

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	Perce	entiles
1	A	$449/427 \ (105\%)$	444 (99%)	5 (1%)	0	100	100
1	В	443/427 (104%)	437 (99%)	5 (1%)	1 (0%)	47	38
All	All	892/854 (104%)	881 (99%)	10 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	425	HIS



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	Perce	ntiles
1	A	360/336 (107%)	349 (97%)	11 (3%)	40	32
1	В	353/336 (105%)	341 (97%)	12 (3%)	37	28
All	All	713/672 (106%)	690 (97%)	23 (3%)	40	30

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	137[A]	ASN
1	В	184	LEU
1	В	144	LEU
1	В	217	LEU
1	A	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	270	ASN
1	В	355	GLN
1	В	281	ASN
1	В	302	GLN
1	В	393	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)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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).

N / - 1	Т	Clasies	Das	T : 1-	Во	ond leng	ths	В	ond ang	les
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C8E	A	439	-	20,20,20	0.36	0	19,19,19	0.40	0
4	LDA	A	432	-	9,9,15	0.27	0	8,8,17	0.52	0
3	C8E	В	433	-	20,20,20	0.36	0	19,19,19	0.40	0
3	C8E	A	441	-	20,20,20	0.37	0	19,19,19	0.49	0
4	LDA	A	435	-	6,6,15	0.27	0	5,5,17	0.42	0
4	LDA	В	430	-	9,9,15	0.27	0	8,8,17	0.53	0
4	LDA	A	434	-	9,9,15	0.24	0	8,8,17	0.57	0
3	C8E	В	435	-	20,20,20	0.34	0	19,19,19	0.56	0
6	2PE	В	436	-	27,27,27	0.69	0	26,26,26	1.54	0
4	LDA	A	437	-	9,9,15	0.27	0	8,8,17	0.49	0
3	C8E	A	443	-	12,12,20	0.33	0	11,11,19	0.38	0
5	ACT	В	1428	-	3,3,3	0.82	0	3,3,3	1.42	0
3	C8E	A	430	-	13,13,20	0.39	0	12,12,19	0.41	0
4	LDA	В	429	-	9,9,15	0.27	0	8,8,17	0.55	0
3	C8E	A	440	-	20,20,20	0.34	0	19,19,19	0.54	0
4	LDA	A	433	-	11,11,15	0.28	0	10,10,17	0.49	0
3	C8E	В	434	-	14,14,20	0.42	0	13,13,19	0.45	0
4	LDA	A	431	-	10,10,15	0.27	0	9,9,17	0.51	0
3	C8E	В	431	-	20,20,20	0.38	0	19,19,19	0.62	0
3	C8E	A	438	-	19,19,20	0.40	0	18,18,19	0.53	0
3	C8E	A	442	-	20,20,20	0.38	0	19,19,19	0.47	0
3	C8E	В	432	-	20,20,20	0.39	0	19,19,19	0.33	0
5	ACT	A	1428	-	3,3,3	0.79	0	3,3,3	1.12	0
3	C8E	A	429	-	12,12,20	0.39	0	11,11,19	0.47	0
4	LDA	A	436	-	6,6,15	0.27	0	5,5,17	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
3	C8E	A	439	-	-	12/18/18/18	-
4	LDA	A	432	-	-	5/7/7/13	-
3	C8E	В	433	-	-	14/18/18/18	-
3	C8E	A	441	-	-	11/18/18/18	-
4	LDA	A	435	-	-	3/4/4/13	-
4	LDA	В	430	-	-	3/7/7/13	-
4	LDA	A	434	-	-	5/7/7/13	-
3	C8E	В	435	-	-	6/18/18/18	-
6	2PE	В	436	-	-	12/25/25/25	-
4	LDA	A	437	-	-	3/7/7/13	-
3	C8E	A	443	-	-	7/10/10/18	-
3	C8E	A	430	-	-	7/11/11/18	-
4	LDA	В	429	-	-	1/7/7/13	-
3	C8E	A	440	-	-	14/18/18/18	-
4	LDA	A	433	-	-	6/9/9/13	-
3	C8E	В	434	-	-	8/12/12/18	-
4	LDA	A	431	-	-	3/8/8/13	-
3	C8E	В	431	-	-	12/18/18/18	-
3	C8E	A	438	-	-	6/17/17/18	-
3	C8E	A	442	-	-	14/18/18/18	-
3	C8E	В	432	-	-	12/18/18/18	-
3	C8E	A	429	-	-	6/10/10/18	-
4	LDA	A	436	-	-	2/4/4/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 172 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	433	C8E	C16-C17-O18-C19
3	A	442	C8E	C3-C4-C5-C6
3	В	431	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	440	C8E	O12-C13-C14-O15
3	A	439	C8E	O9-C10-C11-O12

