



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2024 – 04:15 PM JST

PDB ID : 8JFF
Title : Crystal structure of Catabolite repressor acivator from E. coli in complex with HEPES
Authors : Neetu, N.; Katiki, M.; Kumar, P.
Deposited on : 2023-05-18
Resolution : 2.89 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 ⓘ 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 : 4.02b-467
Mogul : 1.8.5 (274361), 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

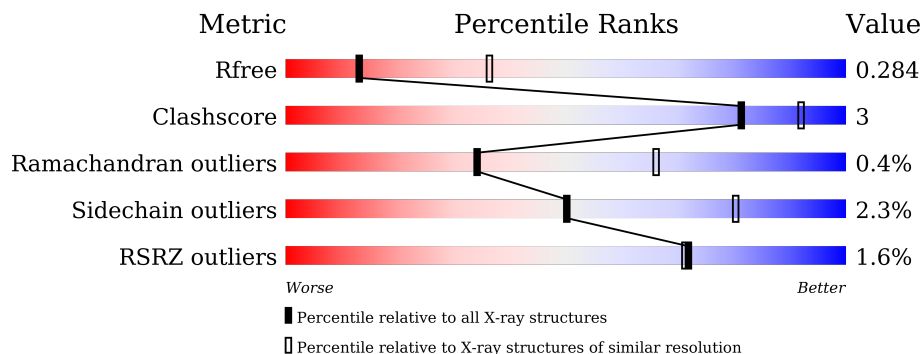
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	334	 2% 73% 8% 18%
1	B	334	 2% 75% 7% 18%

2 Entry composition [i](#)

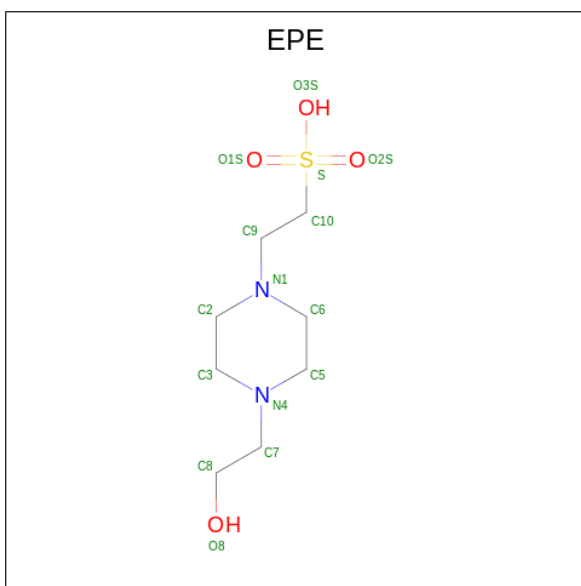
There are 3 unique types of molecules in this entry. The entry contains 4511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catabolite repressor/activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	Total 2220	C 1404	N 398	O 411	S 7	0	0	0
1	B	274	Total 2220	C 1404	N 398	O 411	S 7	0	0	0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 15	C 8	N 2	O 4	S 1	0	0
2	A	1	Total 15	C 8	N 2	O 4	S 1	0	0

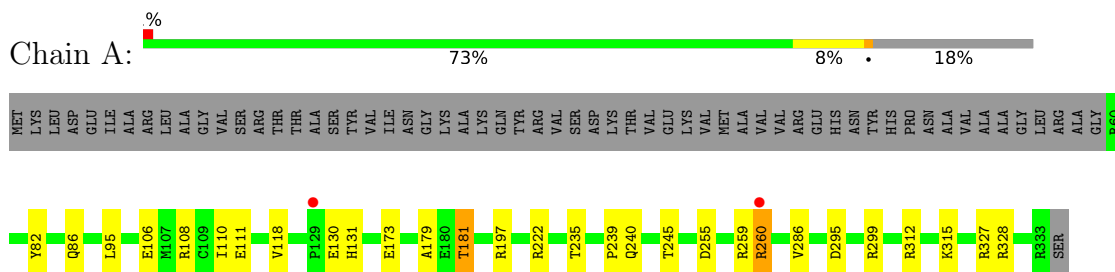
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	16	Total 16	O 16	0	0

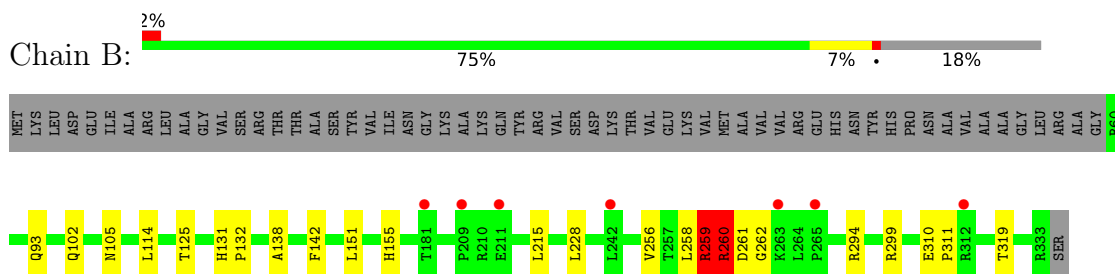
3 Residue-property plots [i](#)

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: Catabolite repressor/activator



- Molecule 1: Catabolite repressor/activator



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.33Å 108.90Å 123.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.51 – 2.89 54.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	89.5 (54.51-2.89) 89.5 (54.45-2.89)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.224 , 0.283 0.227 , 0.284	Depositor DCC
R_{free} test set	590 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtrriage
Anisotropy	0.280	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4511	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: EPE

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	0.25	0/2268	0.48	0/3079
1	B	0.25	0/2268	0.50	0/3079
All	All	0.25	0/4536	0.49	0/6158

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	259	ARG	Sidechain
1	B	260	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	2220	0	2206	12	0
1	B	2220	0	2206	12	0
2	A	30	0	35	0	0
3	A	25	0	0	0	0
3	B	16	0	0	0	0
All	All	4511	0	4447	23	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 3.

All (23) 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:B:259:ARG:O	1:B:261:ASP:N	2.32	0.62
1:B:310:GLU:HG3	1:B:311:PRO:HD2	1.89	0.55
1:A:179:ALA:HB1	1:A:240:GLN:HB2	1.92	0.52
1:A:181:THR:HG23	1:A:239:PRO:HA	1.92	0.51
1:B:102:GLN:HB2	1:B:105:ASN:HD22	1.79	0.47
1:A:108:ARG:HA	1:A:111:GLU:HG2	1.96	0.47
1:A:259:ARG:O	1:A:260:ARG:HB3	2.15	0.47
1:B:125:THR:HG21	1:B:151:LEU:HD23	1.97	0.46
1:B:258:LEU:O	1:B:262:GLY:HA2	2.16	0.46
1:A:197:ARG:NH1	1:A:245:THR:O	2.50	0.44
1:A:286:VAL:CG2	1:A:328:ARG:HB2	2.49	0.43
1:A:173:GLU:OE2	1:A:327:ARG:NH2	2.52	0.42
1:A:95:LEU:HD23	1:B:93:GLN:HG2	2.02	0.42
1:B:131:HIS:CG	1:B:132:PRO:HD2	2.54	0.42
1:B:299:ARG:HB2	1:B:299:ARG:NH1	2.35	0.41
1:B:215:LEU:HG	1:B:228:LEU:HD21	2.02	0.41
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.85	0.41
1:A:130:GLU:O	1:A:131:HIS:C	2.59	0.41
1:B:114:LEU:HD21	1:B:142:PHE:CE2	2.56	0.40
1:B:138:ALA:HB1	1:B:155:HIS:HD2	1.86	0.40
1:A:106:GLU:O	1:A:110:ILE:HG12	2.21	0.40
1:A:222:ARG:NH2	1:A:255:ASP:OD1	2.54	0.40
1:A:82:TYR:O	1:A:86:GLN:HB2	2.22	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	272/334 (81%)	259 (95%)	12 (4%)	1 (0%)	34	66
1	B	272/334 (81%)	256 (94%)	15 (6%)	1 (0%)	34	66
All	All	544/668 (81%)	515 (95%)	27 (5%)	2 (0%)	34	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	ARG
1	A	312	ARG

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	239/286 (84%)	232 (97%)	7 (3%)	42	76
1	B	239/286 (84%)	235 (98%)	4 (2%)	60	86
All	All	478/572 (84%)	467 (98%)	11 (2%)	50	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	A	181	THR
1	A	235	THR
1	A	260	ARG