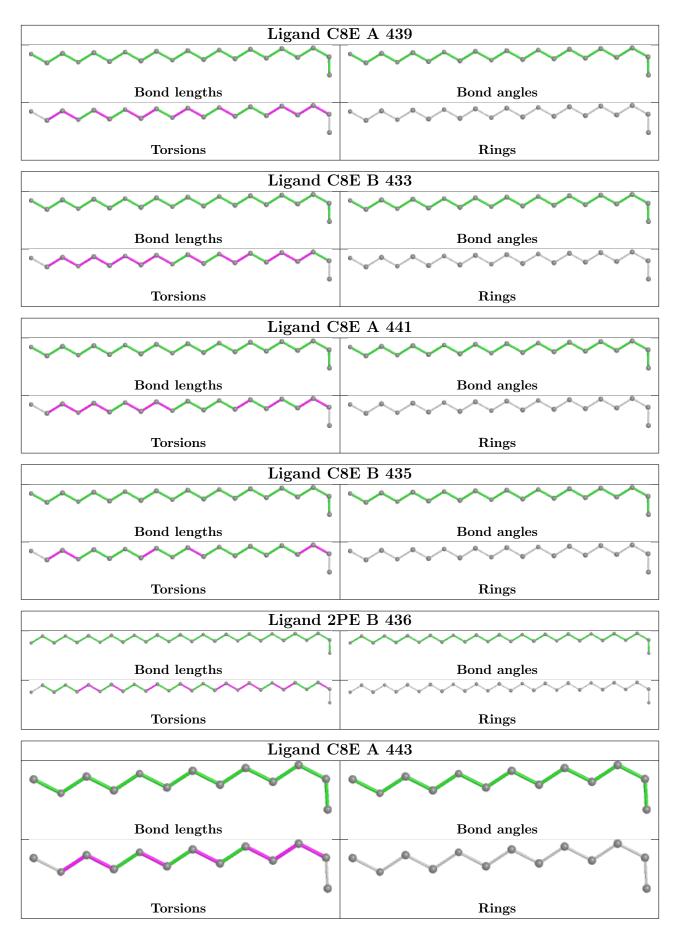
There are no ring outliers.

19 monomers are involved in 47 short contacts:

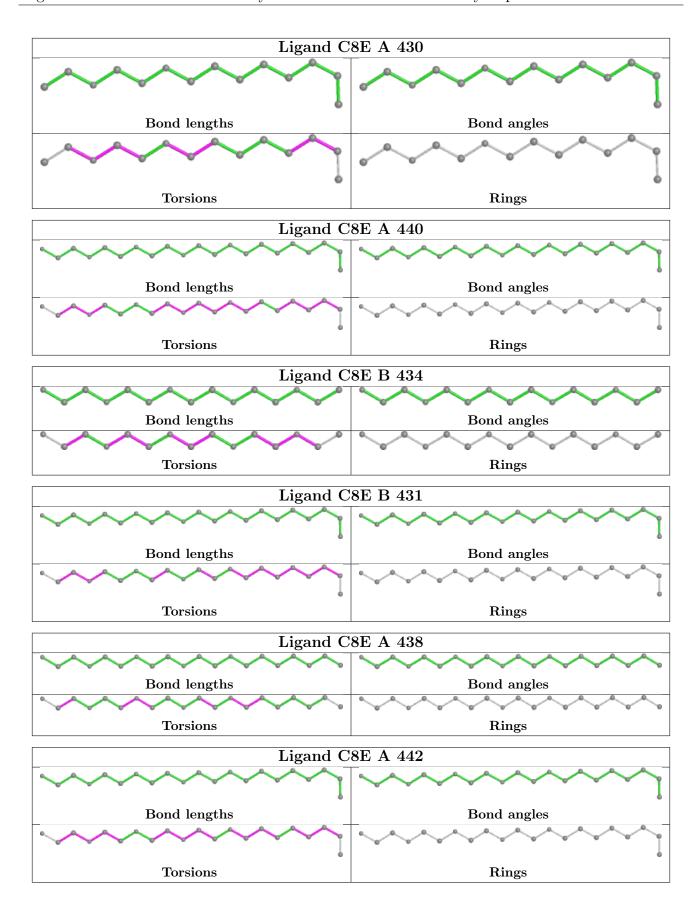
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	C8E	1	0
4	A	432	LDA	1	0
3	В	433	C8E	3	0
3	A	441	C8E	2	0
4	В	430	LDA	2	0
4	A	434	LDA	1	0
3	В	435	C8E	4	0
6	В	436	2PE	2	0
3	A	443	C8E	4	0
3	A	430	C8E	2	0
4	В	429	LDA	1	0
3	A	440	C8E	6	0
4	A	433	LDA	3	0
3	В	434	C8E	3	0
3	В	431	C8E	5	0
3	A	438	C8E	3	0
3	A	442	C8E	5	0
3	В	432	C8E	2	0
5	A	1428	ACT	1	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.