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Mol	Chain	Res	Type
1	A	295	ASP
1	A	299	ARG
1	A	315	LYS
1	B	256	VAL
1	B	259	ARG
1	B	260	ARG
1	B	319	THR

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	291	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](#)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EPE	A	402	-	15,15,15	0.29	0	18,20,20	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	A	401	-	15,15,15	0.58	0	18,20,20	1.16	2 (11%)

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	EPE	A	402	-	-	2/9/19/19	0/1/1/1
2	EPE	A	401	-	-	7/9/19/19	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	EPE	O2S-S-C10	-3.60	102.58	106.92
2	A	401	EPE	O3S-S-O1S	2.85	118.24	111.27
2	A	402	EPE	O3S-S-C10	-2.34	101.98	105.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

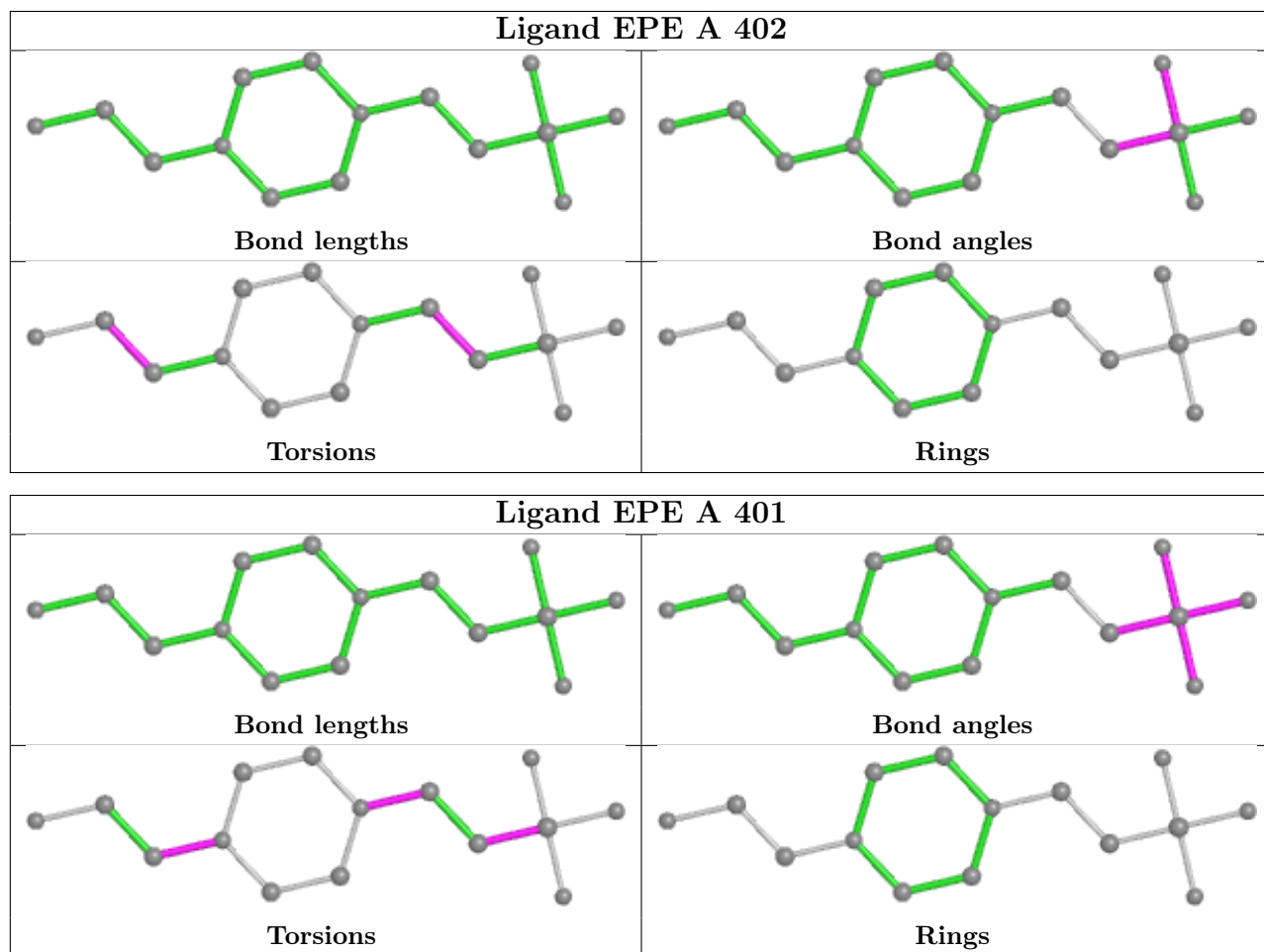
Mol	Chain	Res	Type	Atoms
2	A	401	EPE	C10-C9-N1-C2
2	A	401	EPE	C10-C9-N1-C6
2	A	401	EPE	C9-C10-S-O2S
2	A	401	EPE	C9-C10-S-O3S
2	A	402	EPE	N4-C7-C8-O8
2	A	402	EPE	S-C10-C9-N1
2	A	401	EPE	C9-C10-S-O1S
2	A	401	EPE	C8-C7-N4-C3
2	A	401	EPE	C8-C7-N4-C5