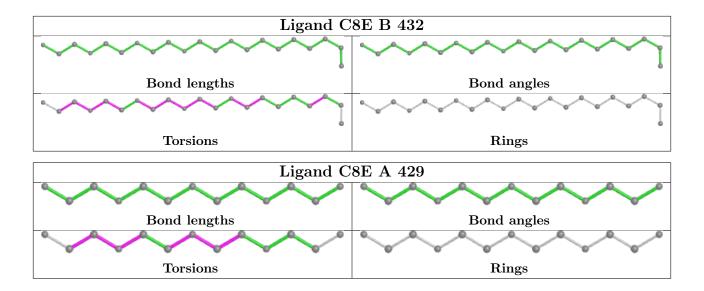












5.7 Other polymers (i)

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 > 2	$OWAB(Å^2)$	Q<0.9
1	A	$427/427 \; (100\%)$	-0.41	7 (1%) 72 74	17, 28, 47, 67	0
1	В	$426/427\ (99\%)$	-0.28	13 (3%) 49 51	17, 29, 49, 110	1 (0%)
All	All	853/854 (99%)	-0.35	20 (2%) 60 63	17, 29, 49, 110	1 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	426	HIS	10.2
1	В	423	HIS	7.5
1	В	424	HIS	4.4
1	В	419	TYR	4.3
1	В	422	HIS	3.9

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.



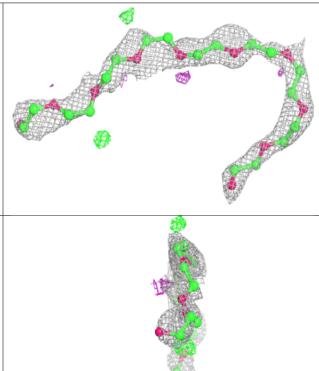
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	C8E	A	430	14/21	0.67	0.24	64,72,88,89	0
4	LDA	A	437	10/16	0.75	0.18	50,57,58,59	0
6	2PE	В	436	28/28	0.75	0.28	75,88,96,97	0
3	C8E	A	441	21/21	0.76	0.23	54,77,89,95	0
3	C8E	A	443	13/21	0.76	0.23	32,49,57,59	0
3	C8E	В	432	21/21	0.77	0.22	51,72,83,86	0
3	C8E	A	442	21/21	0.79	0.25	37,69,78,79	0
4	LDA	A	432	10/16	0.82	0.23	44,60,63,66	0
4	LDA	A	433	12/16	0.82	0.17	41,49,53,54	0
5	ACT	В	1428	4/4	0.84	0.14	39,42,45,48	0
4	LDA	В	429	10/16	0.85	0.28	40,49,53,54	0
3	C8E	В	434	15/21	0.85	0.21	39,48,73,76	0
3	C8E	A	439	21/21	0.85	0.22	56,67,74,77	0
4	LDA	В	430	10/16	0.86	0.13	36,53,70,70	0
3	C8E	В	433	21/21	0.86	0.19	38,52,62,78	0
4	LDA	A	434	10/16	0.86	0.27	58,65,72,74	0
4	LDA	A	431	11/16	0.88	0.18	36,47,52,54	0
3	C8E	В	431	21/21	0.89	0.19	37,50,57,59	0
3	C8E	A	429	13/21	0.90	0.12	31,42,51,64	0
3	C8E	В	435	21/21	0.91	0.20	22,45,93,94	0
3	C8E	A	438	20/21	0.91	0.14	27,44,62,62	0
3	C8E	A	440	21/21	0.92	0.24	35,53,96,102	0
4	LDA	A	436	7/16	0.93	0.15	43,49,54,55	0
5	ACT	A	1428	4/4	0.93	0.15	45,47,48,49	0
4	LDA	A	435	7/16	0.94	0.18	50,56,60,64	0
2	CA	A	428	1/1	0.98	0.04	30,30,30,30	0

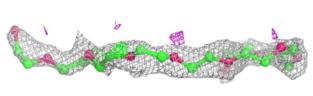
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around 2PE B 436:

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

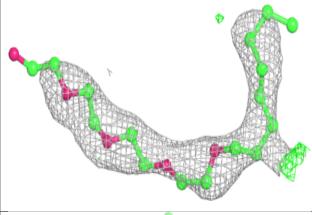


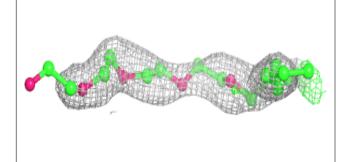


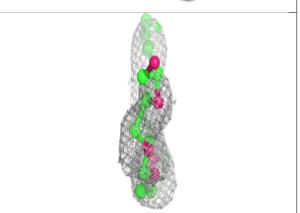


Electron density around C8E A 441:

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

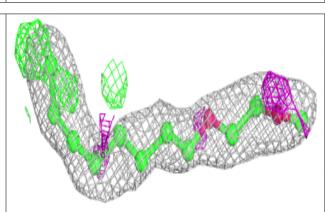


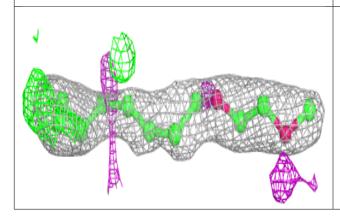


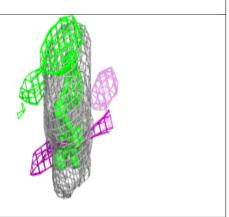


Electron density around C8E A 443:

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





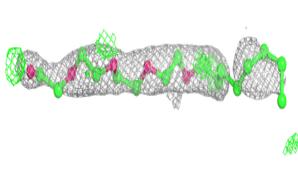


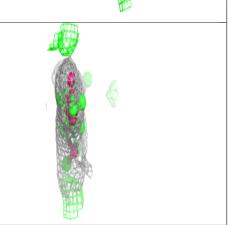


Electron density around C8E A 442: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around C8E B 434: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around C8E A 439: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)

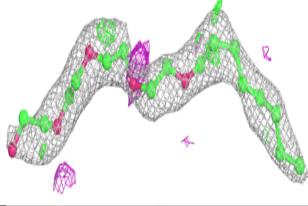


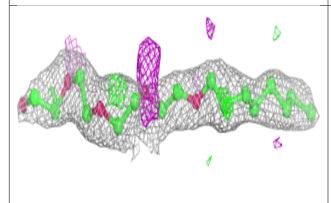


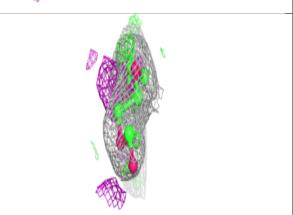


Electron density around C8E B 433:

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

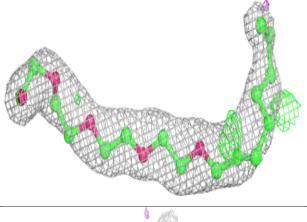


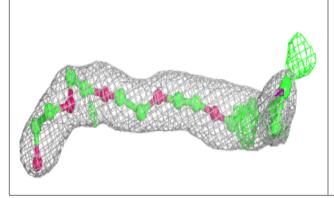


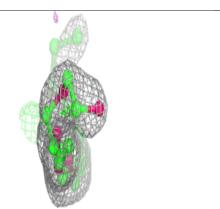


Electron density around C8E B 431:

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



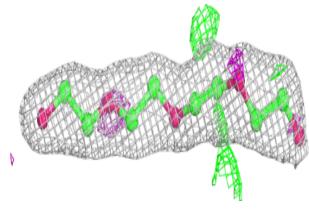


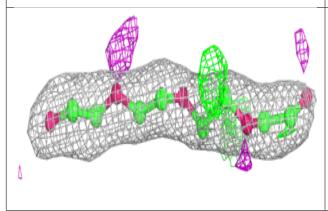


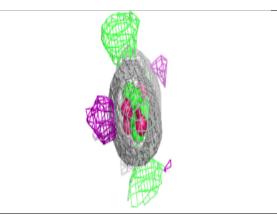


Electron density around C8E A 429:

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

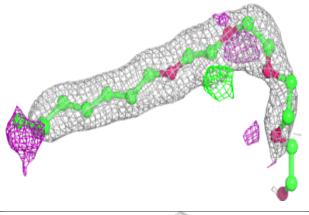


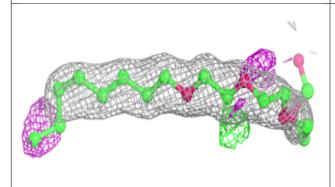


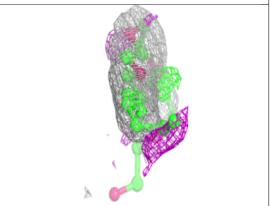


Electron density around C8E B 435:

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









Electron density around C8E A 438: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around C8E A 440: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