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 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	274/334 (82%)	0.09	2 (0%) 87 87	52, 76, 101, 115	0
1	B	274/334 (82%)	0.19	7 (2%) 56 52	57, 78, 103, 123	0
All	All	548/668 (82%)	0.14	9 (1%) 72 71	52, 77, 102, 123	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	PRO	2.9
1	A	129	PRO	2.9
1	A	260	ARG	2.4
1	B	211	GLU	2.2
1	B	263	LYS	2.2
1	B	312	ARG	2.1
1	B	181	THR	2.0
1	B	209	PRO	2.0
1	B	242	LEU	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.

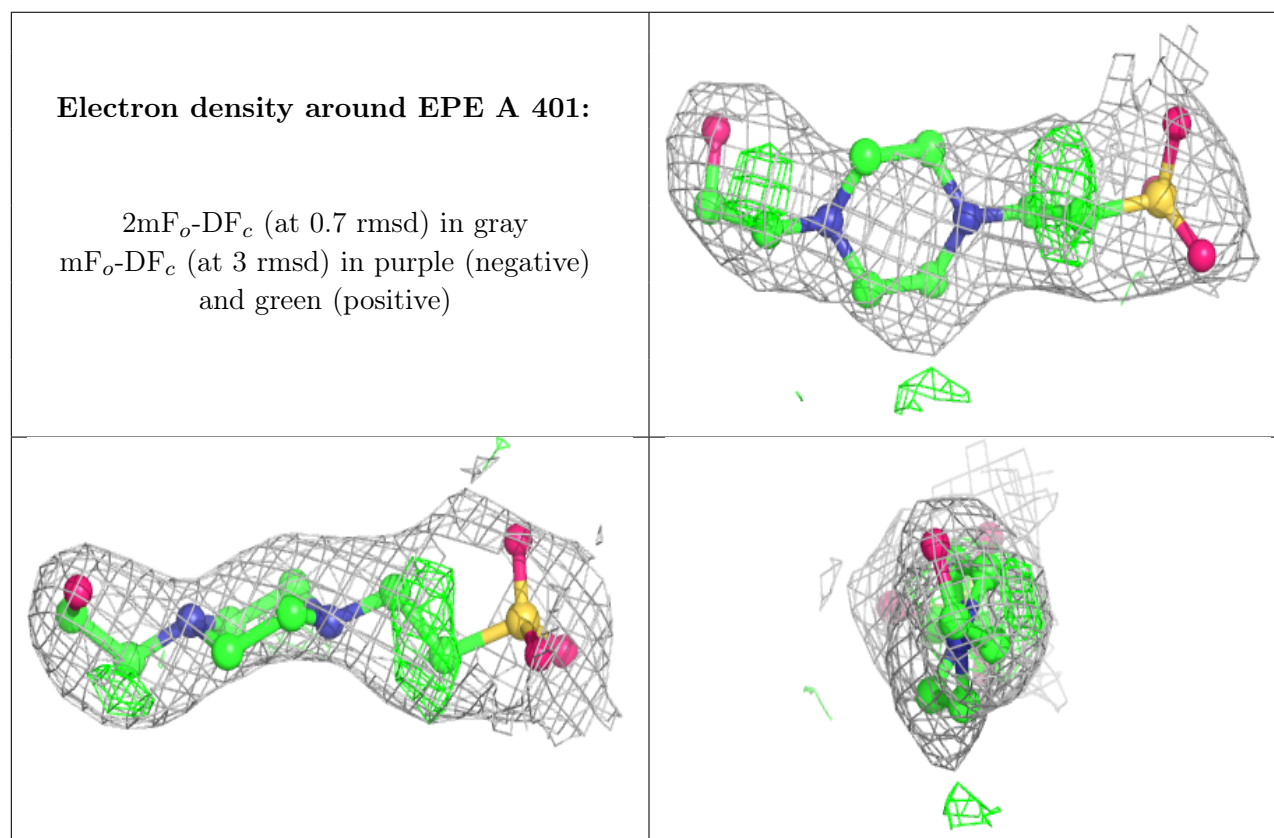
6.4 Ligands [i](#)

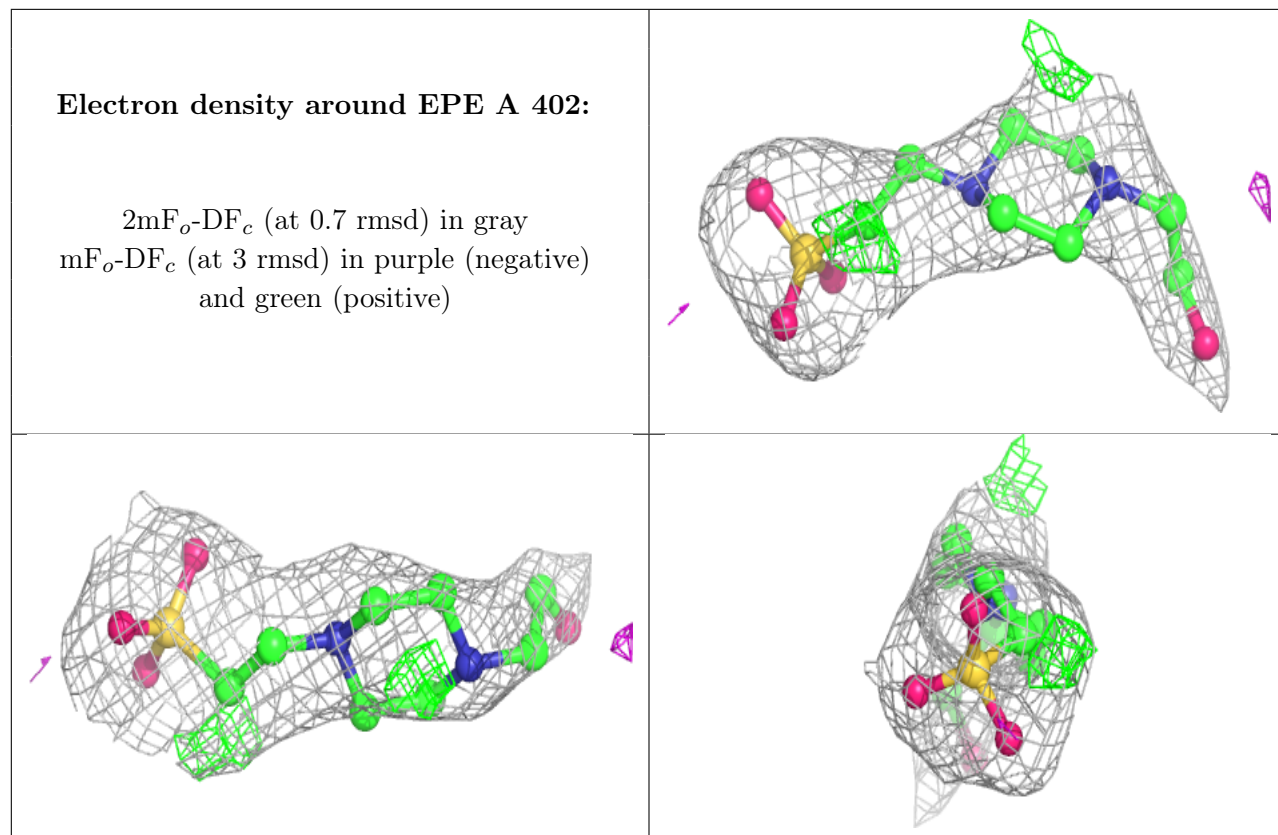
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
2	EPE	A	401	15/15	0.86	0.22	79,88,100,100	0
2	EPE	A	402	15/15	0.89	0.29	80,85,88,88	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.